Initial Entry: Mary Ann Clarke
Date: 18 April 2005

Title: Technical Development and Evaluation of computational fluid dynamics (CFD) models related to Hi-Star 100 transportation cask thermal calculations as processed through a dry transfer facility (DTF)

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Project: This notebook documents thermal and geometric data selection, input deck development, and analyses of results as part of the Hi-Star 100 and DTF CFD thermal modeling effort

Data: Bounding thermal characteristic data for a variety of fuel assemblies and Hi-Star 100 cask can be found in HI-STAR FSAR HI-2012610, chapter 2. Geometric data for the Hi-Star 100 cask can be found in HI-STAR FSAR HI-201260, chapter 4. Waste Package information is given in ANL-XCS-ME-000001 REV00.

Date: 24 June 2005

NOTE: The management of this scientific notebook will be acquired by:
Sidney Chocron, Southwest Research Institute, Division 18, CFD modeling
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Date: 19 April 2005 Entry By: Mary Ann Clarke
Supposed thermal conductivity values:
From HI-STAR FSAR Report HI-2012610, Rev.1

Conversions:
Temperature:
Fahrenheit to Celsius Celsius to Kelvin

$$^{\circ}C = \frac{5}{9}\left(^{\circ}F - 32\right) \qquad K = {}^{\circ}C + 273.15$$

Thermal Conductivity:
Btu/ft-hr-°F to J/m-s-K

$$1.0\frac{Btu}{ft-hr-^{\circ}F} \times \frac{1055.0559J}{1.0Btu} \times \frac{1.0ft}{0.3048m} \times \frac{1.0hr}{3600s} \times \frac{\Delta 1^{\circ}F}{\Delta 0.55555555K} = 1.7307349\frac{J}{m-s-K}$$

Values:
MPC-68 using Stainless Steel Clad Fuel, from Table 4.4.7 with conversions

Temperature			Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	0.931	1.611
450	232.22	505.37	1.125	1.947
700	371.11	644.26	1.311	2.268

Linearization: coordinates (k (J/m-s-K), T (K)): y = 0.0024x + 0.7467

MPC-68 using Zircaloy Clad Fuel, from Table 4.4.7 with conversions

Temperature			Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	1.014	1.754
450	232.22	505.37	1.226	2.121
700	371.11	644.26	1.428	2.471

Linearization: coordinates (k (J/m-s-K), T (K)): y = 0.0026x + 0.8109

Effective thermal conductivity of **Neutron Shield and Radial Channel Region**, Table 4.4.8 with conversions

Temperature	(under normal condition)		Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	1.953	3.380
450	232.22	505.37	1.812	3.136
700	371.11	644.26	1.645	2.847

Linearization: coordinates (k (J/m-s-K), T (K)): y = -0.0019x + 4.0907

Temperature	(under fire condition)		Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	3.012	5.212
450	232.22	505.37	2.865	4.958
700	371.11	644.26	2.689	4.653

Linearization: coordinates (k (J/m-s-K), T (K)): y = -0.0020x + 5.958

General Materials (non-homogenized) from Table 4.2.2

Air

Temperature			Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	0.0976	0.1689
450	232.22	505.37	0.1289	0.2230
700	371.11	644.26	0.1575	0.2725

Linearization: coordinates (k (J/m-s-K), T (K)): $y = 0.0004x + 0.033$

Alloy X

Temperature			Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	0.0173	0.0299
450	232.22	505.37	0.0225	0.0389
700	371.11	644.26	0.0272	0.0470

Linearization: coordinates (k (J/m-s-K), T (K)): $y = 6e\text{-}5x + 0.0075$

Carbon Steel Radial Connectors

Temperature			Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	29.2	50.53
450	232.22	505.37	27.1	46.90
700	371.11	644.26	24.6	42.57

Linearization: coordinates (k (J/m-s-K), T (K)): $y = -0.0287x + 61.148$

Carbon Steel Gamma Shield Layers

Temperature			Thermal Conductivity (k)	
(°F)	(°C)	(K)	(Btu/ft-hr-°F)	(J/m-s-K)
200	93.33	366.48	24.4	42.22
450	232.22	505.37	23.9	41.36
700	371.11	644.26	22.4	38.76

Linearization: coordinates (k (J/m-s-K), T (K)): $y = -0.0125x + 47.075$

Date: 19 April 2005 Entry By: Mary Ann Clarke
Density and Heat Capacity properties summary:
From: HI-STAR FSAR Report HI-2012610, Rev.1

Conversions:
Heat Capacity:
Btu/lbm-°F to J/kg-K

$$1.0\frac{Btu}{lbm-^{\circ}F}\times\frac{1055.0559J}{1.0Btu}\times\frac{1lbm}{0.4535924kg}\times\frac{\Delta 1^{\circ}F}{\Delta 0.55555555K}=4186.7999\frac{J}{kg-K}$$

Density:
lbm/ft^3 to kg/m^3

$$1.0\frac{lbm}{ft^3}\times\frac{0.4535924kg}{1.0lbm}\times\left(\frac{1.0ft}{0.3048m}\right)^3=16.018464\frac{kg}{m^3}$$

Notation:
Specific Heat = (Heat Capacity of a substance)/(Heat Capacity of a reference substance)
The reference substance is usually water unless otherwise specified. In CFD calculations, we use specific heat with water as the reference value.

From Table 4.2.5 with conversions

Material	Density (lbm/ft^3)	(kg/m^3)	Heat Capacity (Btu/lbm-°F)	(J/kg-K)
Zircaloy cladding	409	6551	0.0728	304.79
Fuel (UO_2)	684	10956	0.056	234.46
Carbon Steel	489	7833	0.1	418.67
Stainless Steel	501	8025	0.12	502.41
Boral	154.7	2478	0.13	544.28
Al Alloy 1100	169.9	2721	0.23	962.96
Holtite-A	105.0	1681	0.39	1632.85

Date: 20 April 2005 Entry By: Mary Ann Clarke
CFD grid plane placements for Hi-Star 100 Cask – MPC 68 Basket

Flow-3D has been chosen as the CFD solver for the generalized task of thermally evaluating the Hi-Star 100 Cask in the dry transfer facility. As such, the geometry of the cask must be brought into the program's preprocessor. Since no CAD documents exist in an electronic format such that the cask specifications can be included explicitly, the critical cask components are incorporated into a three-dimensional space by hand (through an input deck) and then a Cartesian mesh is overlaid for computational work. This entry explicitly notates the mesh planes that demarcate specific structural components of the Hi-Star 100 Cask with an MPC-68 basket.

X and Y Space

Location (m)	Component Begins
-1.2144375	overpack neutron shielding outside diameter
-1.089025	overpack multi-layer shell outside diameter
-1.057275	overpack base plate diameter
-0.936625	overpack inner shell outside diameter
-0.873125	overpack inner shell inside diameter
-0.868365	MPC base plate outside diameter
-0.854075	outside MPC shell diameter
-0.847725	inside MPC shell diameter
-0.827405	begin fuel basket orthogonal planes
-0.821055	air gap
-0.816102	fuel assembly
-0.667512	air gap
-0.662559	basket plane
-0656209	air gap
-0.651256	fuel assembly
-0.502666	air gap
-0.497713	basket plane
-0.491363	air gap
-0.486410	fuel assembly
-0.337820	air gap
-0.332867	basket plane
-0.326517	air gap
-0.321564	fuel assembly
-0.172974	air gap
-0.168021	basket plane
-0.161671	air gap
-0.156718	fuel assembly
-0.008128	air gap
-0.003175	basket plane
+0.003175	air gap
+0.008128	fuel assembly
+0.156718	air gap
+0.161671	basket plane

X and Y Space (cont'd)

Location (m)	Component Begins
+0.168021	air gap
+0.172974	fuel assembly
+0.321564	air gap
+0.326517	basket plane
+0.332867	air gap
+0.337820	fuel assembly
+0.486410	air gap
+0.491363	basket plane
+0.497713	air gap
+0.502666	fuel assembly
+0.651256	air gap
+0.656209	basket plane
+0.662559	air gap
+0.667512	fuel assembly
+0.816102	air gap
+0.821055	basket plane
+0.827405	end basket planes
+0.847725	inside MPC shell diameter
+0.854075	outside MPC shell diameter
+0.868365	MPC base plate outside diameter
+0.873125	overpack inner shell inside diameter
+0.936625	overpack inner shell outside diameter
+1.057275	overpack base plate diameter
+1.089025	overpack multi-layer shell outside diameter
+1.2144375	overpack neutron shielding outside diameter

Z Space

Location (m)	Component Begins
-0.215900	bottom overpack base plate
-0.063500	top overpack base plate
0.000000	bottom of fuel basket/bottom of MPC
+0.063500	bottom overpack neutron shielding
+4.403725	top overpack neutron shielding
+4.470400	top of fuel basket
+4.521200	top of MPC shell
+4.791075	top overpack layering system
+4.943475	top overpack idealized lid edge

Date: 28 April 2005 Entry By: Mary Ann Clarke
CFD grid plane placements for Dry Transfer Facility

Because of the disparity between the scale detail of a cask and the scale detail of a room, separate CFD simulations are formulated with separate grids to track thermal effects at room scale. Also, there is no clear documentation (at this point) from NRC that indicates actual room dimensioning. This entry documents the current suppositions regarding room dimensions and explicitly demarcates the mesh planes that define the Dry Transfer Facility.

The mesh is created in a multi-block format so that different rooms within the facility can be easily added in and taken out without having to maintain a very large grid. One unique feature is that the hot cell itself is divided into 4 multi-blocks to better coincide with the rooms beneath. The (0,0,0) point of the mesh is at the bottom center of the CASK. It does not coincide with a wall. This is done for easiest reference between the refined mesh of the cask scale model with the coarse scale of this room scale model.

The Hot Cell

Grid 1 (the region above the staging rack)

X Space

Location (m)	Component Begins
34.1376	112ft right of cask center
49.3776	162ft right of cask center (the farthest wall)

Y Space

Location (m)	Component Begins
-5.7912	19ft front of cask center
-1.22	plane just outside of cask radius
1.22	plane just outside of cask radius
5.7912	19ft behind of cask center

Z Space

Location (m)	Component Begins
5.16255	18ft roof of 1st floor; begin concrete separation
5.4864	18in concrete barrier
6.0	arbitrary transition for heat transfer analysis
21.3360	70ft head space

Grid 2 (the region above waste package 2; 2 rooms away from the cask)

X Space

Location (m)	Component Begins
26.2128	86ft right of cask center
34.1376	112ft right of cask center

Y Space

Location (m)	Component Begins
-5.7912	19ft front of cask center

-1.22	plane just outside of cask radius
1.22	plane just outside of cask radius
5.7912	19ft behind of cask center

Z Space

Location (m)	Component Begins
5.16255	18ft roof of 1st floor; begin concrete separation
5.4864	18in concrete barrier
6.0	arbitrary transition for heat transfer analysis
21.3360	70ft head space

Grid 3 (the region above waste package 1; 1 room away from the cask)

X Space

Location (m)	Component Begins
17.6784	58ft right of cask center
26.2128	86ft right of cask center

Y Space

Location (m)	Component Begins
-5.7912	19ft front of cask center
-1.22	plane just outside of cask radius
1.22	plane just outside of cask radius
5.7912	19ft behind of cask center

Z Space

Location (m)	Component Begins
5.16255	18ft roof of 1st floor; begin concrete separation
5.4864	18in concrete barrier
6.0	arbitrary transition for heat transfer analysis
21.3360	70ft head space

Grid 4 (the region above the cask room)

X Space

Location (m)	Component Begins
-15.8496	-52ft left of cask center
-1.22	plane just outside of cask radius
1.22	plane just outside of cask radius
17.6784	58ft right of cask center

Y Space

Location (m)	Component Begins
-5.7912	19ft front of cask center
-1.22	plane just outside of cask radius
1.22	plane just outside of cask radius
5.7912	19ft behind of cask center

Z Space

Location (m)	Component Begins
5.16255	18ft roof of 1st floor; begin concrete separation
5.4864	18in concrete barrier
6.0	arbitrary transition for heat transfer analysis
21.3360	70ft head space

The Cask Room

presently this is visualized as a lower level chimney, but may change later on to include outside dimensioning of room

X and Y Space

Location (m)	Component Begins
-1.22	plane just outside of cask radius
-1.21920	cask outside radius
-1.095375	overpack secondary radius
-1.057275	overpack base plate radius
-0.873125	overpack inside radius
-0.8683625	MPC outside radius
-0.8556625	MPC inside radius
0.8556625	MPC inside radius
0.8683625	MPC outside radius
0.873125	overpack inside radius
1.057275	overpack base plate radius
1.095375	overpack secondary radius
1.21920	cask outside radius
1.22	plane just outside of cask radius

Z Space

Location (m)	Component Begins
0.0	base of cask (outside overpack)
0.1524	top of overpack base plate
0.2159	top of MPC base plate
4.619625	top of fattest part of overpack
4.69265	top of basket
4.9863375	top of MPC
5.16255	bottom of concrete block interface

Date: 02 May 2005 Entry By: Mary Ann Clarke
Installation Procedure for FLOW-3D

After request from Bis Dasgupta, on 29 April 2005, I completed Installation Testing for FLOW-3D version 9.0 on a Dell OptiPlex GX400 PC with an Intel Pentium 4 – 1.7GHz processor utilizing a Suse Linux Enterprise 9.0 operating system. In particular I utilized the computer padme as an interfacial device.

The test benchmark was provided by FlowScience, the maker of FLOW-3D. Steve Green provided the benchmark data to me after consult with FlowScience. The input deck is written out below:

NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH)
This test calculation is based on a benchmark defined in:
G DE VAHL DAVIS AND I P JONES, "NATURAL CONVECTION IN A SQUARE CAVITY: A COMPARISON EXERCISE", INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 3, PP 227-248, 1983.
We have chosen the low rayleigh number case to reduce computational cost.
The problem definition has been "non-dimensionalized" by selecting lengths and physical properties equal to 1, except for the viscosity and thermal expansion coefficient. The rayleigh number is controlled by varying the value of gz.

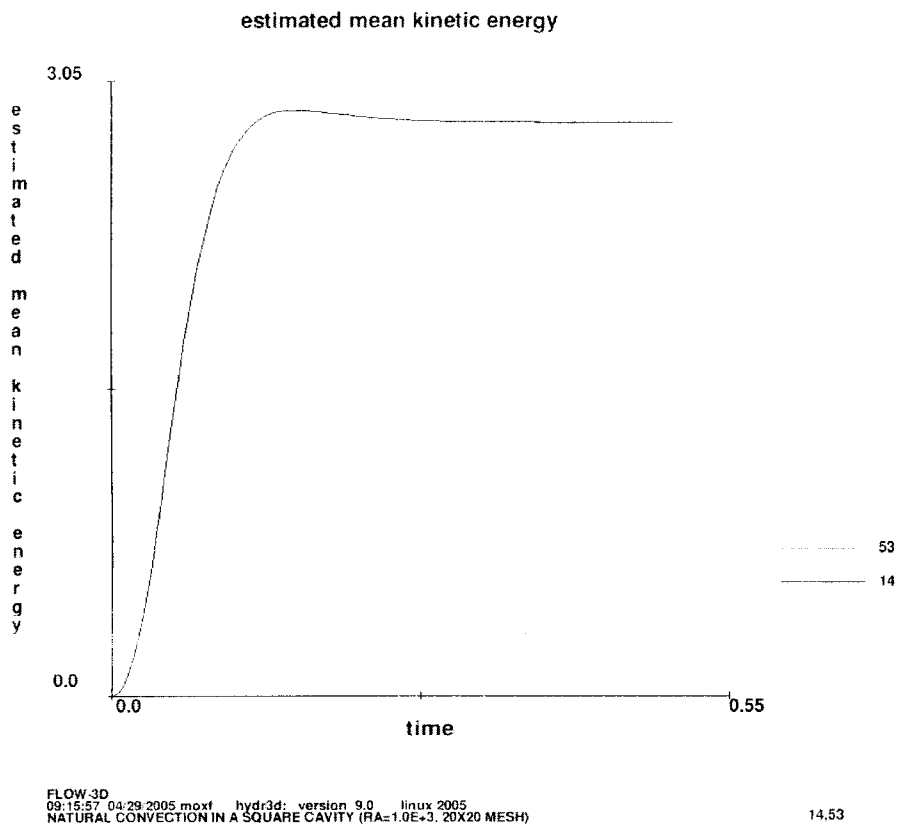
```
$xput
   ipdis=1,          remark=' initial hydrostatic pressure distribution',
   ifenrg=3,         remark=' solve for internal energy and temperature',
   ifrho=1,          remark=' evaluate density from temperature ',
   itb=0,            remark=' no free surface ',
   nmat=1,           remark=' one fluid',
   iwsh=1,           remark=' include wall shear ',
   gz=-7.1e+4,       remark=' gz gives rayleigh number = 1000 ',
   delt=0.001,       remark=' initial time step size ',
   twfin=0.5,        remark=' this is a short final time ',
                     remark='   it is chosen to reduce cpu time ',
   prtdt=0.5,        remark=' only print at end of calculaiton ',
   pltdt=0.1,        remark=' only plot at end of calculation ',
   ihtc=1,           remark=' evaluate wall heat transfer ',
 $end

 $limits
 $end

 $props
                     remark=' equation of state parameters ',
   cv1=1.0,          remark=' non-dimensional specific heat ',
   rhof=1.0,         remark=' non-dimensional density ',
   thc1=1.0,         remark=' non-dimensional conductivity',
```

```
  mui=0.71,          remark=' viscosity set to give the ',
                     remark=' correct prandtl number ',
  thexf1=0.01,       remark=' thermal expansion coefficient ',
                     remark=' must be small ',
  tstar=0.0,         remark=' reference temperature for thermal',
                     remark=' expansion',
$end

$bcdata
                     remark=' walls on physical edges of the box ',
    wl=2,
    tbc(1)=1.0,      remark=' non-dimensional left boundary',
                     remark='  temperature ',
    hwall1(1)=1.e4,  remark=' effective heat transfer ',
                     remark=' coefficient for conduction ',
    wr=2,
    tbc(2)=1.0e-10,  remark=' a non-zero value is needed',
                     remark=' because zero indicates an '.
                     remark=' insulated boundary ',
    hwall1(2)=1.e4,  remark=' effective heat transfer ',
                     remark=' coefficient for conduction ',

    wb=2,  rwall(5)=0.0,      remark=' insulated bottom boundary ',
    wt=2,  rwall(6)=0.0,      remark=' insulated top boundary',


                     remark=' symmetry conditions for 2d approximation ',
    wf=1,
    wbk=1,
$end

$mesh
                     remark=' define a simple, uniform mesh ',
  nxcelt=20,   px(2)=1.0,
  nzcelt=20,   pz(2)=1.0,
$end

$obs
$end

$fl
  flht=1.0,
$end

$bf
$end
```

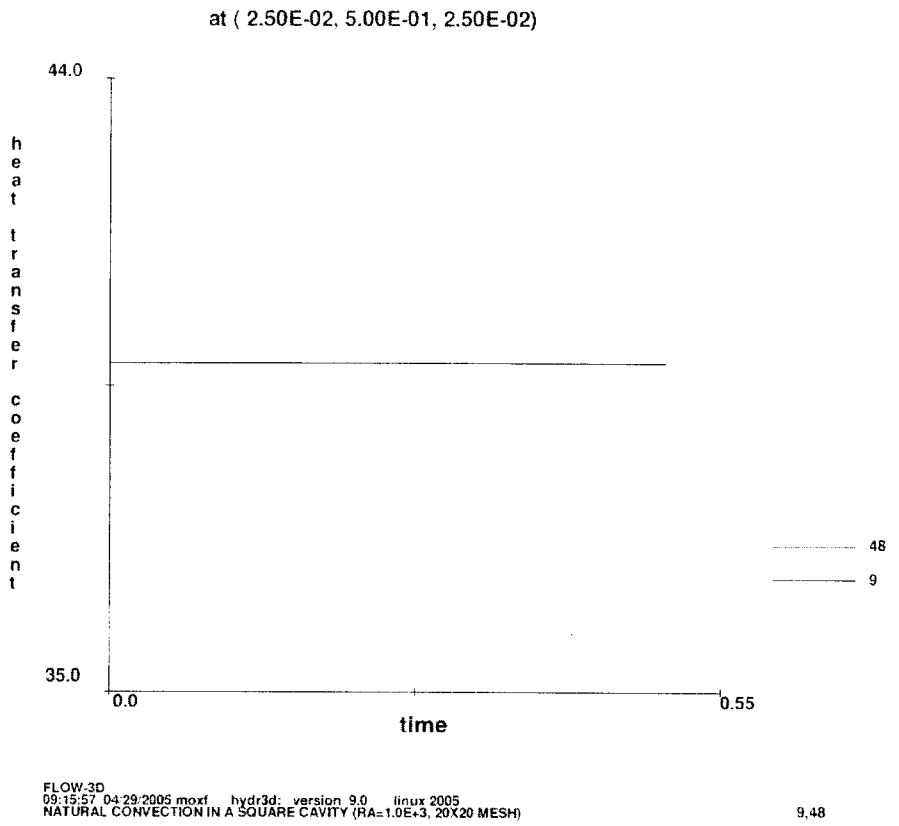
```
$temp
                        remark=' start from uniform temperature ',
   tempi=0.5,
$end

$grafic
                        remark=' place a history probe in the lower left corner ',
   xloc(1)=0.025,   zloc(1)=0.025,   yloc(1)=0.5,
   nvplts=2,            remark='2  velocity vector plots ',
   contpv(1)='tn',      remark=' fluid temperature ',
   contpv(2)='p',       remark=' pressure ',
   ncplts=2,            remark='2 contour plots ',
   ictyp(1)=5,          remark=' color contour lines ',
   contyp(1)='tn',      remark='   of fluid temperature ',
   ictyp(2)=5,          remark=' color contour lines ',
   contyp(2)='p',       remark='   of pressure ',
$end

$parts
$end
```

This input deck was taken from the start-up section of FLOW-3D under the ~/rusr/Flow3d/examples/nconxz/ directory. The file is identified as prepin.inp. Comparative solution data was provided directly from Flowscience through Steve Green (x3519) of Division 18, Southwest Research Institute. Steve had similarly conducted an installation test of FLOW-3D, but on a different computer platform and operating system using the same input deck and comparative benchmark data.

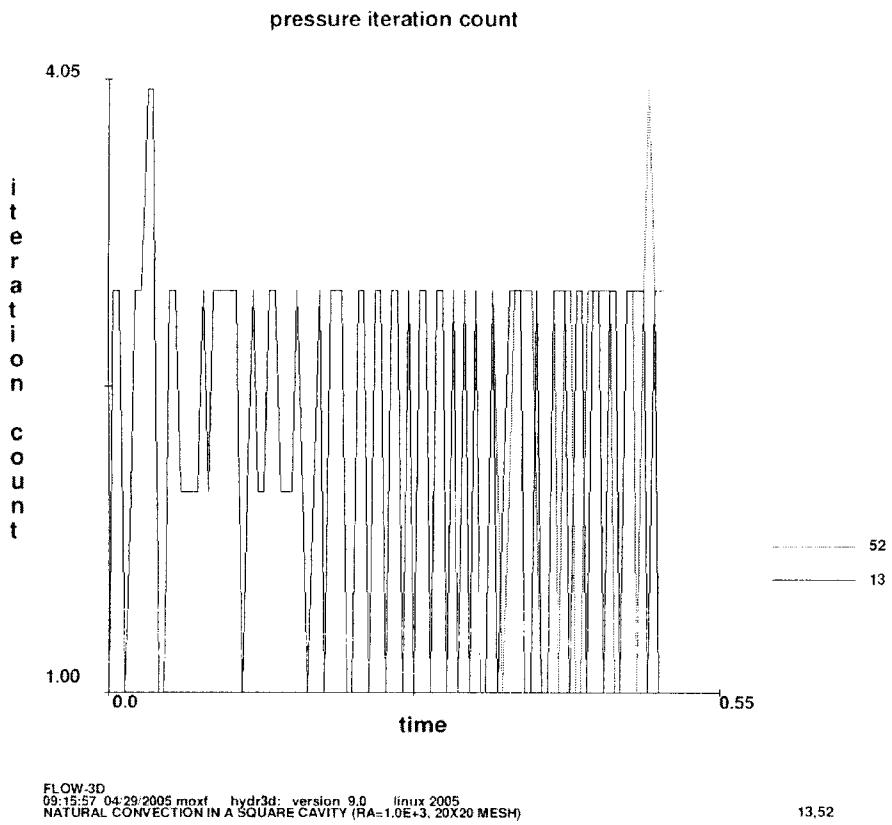
Following is the comparative data from the analysis. Grey lines are the current study. Blue lines are the benchmark study. The graphs were generated by FLOW-3D's interactive GUI by importing the output plot files from both studies and overlaying them when appropriate.



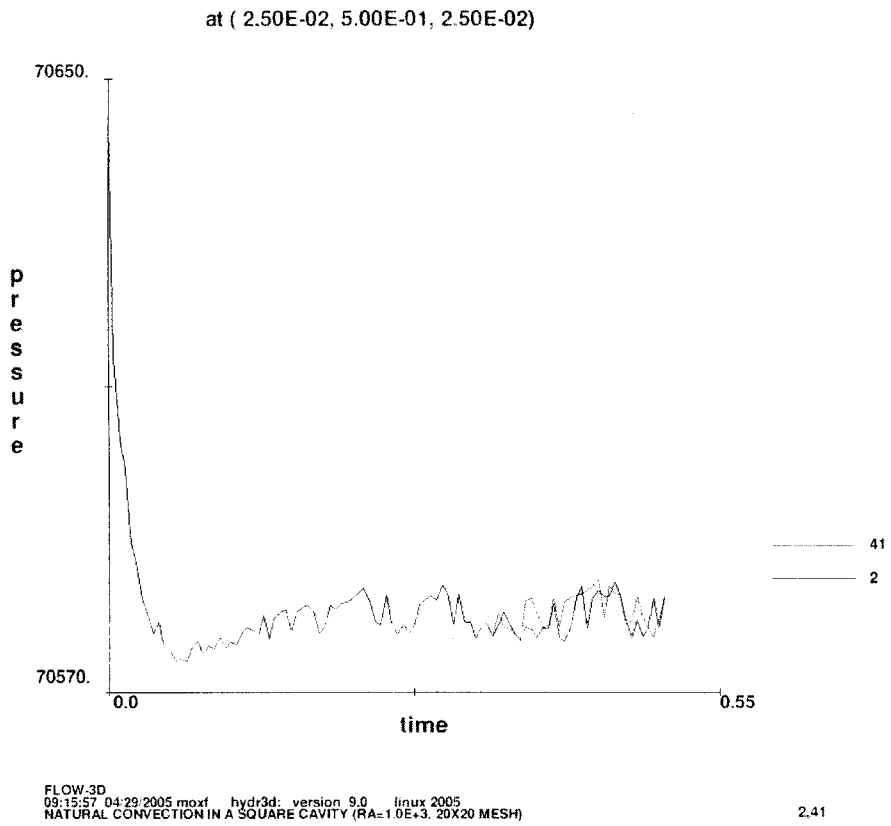
Estimated kinetic energy is a global parameter for the system. There is little difference between the runs.



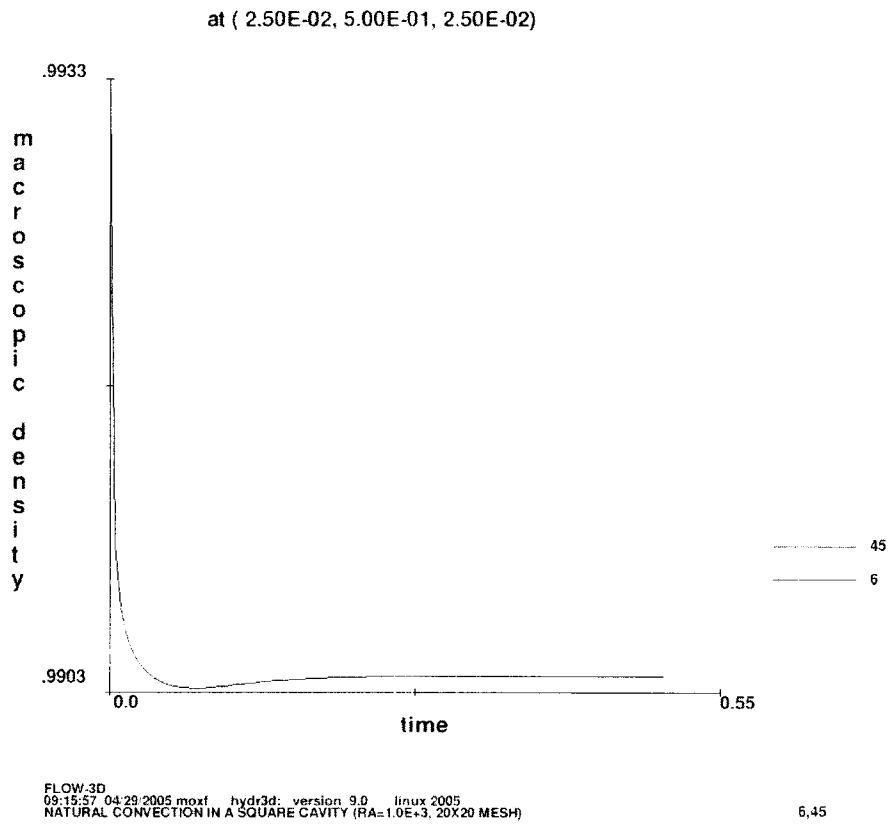
Heat transfer coefficient (in this case) is a global parameter being calculated interactively by the code. There is little difference between the runs.



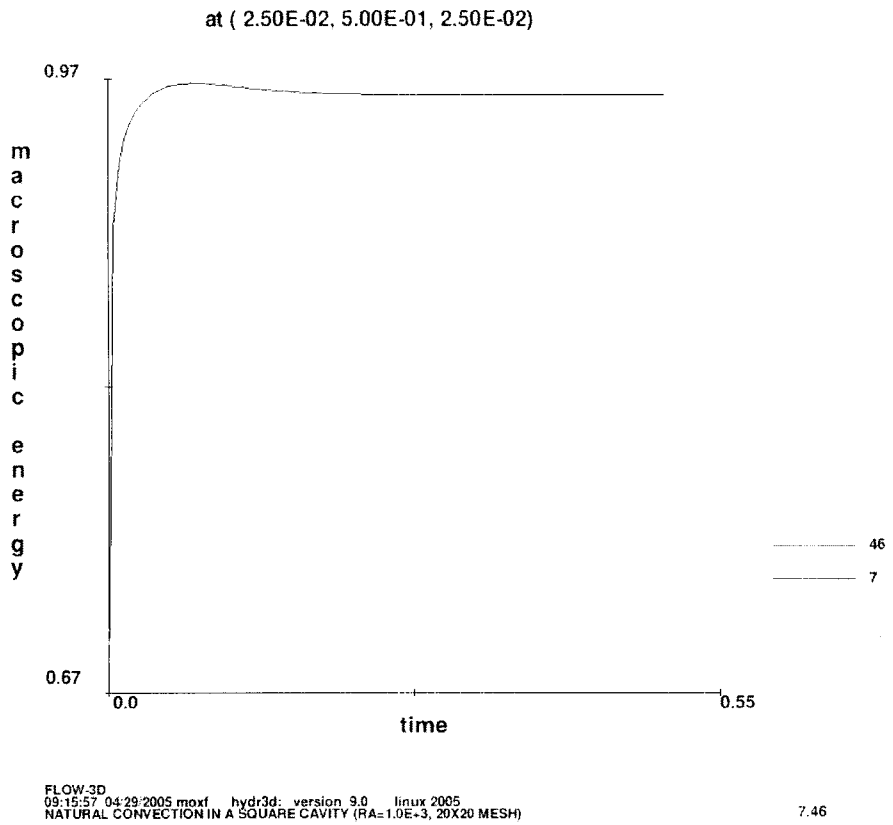
Pressure iteration count is related to the number of times the code goes through the calculations for pressure at any given timestep. The number of these iterations can vary widely from code to code or system to system and still produce the same results. Here we see relatively similar results from the pressure iteration count, although near the end of the simulation, the bench mark and test run do deviate slightly. However, there is no visible effect on measured results quantities so this deviation is of no concern.



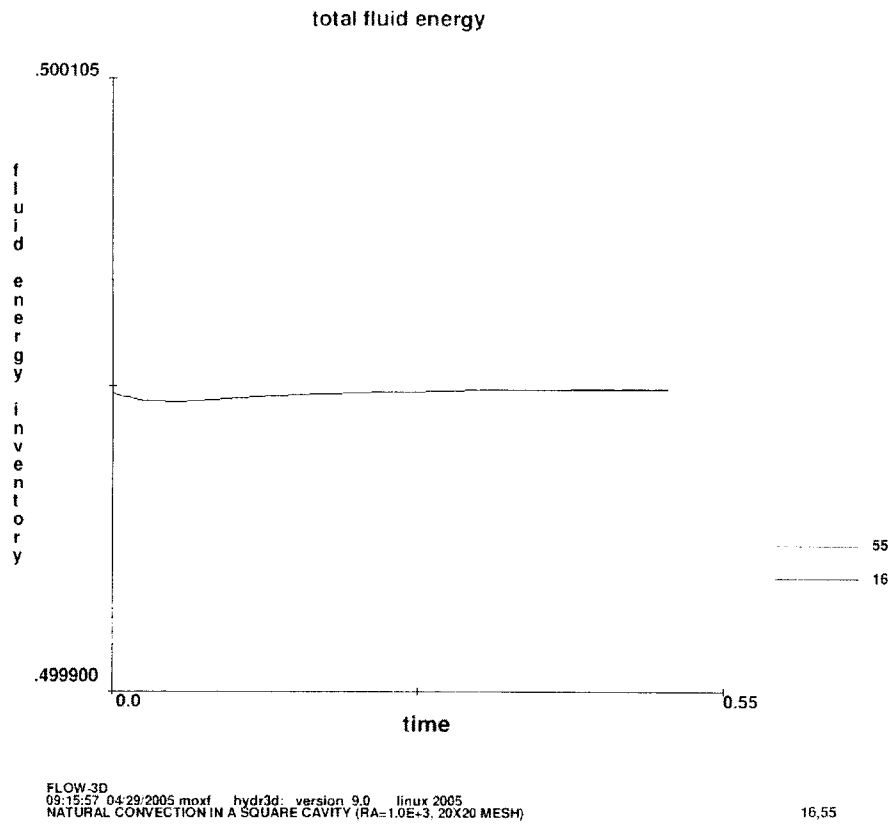
Pressure is a point specific property. Here pressure is shown at (2.5e-02, 5.0e-01, 2.5e-02) roughly the center of the hot panel in the problem. We see good agreement between the two runs, with very minor deviation in the same area as the iteration count differential.



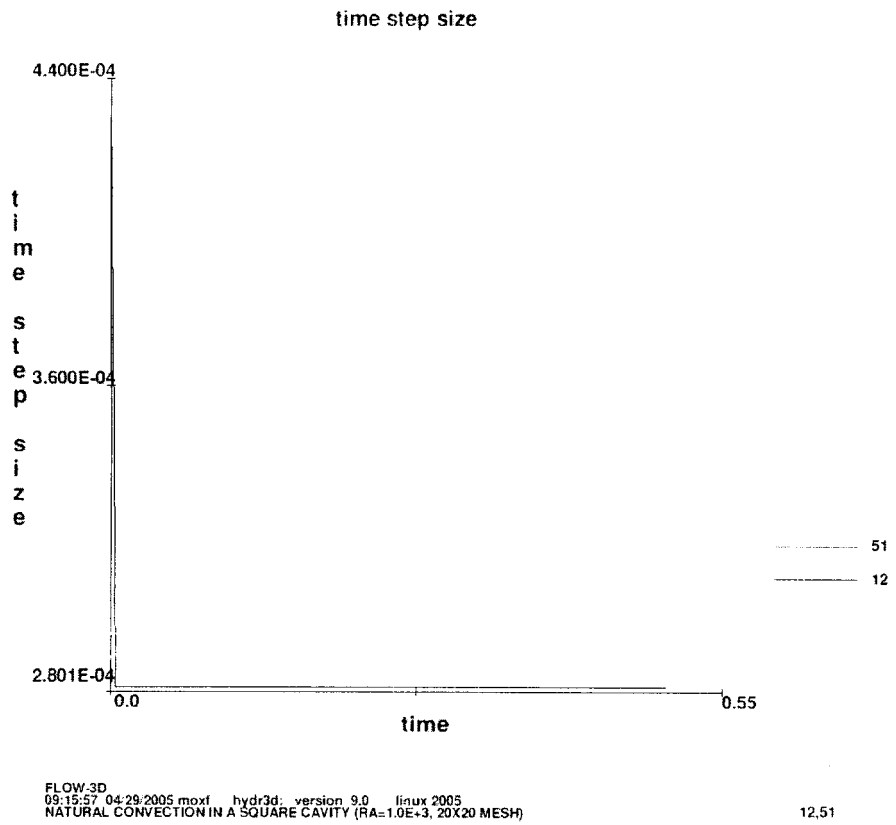
Macroscopic density is a point specific property. Here macroscopic density is shown at (2.5e-02, 5.0e-01, 2.5e-02) roughly the center of the hot panel in the problem. We see excellent agreement in this parameter.



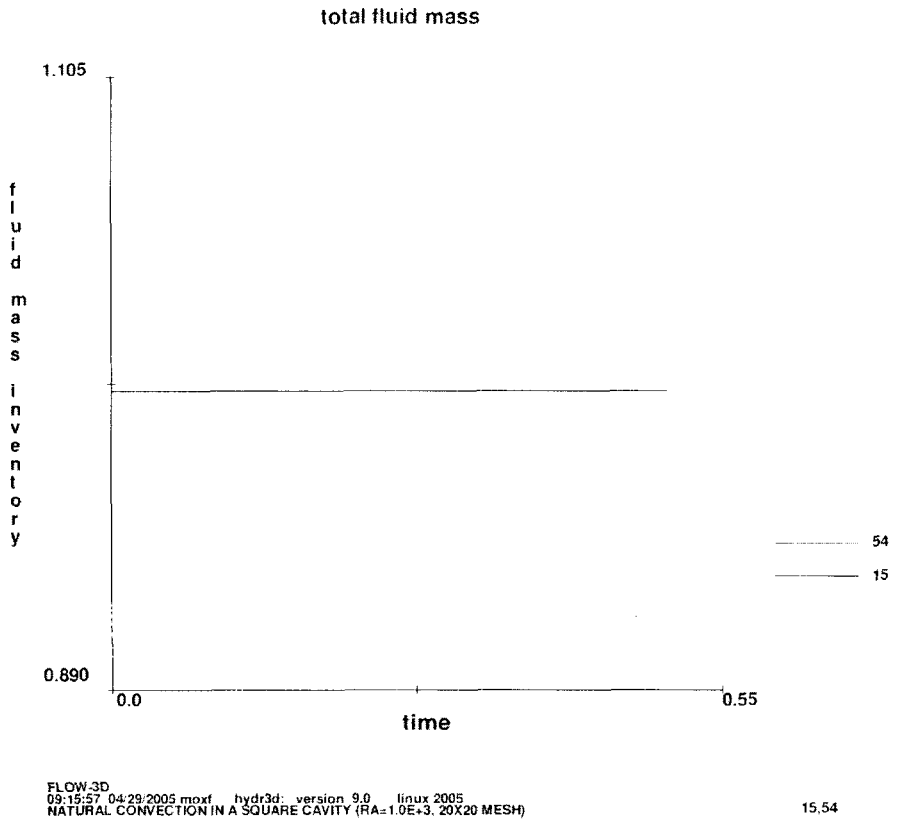
Macroscopic energy is a global property. We see good agreement between the test set and bench mark data.



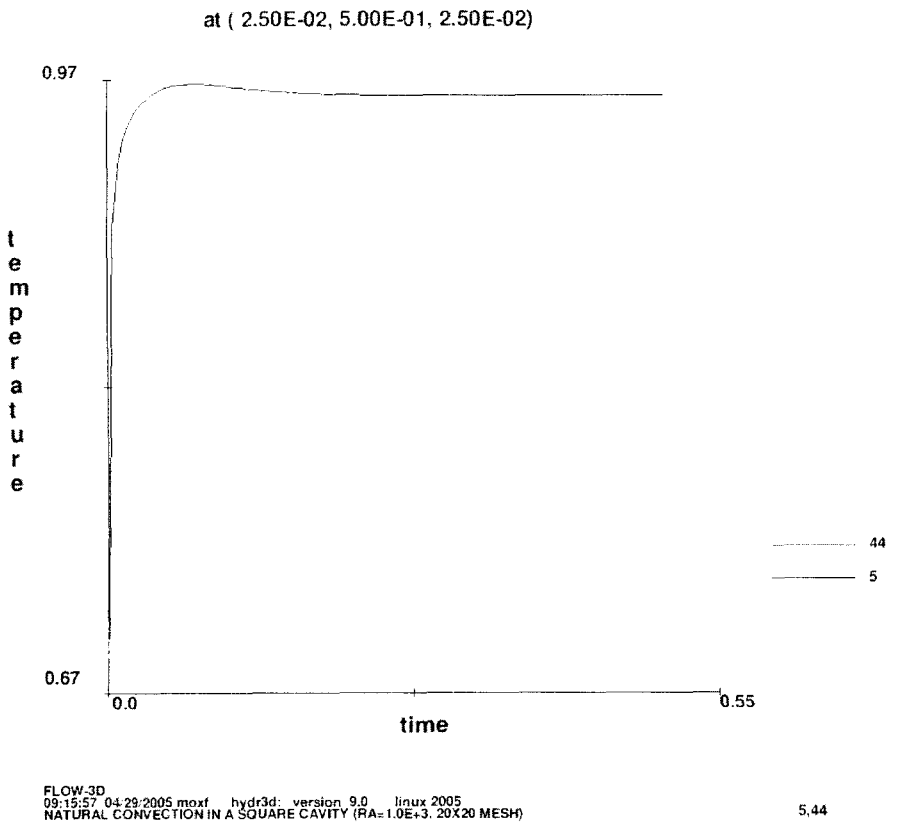
Fluid energy inventory is a global parameter. We show excellent agreement between benchmark and installation data.



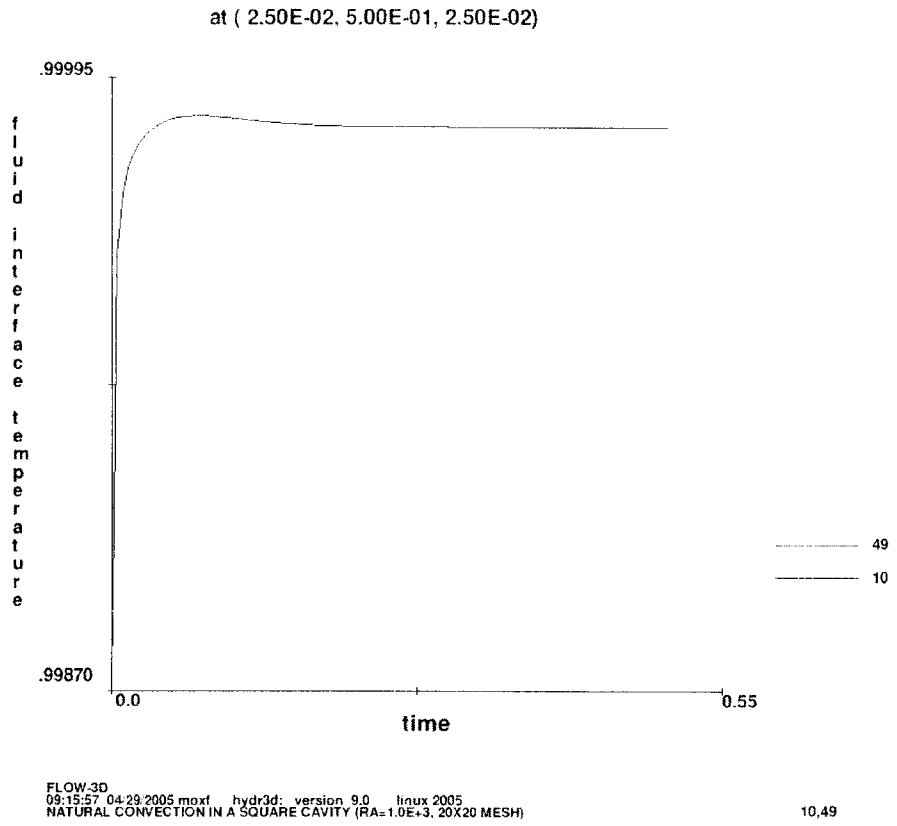
Time step size is dependent on convergence and may vary code to code. Here, however, we see excellent agreement through the runs.



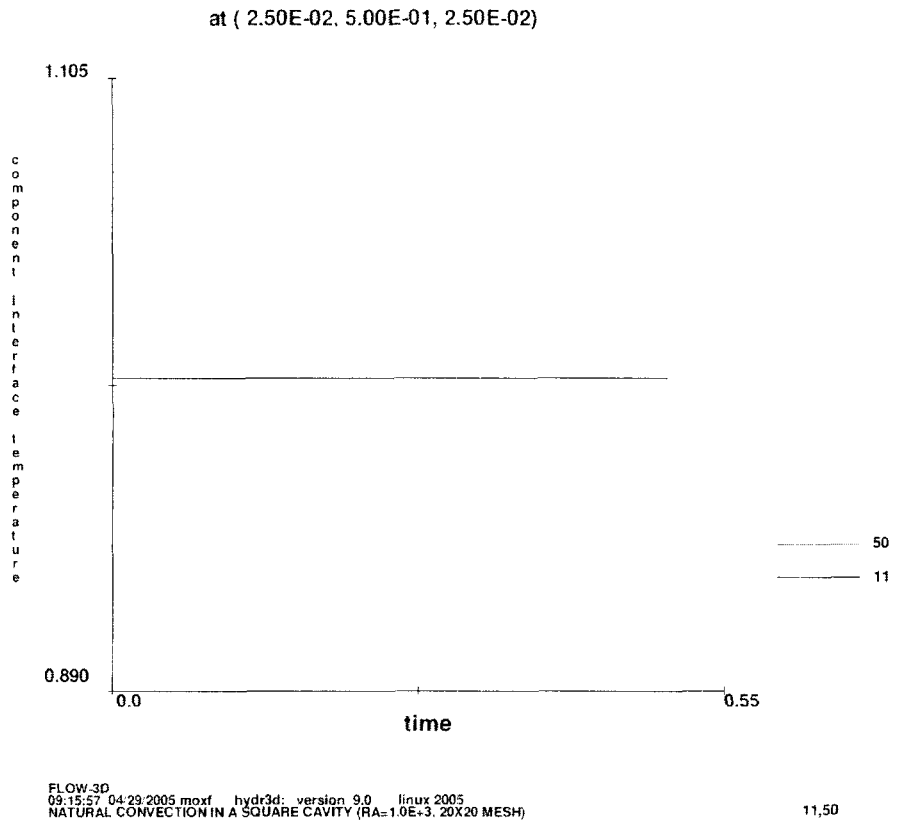
Fluid mass inventory should be a constant in a closed system and that is exactly what we see for both the benchmark and test case.



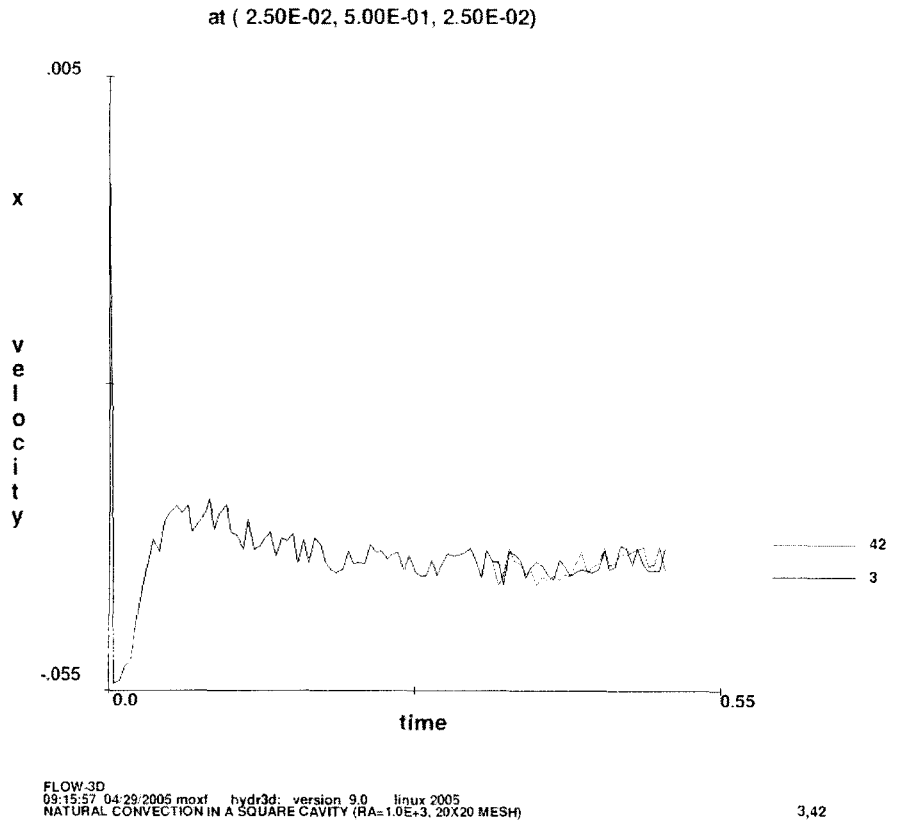
Temperature is a point specific property. Here temperature is shown at (2.5e-02, 5.0e-1, 2.5e-02) roughly the center of the hot panel in the problem. There is good agreement between the test case and the benchmark case.



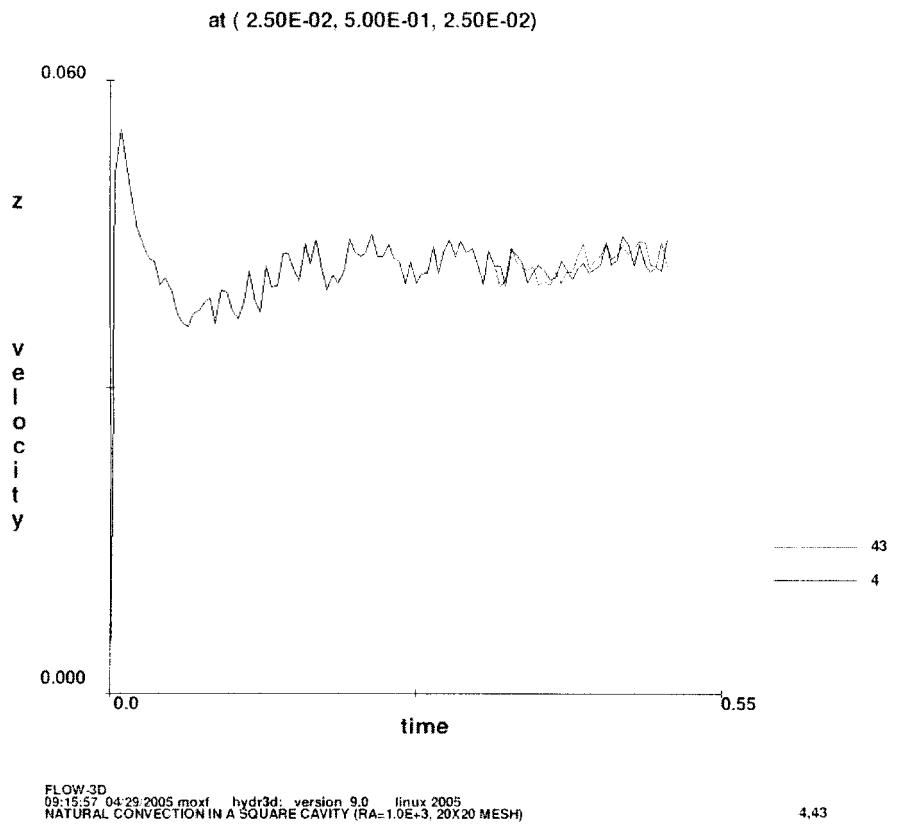
Fluid interface temperature is a point specific parameter. Here fluid interface temperature is shown at (2.5e-02, 5.0e-1, 2.5e-02) roughly the center of the hot panel in the problem. We see excellent agreement between test and benchmark data.



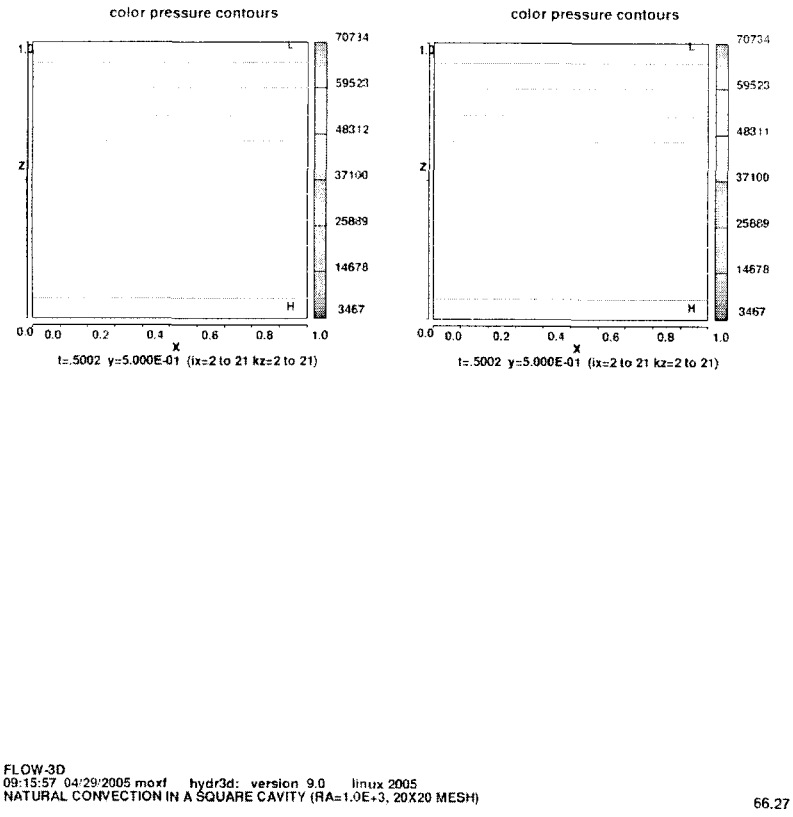
Component interface temperature is point specific. Here component interface temperature is shown at (2.5e-02, 5.0e-1, 2.5e-02) roughly the center of the hot panel in the problem.



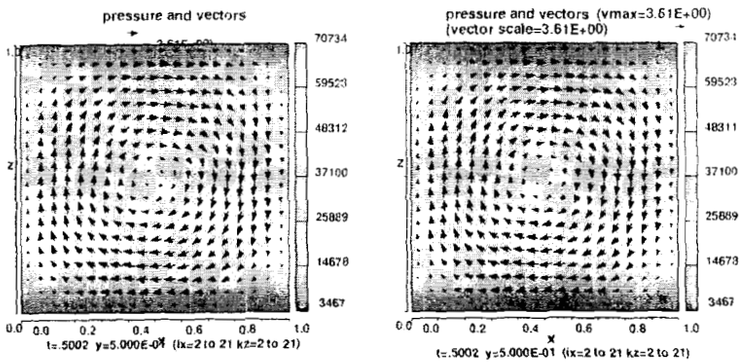
X-velocity is a point specific quantity. Here x-velocity is shown at (2.5e-02, 5.0e-1, 2.5e-02) roughly the center of the hot panel in the problem. We have some deviation toward the end of the simulation, but the magnitude remains reasonable and does not affect overall results.



W-velocity is a point specific quantity. Here w-velocity is shown at (2.5e-02, 5.0e-1, 2.5e-02) roughly the center of the hot panel in the problem. We have some deviation toward the end of the simulation, but the magnitude remains reasonable and does not affect overall results.

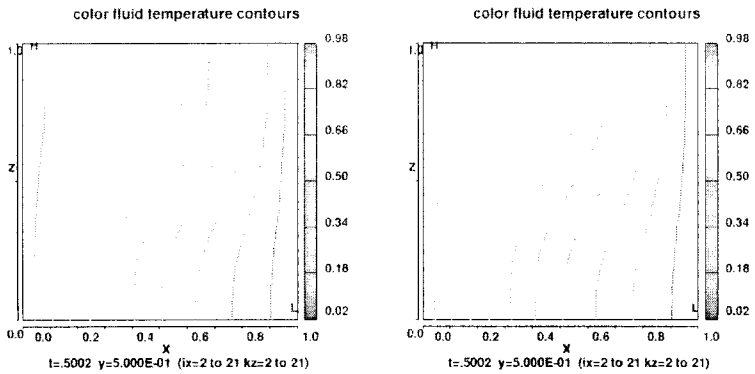


Pressure is a local quantity but can be inspected globally as a results parameter. Here pressure is shown evaluated everywhere in a 2-D visualization. As one can clearly see, there is little difference between calculated pressure at specific points throughout the domain.



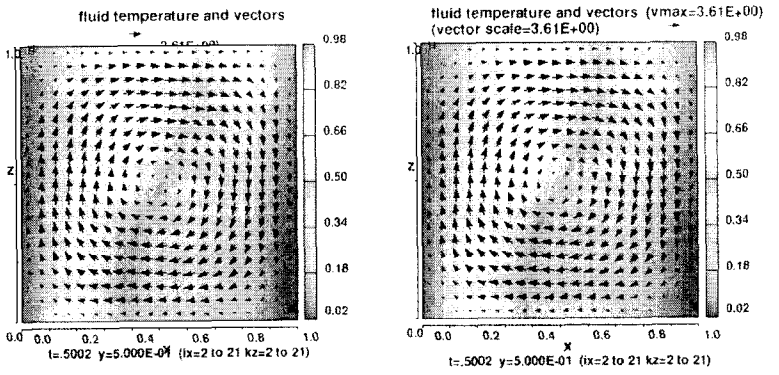
FLOW-3D
09:15:57 04/29/2005 moxf hydr3d: version 9.0 linux 2005
NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH) 78.39

Here we look at velocity vectors over a fully colored pressure field. Once again, there is little difference between the two simulations. Velocity intensity as well as global pressure calculations match well.



FLOW-3D
09:15:57 04/29/2005 moxf hydr3d: version 9.0 linux 2005
NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH) 60.21

Here temperature is shown over the global field as contour lines. As you can readily see, there is little difference in temperature quantities on a global scale.



FLOW-3D
09:15:57 04/29/2005 mext hydr3d: version 9.0 linux 2005
NATURAL CONVECTION IN A SQUARE CAVITY (RA=1.0E+3, 20X20 MESH) 72.33

Here temperature is shown with velocity vectors. The temperature field of the previous graphic is colored in and the velocity vectors overlaid. The circulation pattern is in the direction obvious by physics, and the two cases match very well.

In lieu of these comparisons between a test installation run and a benchmark data set, it was determined that the code FLOW-3D version 9.0 was correctly installed on a Dell OptiPlex GX 400 PC with an Intel Pentium 4 1.7GHz processor utilizing Suse Linux Enterprise 9.0. Data was forwarded to Bis Dasgupta to associate correctly with a software release notice.

Date: 13 May 2005 Entry By: Mary Ann Clarke
Information and redirection from Chris Ryder (NRC)

Chris Ryder sent a hand-out entitled: Bounding Conditions for Thermal Calculations of Fuel Temperature in a Cask and Waste Package (May 12, 2005, revised) via email. I iterate its contents here, typographical errors included.

Fuel rod determination due to oxidation especially in MPC of transportation cask or in transient to waste package may develop fine particulates that could be released to the transfer room. Temperature must be controlled for two reasons:
. Limit oxidation
. Protection instrumentation, controls, monitors, and in some case motors
The potential damage due to temperature rise may make the HVAC or cooling system components ITS.

Assumptions.
1. When helium is vented from a transportation cask, the fuel temperature will start to rise. The helium cover gas would be less dense, and hence, less conductive to draw heat from the fuel to the overpack.
2. When the seal welds are ground off and the lid is removed, the helium migrates out of the cask and air takes its place. Compared to helium under pressure, air is a relatively good insulator.
3. Heat loss to the transfer room will be by natural convection from the open top of the cask. Heat loss to room housing the cask will be from the walls and bottom of the cask. The walls by natural convection. The bottom by conduction to the lift. The bottom heat rejection may be small enough to ignore.
4. The waste package does not add additional heat load to the room. Its heat load comes from the fuel moved from the MPC to the WP. Less heat in MPC, more in WP.
5. The rooms are large enough that air velocities in the room will be small. Heat transfer by natural convection is anticipated.

Suppositions.
NOTE: Some inputs are to be taken as place holders. Such a value is indicated by an asterisk. When more accurate information is known, the values can be changed. The model should be made with this capability.
1. HI-STAR 100 Cask. The FSAR has substantial data, material parameters, et.al that may be useful in your analysis.
2. PWR fuel in MPC-24 of the cask
3. Maximum decay heat load per assembly allowable in the cask.
4. The temperature in the room housing the cask is maintained at 80deg F by sufficient air supply and exits from the secondary at 90deg F.
5. The temperature in the transfer cell is maintained at 85deg F and exits the primary at 95deg F.
6. The maximum design temperature of the transfer cell is 105deg F.
7. The maximum design temperature of the room housing the cask is 95deg F.
8. In the event of a loss of HVAC, operations are halted.

9. Though oxidation is an exothermic reaction, its contribution to the heat load of an assembly is taken to be negligible.
10. Begin with a fully loaded cask.
11. Double the heat load to each room to account for lights, instruments, motors, equipment. Calculate an air flow based on sensible heat removal. Round up the air flow to the next 1000cfm.

Determinations.
1. Determine the time-temperature profile a significant points (eg hottest location along an assembly) in the cask.
2. Determine natural convection in and out of the cask.
3. Given that a fuel rod splits and releases U3O8 powder of a particle sizes of 3, and 0.03 microns, determine if the convection currents are sufficient to carry the powder out of the cask. The amounts of each size particles will be determined by the NRC staff in a separate calculation.
4. Determine, if possible, an optimum way of unloading the cask.
5. Cask temperatures are expected to drop as fuel assemblies are removed. At some point sufficient fuel assemblies will be removed to eliminate temperature rise concerns. How many assemblies need to be removed to reach the point at which heat lost to both rooms exceeds heat generation in the cask?
6. In the event the HVAC system is isolated or fails, what is the effect on temperature of fuel assemblies as a function of time. What is the effect on the transfer cell? What is the effect on the cask room?
7. Determine the time-temperature profile of hottest fuel assemblies in the waste package at significant locations when the waste package is fully loaded.
8. Determine the extent to which the air velocity in the transfer cell is sufficient to keep aerosols aloft.

Date: 19 May 2005 Entry By: Mary Ann Clarke
Calculating porosity values for MPC-24 basket

Using Table 4.4.13 from Hi-Star FSAR Report HI-2012610

Metric conversion: 1 ft^3 = 0.02831685 m^3

(re-created here + augmented with metric values)
Summary of MPC-24 Free Volume Calculations

Item	Volume (ft^3)	Volume (m^3)
Cavity Volume	367.9	10.4177
Basket Metal Volume	37.9	1.07320
Bounding Fuel Assemblies Volume	78.8	2.23136
Basket Supports and Fuel Spacers Volume	6.1	0.17273
Aluminum Conduction Elements	5.9	0.16706
Net Free Volume	237.5	6.72525

Total Net Porosity = Net Free Volume / Cavity Volume = 6.72525/10.4177 = 0.64555

As a simplication, and because the basket is NOT porous to flow in the cross axial direction local to the assemblies (i.e. there is no air flow between assemblies *because of* the basket), an axial porosity is also calculated. This is evaluated by noting the size of basket and assembly components with respect to the cross section of the MPC. These values are taken from HOLTEC International drawing number 3926, "MPC-24 Fuel Basket Arrangement."

Item	Volume (m^3)
Cross sectional area of the basket	0.1606448
Cross sectional area of the assemblies	1.2482220
Cross sectional area of cavity	2.2576668
Net Free Area	0.8488000

Total Cross Sectional Porosity = Net Free Area/Cross sectional area of cavity
= 0.8488000/2.2576668 = 0.37596

Date: 20 May 2005 Entry By: Mary Ann Clarke
CFD grid plane placements MPC-24

Flow-3D has been chosen as the CFD solver for the generalized task of thermally evaluating the Hi-Star 100 Cask in the dry transfer facility. As such, the geometry of the cask must be brought into the program's preprocessor. Since no CAD documents exist in an electronic format such that the cask specifications can be included explicitly, the critical cask components are incorporated into a three-dimensional space by hand (through an input deck) and then a Cartesian mesh is overlaid for computational work. This entry explicitly notates the mesh planes that demarcate specific structural components of the Hi-Star 100 Cask with an MPC-24 basket.

X Space

Location (m)	Component Begins
-2.4336375	4ft air gap beyond cask
-1.2144375	overpack neutron shielding outside radius
-1.0890250	overpack multi-layer shell outside radius
-1.0572750	overpack baseplate radius
-0.9366250	overpack inner shell outside radius
-0.8731250	overpack inner shell inside radius
-0.8683650	MPC base plate outside radius
-0.8540750	outside MPC shell radius
-0.8477250	inside MPC shell radius
-0.8216900	begin fuel basket
-0.8137525	end basket edge, left edge in assemblies 7,13
-0.5842000	begin basket edge, right edge in assemblies 7,13
-0.5762625	end basket edge, left edge in assemblies 3,19
-0.5288280	left edge in assemblies 8,14
-0.3496945	right edge in assemblies 3,19
-0.3022600	begin basket edge, right edge in assemblies 8,14
-0.2943225	end basket edge, left edge in assemblies 4,20
-0.2517902	left edge in assemblies 1,9,15,23
-0.0677545	right edge in assemblies 4,20
-0.0252222	right edge in assemblies 1,9,15,2333, begin basket edge
-0.0172847	end basket edge (air gap)
0.0000000	air gap and center of cask
0.0172847	begin basket edge
0.0252222	end basket edge, left edge in assemblies 2,10,16,24
0.0677545	left edge in assemblies 5,21
0.2517902	right edge in assemblies 2,10,16,24
0.2943225	right edge in assemblies 5,21, begin basket edge
0.3022600	end basket edge, left edge assemblies 11,17
0.3496945	left edge in assemblies 6,22
0.5288280	right edge in assemblies 11,17
0.5762625	right edge in assemblies 6,22, begin basket edge
0.5842000	end basket edge, left edge assemblies 12,18
0.8137525	right edge assemblies 12,18, begin basket edge

X Space (cont'd)

Location (m)	Component Begins
0.8216900	end fuel basket
0.8477250	inside MPC shell radius
0.8540750	outside MPC shell radius
0.8683650	MPC base plate outside radius
0.8731250	overpack inner shell inside radius
0.9366250	overpack inner shell outside radius
1.0572750	overpack base-plate radius
1.0890250	overpack multi-layer shell outside radius
1.2144375	overpack neutron shielding outside radius
2.4336375	4ft air gap beyond cask

Y Space

Location (m)	Component Begins
-2.4336375	4ft air gap beyond cask
-1.2144375	overpack neutron shielding outside radius
-1.0890250	overpack multi-layer shell outside radius
-1.0572750	overpack baseplate radius
-0.9366250	overpack inner shell outside radius
-0.8731250	overpack inner shell inside radius
-0.8683650	MPC base plate outside radius
-0.8540750	outside MPC shell radius
-0.8477250	inside MPC shell radius
-0.8216900	end fuel basket edge
-0.8137525	begin basket edge, bottom edge in assemblies 23,24
-0.5842000	end basket edge, top edge in assemblies 23,24
-0.5762625	begin basket edge, bottom edge in assemblies 19,22
-0.5288280	bottom edge in assemblies 20,21
-0.3496945	top edge in assemblies 19,22
-0.3022600	end basket edge, top edge in assemblies 20,21
-0.2943225	begin basket edge, left edge in assemblies 14,17
-0.2517902	bottom edge in assemblies 13,15,16,18
-0.0677545	top edge in assemblies 14,17
-0.0252222	top edge in assemblies 13,15,16,18, begin basket edge
-0.0172847	end basket edge (air gap)
0.0000000	air gap and center of cask
0.0172847	begin basket edge
0.0252222	end basket edge, bottom edge in assemblies 7,9,10,12
0.0677545	bottom edge in assemblies 8,11
0.2517902	top edge in assemblies 7,9,10,12
0.2943225	top edge in assemblies 8,11, begin basket edge
0.3022600	end basket edge, bottom edge assemblies 4,5
0.3496945	bottom edge in assemblies 3,6
0.5288280	top edge in assemblies 4,5
0.5762625	top edge in assemblies 3,6 begin basket edge

Y Space (cont'd)

Location (m)	Component Begins
0.5842000	end basket edge, bottom edge assemblies 1,2
0.8137525	top edge assemblies 1,2, begin basket edge
0.8216900	end fuel basket
0.8477250	inside MPC shell radius
0.8540750	outside MPC shell radius
0.8683650	MPC base plate outside radius
0.8731250	overpack inner shell inside radius
0.9366250	overpack inner shell outside radius
1.0572750	overpack base-plate radius
1.0890250	overpack multi-layer shell outside radius
1.2144375	overpack neutron shielding outside radius
2.4336375	4ft air gap beyond cask

Z Space

Location (m)	Component Begins
-0.2159000	bottom overpack base plate
-0.0635000	top overpack base plate
0.0000000	bottom of fuel basket
0.0635000	bottom overpack neutron shielding
0.3052800	begin fuel
4.1651200	end fuel
4.4037250	top overpack neutron shielding
4.4704000	top fuel basket
4.5212000	top MPC shell
4.7910750	top overpack layering system
4.9434779	top overpack idealized lid edge
6.0000000	3+ feet higher than the cask

Date: 09 June 2005 Entry By: Mary Ann Clarke
Flow-3D Validation Exercises

Case 1: A comparison of: "Natural convection inside ventilated enclosure heated by downward-facing plate: experiments and numerical simulations"
by: Dubovsky, V., et. al.
from: International Journal of Heat and Mass Transfer, Vol 44, **2001**, pp 3155-3168.

Numerical Comparative: Fluent 4.52 v. Flow-3D 9.0

Physical Model.
This is a scaled room-like event whereby a portion of the "ceiling" of a room is heated and two ceiling sections are open for natural ventilation through in and out air flow. From the point of view of heat transfer into the enclosure, heating from the ceiling is considered a worst case scenario; heat transfer is primarily by conduction between the hot plate and the circulating air. However, it is the temperature differential between the walls of the room that creates a natural circulation in the room; it is this air motion that drives the ventilation.

In the "real" experiment, the hot plate is provided by the bottom of a tin tank filled with boiling water, maintained at temperature by the immersion of two electrical heaters. The walls of the tank that are not part of the hot plate are insulated. Spatial uniformity of the plate temperature was experimentally verified and shown to be constant and uniform at 100°C. The box acting as the experimental room is of dimensions: 60cm (length), 30cm (height), and 24cm (width). Along the top of the box two 5cm openings running the entire width of the box act as the air inflow and outflow regions. Also, an interior wall, running from the air inflow edge to 5cm above the bottom of the box exists. Please see Figure 1 for a visual description of the testing apparatus.

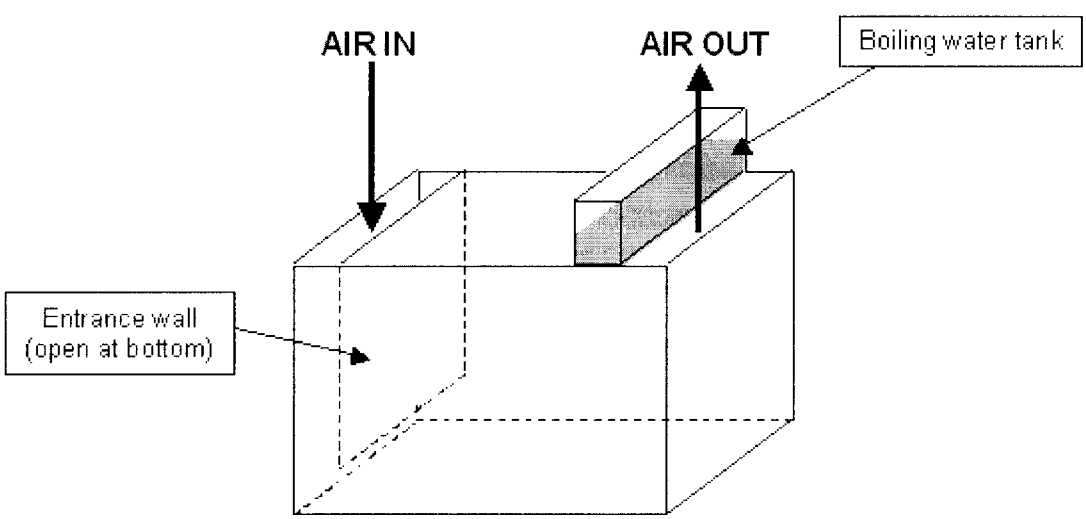


Figure 1: Experimental Apparatus Used in Test Case 1

All walls of the box are thermally insulated with a 0.2cm layer of insulation. The convective heat transfer coefficient measured outside the box was 10-12 W/m2-°C. The convective heat transfer coefficient assumed inside the box was 2-5 W/m2-°C. The heat transfer coefficient based on the thermal resistance of the wall and the convective resistance outside the box was obtained as 0.08 W/m2-°C with an uncertainty of 15%. The heat transfer coefficient for the heated plate was found to be 5 W/m2-°C with a 20% uncertainty (all note, p. 3158).

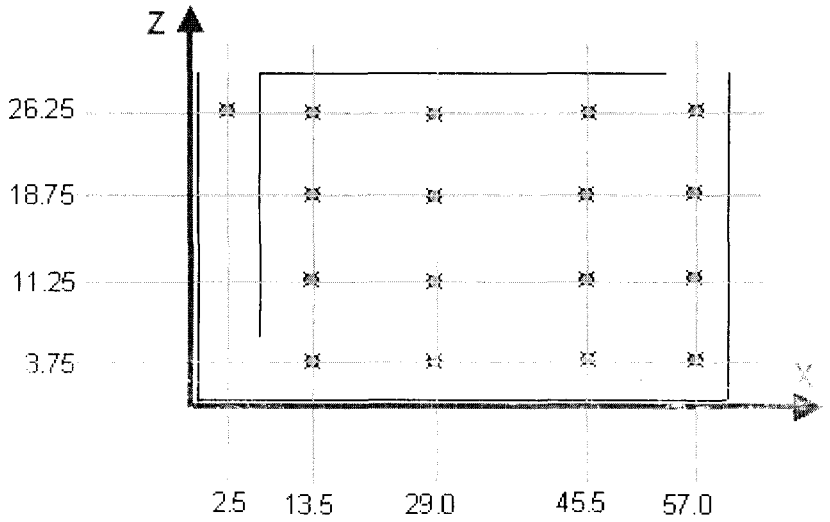


Figure 2: Thermocouple placement along midline (depth) of system. Left and lower inside walls shown at 0 axes location. Offset given is in cm.

Thermocouples were placed along the apparatus width midline as shown in Figure 2. Temperature measurements were made every 15 minutes. Steady state was determined as a point when less that 0.2°C deviation from a previous measurement was made for all thermocouples in the system. Typical times to steady state were on the order of 2 hours.

A more detailed accounting of the test fixture and experimental method can be obtained in the cited paper of Case 1.

Computational Model.

The cited paper incorporates an experimental comparison to a numerical model run in the computational fluid dynamics code, Fluent 4.52. Specifically, they compare to (1) a steady state case when the whole system is sealed, (2) a ventilated steady state when the entrance and exit windows are open, and (3) the early transient between state (1) and state (2). A 2-dimensional grid evaluation was undertaken (eliminating width) using 60 x 30 (length x height) and 120 x 60 grids to determine if temperature effects were significant. There was little difference in the comparative runs so the coarser mesh was extended to the three dimensional calculations. The reported 3-dimensional Fluent 4.52 runs use a grid defined at 60 x 30 x 8 (length x height x width), where each cell is particularly 1 x 1 x 3 cm^3. A grid refinement study was conducted for one case utilizing 60 x 30 x 24; differences were within experimental error so the coarser grid was maintained for the rest of the calculations.

The particular settings used in Fluent 4.52 are not described in the paper, but instead a general description of the heat transfer theory utilized by Fluent 4.52 is offered. This theory, presented on page 3161 is identical to that of our proposed computational fluid dynamics code, Flow-3d 9.0, and will be reiterated here.

The basic conservation equations are solved numerically. The form of these equations is:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \frac{\partial p}{\partial t} + u_i\frac{\partial p}{\partial x_i} + \tau_{ij}\frac{\partial u_i}{\partial x_j}$$

The first equation is for continuity, the second for momentum, and the third for energy. Variable definitions are:

ρ = density, u_i = velocity in the I-direction, p = static pressure, t = time,

x_i = Cartesian location, τ_{ij} = stress tensor, g_i = gravitational acceleration in the I-direction,

h = static enthalpy, k = thermal conductivity, and T = temperature.

The Flow-3d 9.0 model employed a 64 x 34 x 12 grid to include the physical nature of the walls and insulation materials of the test fixture. The original Fluent 4.52 model simplified these boundaries as mesh boundaries with generalized wall properties. The boundary which incorporated the inflow/outflow condition was given the property that p'=0, which is the same as Flow-3d 9.0's continuative condition that we similarly employed. This test, while slightly more computationally expensive, therefore, allows us to examine the walls themselves and the interaction of those walls with a boundary of air in addition to the thermal comparatives registered by the interior thermocouples of the fixture. It also allows us to verify thermal properties as suggested by the experiments. Hence our results are two fold: (1) a comparison to the actual experiments by Dubovsky and (2) a comparison to a different numerical model created in Fluent 4.52, a widely recognized and employed computational fluid dynamics code.

Comparative Results.

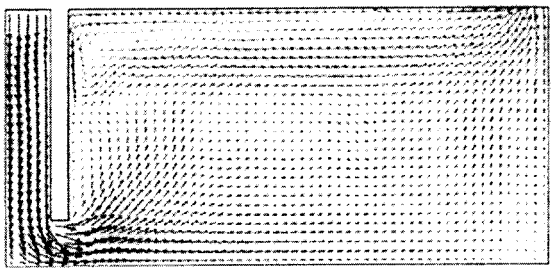
First, the system is brought to a closed steady state. This means that the system is completely closed (the vents are shut) and allowed to equilibrate with the hot plate in place. Equilibration is measured by evaluating the temperature at history points within the system per figure 2. When no change in local temperature is observed (aside from normal and regular numerical oscillation), the system is deemed steady.

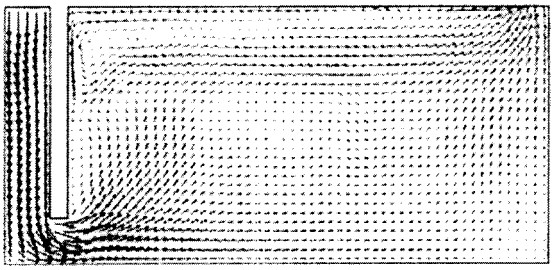
Then, the side vents of the system are opened and the transient is observed and compared. Shown in Figure 3a and 3b is a side by side comparison of the Fluent 4.52 prediction and the Flow-3D 9.0 prediction of the velocity vectors in the flow along the mid-plane through the

system over a reported 20 second transient. Figure 4 is a side by side comparison of the steady state condition. Qualitatively and numerically there is less than 1% difference between the cases.

Fluent 4.52 Flow-3D 9.0

1 sec





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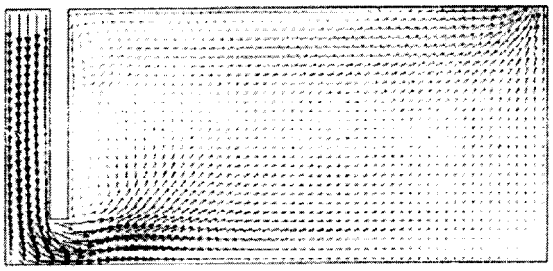

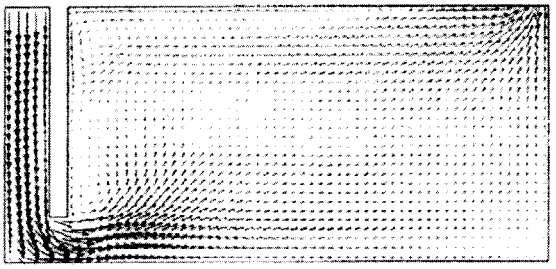

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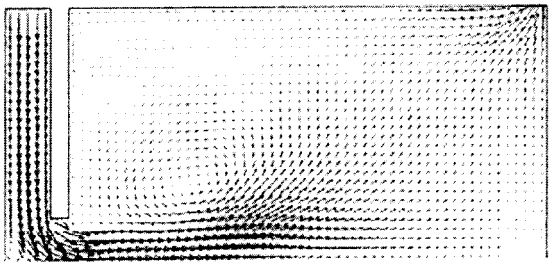
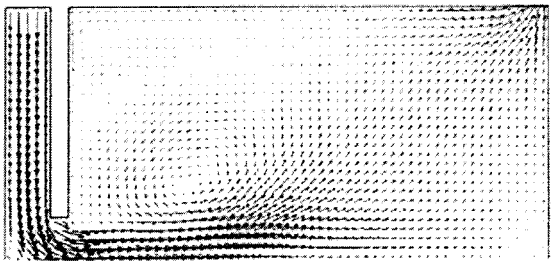
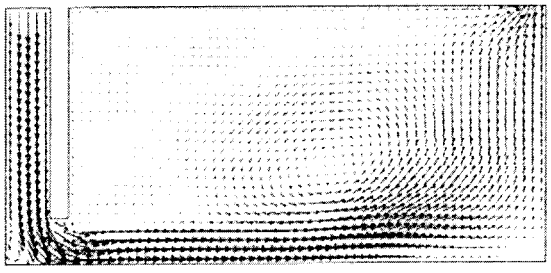
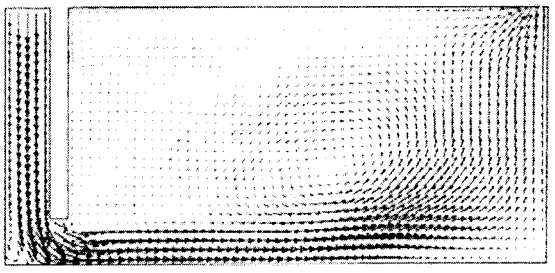




6 sec





8 sec

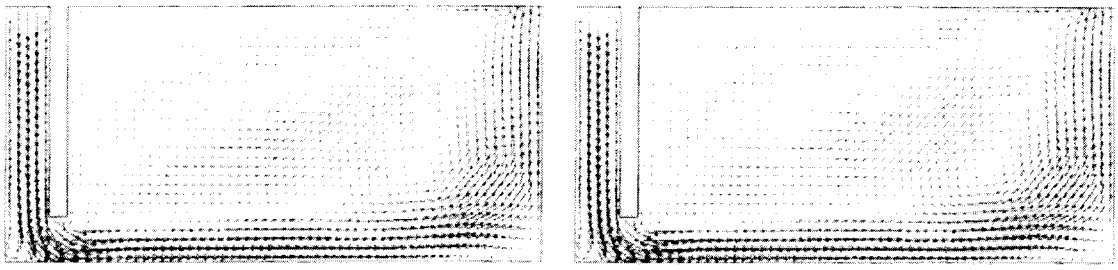
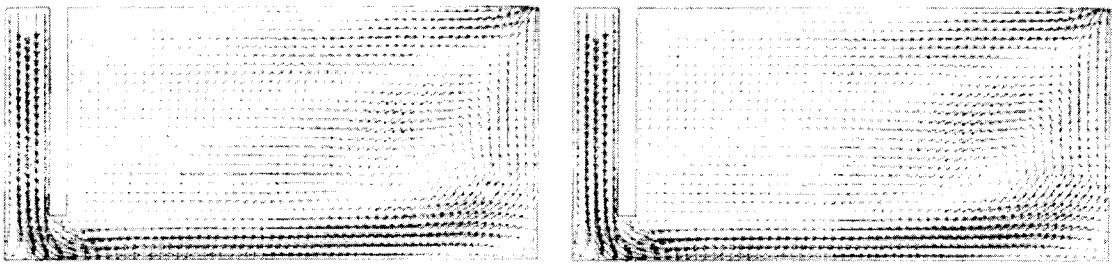


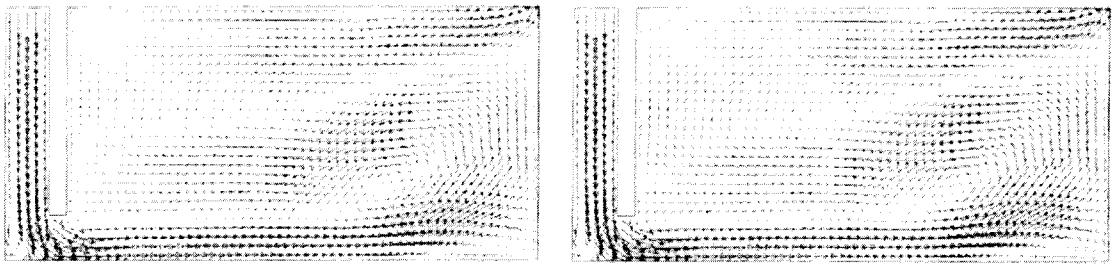
Figure 3a: Transient development of velocity vector flow field. 1 – 8 seconds

Fluent 4.52 Flow-3D 9.0

10 sec



12 sec



20 sec

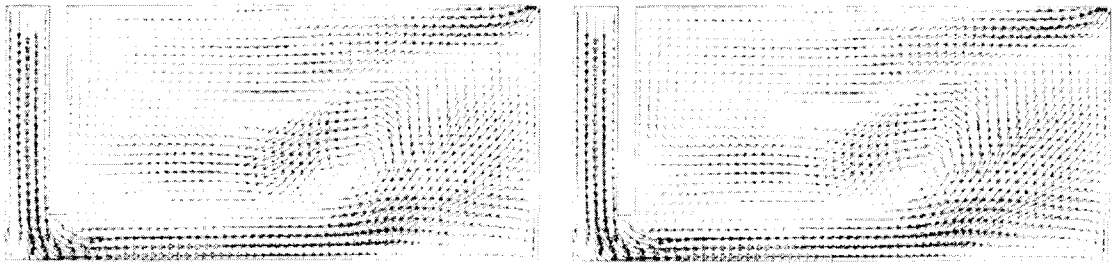


Figure 3b: Transient development of velocity vector flow field, 10 –20 seconds

Fluent 4.52 Flow-3D 9.0

Steady State (time = unk) Steady State (500 sec)

(c)

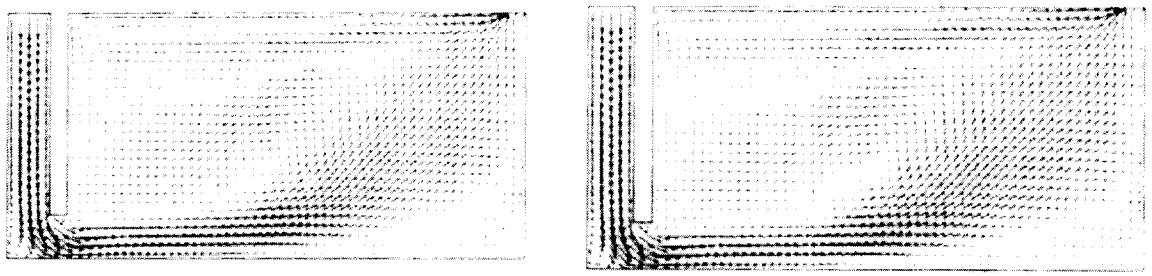


Figure 4: Steady state velocity vector comparison of Fluent 4.52 case and Flow-3D 9.0 Case

In addition to an evaluation of local velocity profile as a comparison to the Fluent 4.52 runs, we also measure the temperature within the fixture at discrete locations at steady state. These locations are the same as those illustrated in Figure 2 along the mid-line of the system. These values are catalogued in Table 1.

Thermocouple Position (x,z) = (cm,cm)	**Measured** Temp (°C)	**Flow-3D 9.0** Temp (°C)
(2.5,26.25)	0.2	0.2
(13.5, 26.25)	2.6	2.5
(29.0, 26.25)	3.3	3.3
(45.5, 26.25)	3.6	3.6
(57.0, 26.25)	3.1	3.2
(13.5, 18.75)	2.3	2.3
(29.0, 18.75)	2.5	2.5
(45.5, 18.75)	2.5	2.6
(57.0, 18.75)	2.4	2.4
(13.5, 11.25)	2.1	2.0
(29.0, 11.25)	2.2	2.2
(45.5, 11.25)	2.0	2.0
(57.0, 11.25)	1.9	1.9
(13.5, 3.75)	1.8	1.9
(29.0, 3.75)	1.5	1.5
(45.5, 3.75)	1.5	1.5
(57.0, 3.75)	1.9	1.9

Table 1: Temperature Distribution Above Ambient (25C) at Steady State along midline xz plane of test fixture. (x,z) notation corresponds to Figure 2.

There is good agreement between actual results and Flow-3D 9.0 predictions.

This is a copy of the Flow-3D input deck used in Case 1:

04 March 2005 - convection in ventilated enclosure

This is a test deck to evaluate natural convection inside a ventilated enclosure.
I am working against an experiment as defined in the paper:

Natural convection inside ventilated enclosure heated by downward-facing plate: experiments and numerical simulations
By: Dubovsky, V.; Ziskand, G.; Druckman, S; Moshka, E; Weiss, Y; Letan, R;
From: International Journal of Heat and Mass Transfer
Volume 44, 2001, pp.3155 - 3168

As a brief description, a sizable box is created with openings on opposite sides of the roof. Air is forced in one side and naturally circulates to the other opening as an exit. There is a good pic of this on p.3157 of the aforementioned paper. Meanwhile, near the exit a region of "boiling water" is maintained to create a hot plate in the roof. Computationally, we don't use water, but we do maintain the plate at 100C. Thermocouples are placed in discrete locations throughout the enclosure and are monitored to compare to the experiment and to a separate numerical analysis described in the paper. Air currents and temperature distributions will be compared.

```
$XPUT

  icmprs  = 1,   remark = 'compressible flow',
  ifrho   = 1,   remark = 'density as function of ff and local T',
  ifenrg  = 3,   remark = 'internal energy, 1st order advection',
  ifvis   = 1,   remark = 'turbulent energy model',
  iorder  = 3,   remark = 'setting iorder = 1 (linear) for start-up',
  itb     = 0,   remark = 'no free surfaces',
  nmat    = 2,   remark = 'compressible option requires using 2 mat',
  iwsh    = 0,   remark = 'turn off wall shear',

  imphtc = 1,    remark = 'fully implicit eval of temp terms',
  ihtc   = 1,    remark = 'turn on heat transfer',

  twfin   = 50.0, remark = 'simulation end, seconds',
  pltdt   = 0.5, remark = 'plotting interval, seconds',
  hpltdt  = 1.0, remark = 'history interval, seconds',
  delt    = 0.1, remark = 'time step, seconds',
  istdy   = 1,   remark = 'accelerate to steady state using non-phys transient',
  autot   = 2.0, remark = 'timestep by stability',
  omega   = 1.7, remark = 'default setting for over-relaxation factor',
```

```
  epsadj  =  1.0, remark = 'standard convergence criterion',

  iadix  =  1,  remark = 'pressure iteration options (x,y,z) ADI',
  iadiy  =  1,
  iadiz  =  1,

$END

$LIMITS

  itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
  itmax  =  100,    remark = 'allowable inner iteration count',
                        remark = 'adjust itmax early to quickly step through start-up',
  negtmx  =  100000,  remark = 'negative rhoe resets',

$END

$PROPS

  remark  = 'set up properties on fluid 2 to allow for compressibility option',

  mu2    = 1.86e-5, remark = 'viscosity air',
  cv2    = 1883.7,  remark = 'specific heat air',
  thc2   = 0.0264,  remark = 'thermal conductivity air',
  tstar  = 293.15,  remark = 'ref temp for air properties',
  rf2    = 287.0,   remark = 'gas constant air',

$END

$SCALAR
  remark = 'none needed for these simulations',
$END

$BCDATA

  remark = 'top wall is continuative (wt) or boundary 6',

  wl    = 2,
  wr    = 2,
  wf    = 2,
  wbk   = 2,
  wb    = 2,
  wt    = 3,  remark = 'change to 3 when chimney open',
  fbc(6) = 1.0,
```

```
$END

$MESH

  remark = 'creating simple mesh for test',
  remark = 'simulations run in metric units',
  remark = 'using uniform mesh spacing = 0.005m in all directions',
  remark = 'total 3 dimensional mesh count = 487424',

  remark = 'original Fluent runs done at 60 x 8 x 30',
  remark = 'second set done at 60 x 24 x 30',
  remark = 'but they dont show walls',

  remark = 'x direction is longest dimension of enclosure corresponding to width',
  nxcelt  = 128,
   px(1) = -0.020,    nxcell(1) = 4,
   px(2) =  0.00,     nxcell(2) = 120,
   px(3) =  0.60,     nxcell(3) = 4,
   px(4) =  0.620

  remark = 'y direction is depth',
  nycelt  = 56,
   py(1) = -0.020,    nycell(1) = 4,
   py(2) =  0.00,     nycell(2) = 48,
   py(3) =  0.24,     nycell(3) = 4,
   py(4) =  0.26,

  remark = 'z direction is height',
  nzcelt  = 68,
   pz(1) = -0.020,    nzcell(1) = 4,
   pz(2) =  0.00,     nzcell(2) = 60,
   pz(3) =  0.30,     nzcell(3) = 4,
   pz(4) =  0.320,

$END

$OBS

  nobs = 11,

  remark = 'create the obstacle field',

  remark = 'first put in the exterior walls, all 2cm thick insulated',
  remark = 'front and back of box',
```

```
iob(1) = 1, ioh(1) = 1, xl(1) = -0.020, xh(1) = 0.620,
            yl(1) = -0.020, yh(1) = 0.000,
            zl(1) = -0.020, zh(1) = 0.320,
            remark = 'heat transfer coefficient W/m2-C, from p3158',
            remark = 'kobs(1) = 0.08',

iob(2) = 2, ioh(2) = 1, xl(2) = -0.020, xh(2) = 0.620,
            yl(2) =  0.240, yh(2) = 0.260,
            zl(2) = -0.020, zh(2) = 0.320,
            remark = 'kobs(2) = 0.08',

remark = 'left and right side of box',
iob(3) = 3, ioh(3) = 1, xl(3) = -0.020, xh(3) = 0.000,
            yl(3) = -0.020, yh(3) = 0.260,
            zl(3) = -0.020, zh(3) = 0.320,
            remark = 'kobs(3) = 0.08',

iob(4) = 4, ioh(4) = 1, xl(4) =  0.600, xh(4) = 0.620,
            yl(4) = -0.020, yh(4) = 0.260,
            zl(4) = -0.020, zh(4) = 0.320,
            remark = 'kobs(4) = 0.08',

remark = 'bottom of box',
iob(5) = 5, ioh(5) = 1, xl(5) = -0.020, xh(5) = 0.620,
            yl(5) = -0.020, yh(5) = 0.260,
            zl(5) = -0.020, zh(5) = 0.000,
            remark = 'kobs(5) = 0.08',

remark = 'top of box, left and excluding hot plate',
iob(6) = 6, ioh(6) = 1, xl(6) =  0.050, xh(6) = 0.400,
            yl(6) = -0.020, yh(6) = 0.260,
            zl(6) =  0.300, zh(6) = 0.320,
            remark = 'kobs(6) = 0.08',

remark = 'top of box, right and excluding hot plate',
iob(7) = 7, ioh(7) = 1, xl(7) =  0.510, xh(7) = 0.550,
            yl(7) = -0.020, yh(7) = 0.260,
            zl(7) =  0.300, zh(7) = 0.320,
            remark = 'kobs(7) = 0.08',

remark = 'the hot plate',
iob(8) = 8, ioh(8) = 1, xl(8) =  0.400, xh(8) = 0.510,
            yl(8) = -0.020, yh(8) = 0.260,
            zl(8) =  0.300, zh(8) = 0.320,
            pobs(1,8) = -1200.0,
            kobs(8) = -5.0,
```

```
                twobs(1,8) = 373.0,
                tobs(1) = 0.0,

  remark = 'inner partition, with opening at bottom',
  iob(9) = 9, ioh(9) = 1, xl(9) =  0.050, xh(9) = 0.070,
                yl(9) = -0.020, yh(9) = 0.260,
                zl(9) =  0.050, zh(9) = 0.320,
                remark = 'kobs(9) = 0.08',

  remark = 'once box at steady state, remove lids',

  remark = 'close the box, left lid',
  remark = 'iob(10) = 10, ioh(10) = 1, xl(10) = -0.020, xh(10) = 0.050,',
  remark = '                    yl(10) = -0.020, yh(10) = 0.260,',
  remark = '                    zl(10) =  0.300, zh(10) = 0.320,',
                  remark = 'kobs(10) = 0.08',

  remark = 'close the box, right lid',
  remark = 'iob(11) = 11, ioh(11) = 1, xl(11) =  0.550, xh(11) = 0.620,',
  remark = '                    yl(11) = -0.020, yh(11) = 0.260,',
  remark = '                    zl(11) =  0.300, zh(11) = 0.320,',
                  remark = 'kobs(11) = 0.08',


$END

$FL

  nfls = 1,

  fioh(1) = 1, freg(1) = 1.0, fxl(1) = 0.0, fxh(1) = 0.60,
                    fyl(1) = 0.0, fyh(1) = 0.24,
                    fzl(1) = 0.0, fzh(1) = 0.30,

$END

$BF
$END

$TEMP

  remark = 'setting initial temps to 25C to get things started',
  tempi = 300,

  remark = 'recreate the hot plate as a temperature region',
  ntmp = 1,
```

```
   txl(1) =  0.400, txh(1) = 0.510,
   tyl(1) = -0.020, tyh(1) = 0.260,
   tzl(1) =  0.300, tzh(1) = 0.320,

   twreg(1) = 373,

$END

$GRAFIC

   icolor = 2,

   jobsbk = 29,  jobsf = 27,

   remark = 'dump out T',
   ncplts = 2,
   contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3, jc1(1) = 27, jc2(1) = 29,
   contyp(2) = 'tn', ictyp(2) = 1, iperc(2) = 3, jc1(2) = 27, jc2(2) = 29,
   contyp(3) = 'vel',ictyp(3) = 1, iperc(3) = 3, jc1(3) = 27, jc2(3) = 29,


   remark = 'lay in history points at all thermocouple locations',
   wintl(1) = 'entry way',
   xloc(1) = 0.025, yloc(1) = 0.120, zloc(1) = 0.2625,

   remark = 'thermocouple number per page 3157, using array notation for local ref',
   wintl(2) = 'top left, (row,col) = (1,1)',
   xloc(2) = 0.135, yloc(2) = 0.120, zloc(2) = 0.2625,

   wintl(3) = '(row,col) = (2,1)',
   xloc(3) = 0.135, yloc(3) = 0.120, zloc(3) = 0.1875,

   wintl(4) = '(row,col) = (3,1)',
   xloc(4) = 0.135, yloc(4) = 0.120, zloc(4) = 0.1125,

   wintl(5) = '(row,col) = (4,1)',
   xloc(5) = 0.135, yloc(5) = 0.120, zloc(5) = 0.0375,

   wintl(6) = '(row,col) = (1,2)',
   xloc(6) = 0.290, yloc(6) = 0.120, zloc(6) = 0.2625,

   wintl(7) = '(row,col) = (2,2)',
   xloc(7) = 0.290, yloc(7) = 0.120, zloc(7) = 0.1875,

   wintl(8) = '(row,col) = (3,2)',
```

```
  xloc(8) = 0.290, yloc(8) = 0.120, zloc(8) = 0.1125,

  wintl(9) = '(row,col) = (4,2)',
  xloc(9) = 0.290, yloc(9) = 0.120, zloc(9) = 0.0375,

  wintl(10) = '(row,col) = (1,3)',
  xloc(10) = 0.455, yloc(10) = 0.120, zloc(10) = 0.2625,

  wintl(11) = '(row,col) = (2,3)',
  xloc(11) = 0.455, yloc(11) = 0.120, zloc(11) = 0.1875,

  wintl(12) = '(row,col) = (3,3)',
  xloc(12) = 0.455, yloc(12) = 0.120, zloc(12) = 0.1125,

  wintl(13) = '(row,col) = (4,3)',
  xloc(13) = 0.455, yloc(13) = 0.120, zloc(13) = 0.0375,

  wintl(14) = '(row,col) = (1,4)',
  xloc(14) = 0.570, yloc(14) = 0.120, zloc(14) = 0.2625,

  wintl(15) = '(row,col) = (2,4)',
  xloc(15) = 0.570, yloc(15) = 0.120, zloc(15) = 0.1875,

  wintl(16) = '(row,col) = (3,4)',
  xloc(16) = 0.570, yloc(16) = 0.120, zloc(16) = 0.1125,

  wintl(17) = '(row,col) = (4,4)',
  xloc(17) = 0.570, yloc(17) = 0.120, zloc(17) = 0.0375,

$END

$PARTS
$END
```

Case 2: Closed form solution of a forced air flow in a confined structure.

Physical Model.

A room having dimension 4m x 2m x 3m (length x depth x height) with a single source of forced ventilation and a single exit for natural exhaust is simulated. Forced ventilation is through a rectangular vent of size 0.4m x 0.4m; exhaust is through a similarly sized vent in the ceiling. The model is maintained at constant temperature and pressure. Any variation in these parameters is an artifact of the compressibility of the gas employed, which in this case is air.

Physics demands that at steady state the mass of gas entering the room is equivalent to the mass of gas exiting the room.

Furthermore, regardless of the physical construct of a problem, a flow can be considered 'one-dimensional' under the following conditions: (1) the flow is normal to the boundary at locations where mass enters or exits the control volume, and (2) all intensive properties, such as velocity and density, are uniform with position over each inlet or exit area through which matter flows.*

In particular, when flow is considered one-dimensional, the mass flow rate ($\dot{m}$) at inlet and outlet is defined by $\dot{m} = \rho A V$, where ρ is density, A is cross sectional area, and V is velocity. Steady state, therefore, in these situations is often regarded as Mass (IN) = Mass (OUT).

Given the construct of this validation run and the definition of one-dimensional flow, we would therefore expect to see both constant velocity and density at the inlet and outlet of this example.

This validation run evaluates this physical phenomenon and ascertains whether or not Flow-3d 9.0 accurately predicts the outcome.

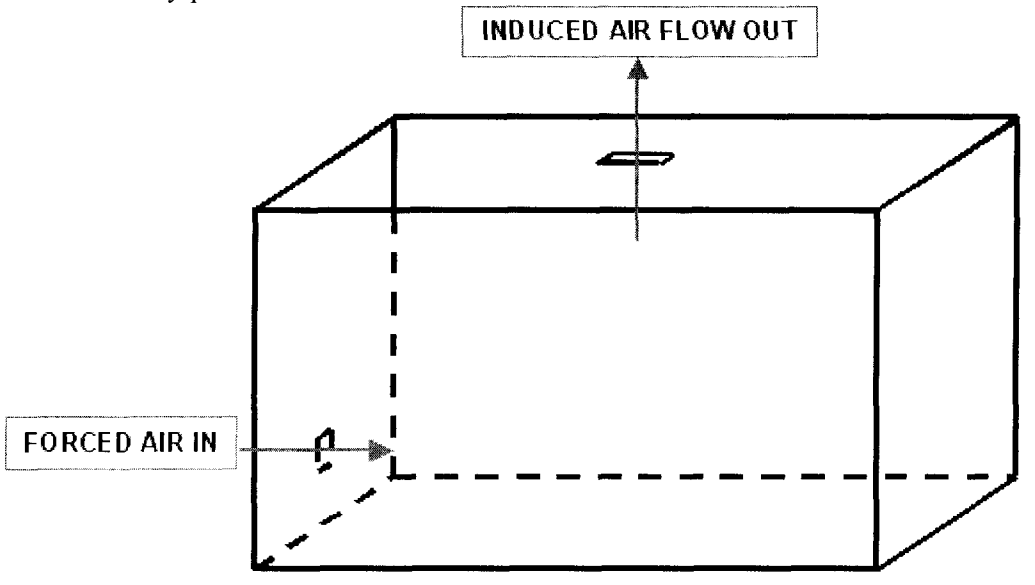
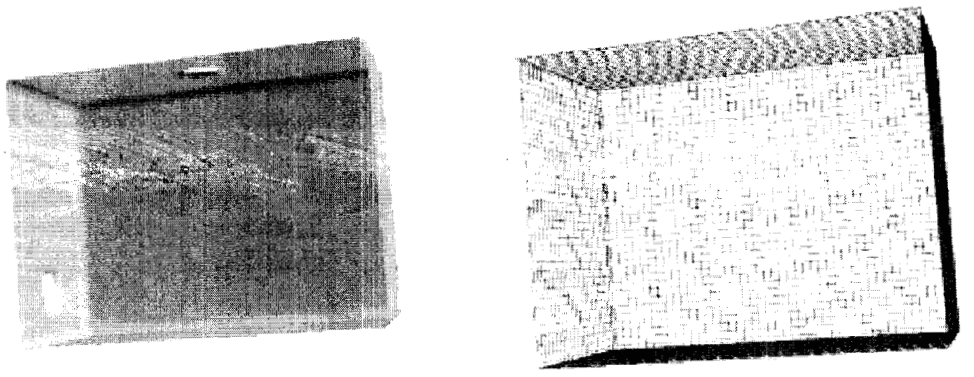


Figure 1: Experimental apparatus used in test case 2.

*Moran, M.J and Shapiro, H.N, "Fundamentals of Engineering Thermodynamics," 4th Edition, John Wiley & Sons, Inc., New York, 2000.

Computational Model.

The computational model is described exactly as the physical model above. Interior dimensions of the room are 4m x 2m x 3m. Computational walls of thickness 0.2m are applied in each direction to simplify visualizations and restrict inflow and outflow properly. Vents are created as 0.4m x 0.4m openings through their respective boundaries. Figure 2 shows a visualization of the computational model. The full model utilizes a mesh of 44 x 24 x 34 indicating a completely uniform grid of individual block size 0.1 x 0.1 x 0.1m. (An additional run at double the resolution was also completed to verify results. Only the coarse mesh solution is given here.)



(a) (b)

Figure 2: Visualization of the computational model, showing both (a) wall structure (front wall removed for clarity) and (b) grid resolution (red is open, blue is closed). For purposes of discussion, air comes in from the left and goes out through the top.

History points, which are numerical markers in the flow, were placed in the center of both inflow and outflow vents. These points were monitored to ascertain when the flow reached steady state.

A forced air in-flow condition equivalent to the application of a constant velocity of 0.25m/s was applied to the in-flow vent as visualized in Figure 1. On the outflow boundary, a continuative condition was applied which indicates that Flow-3D V9.0 will extrapolate local data upstream into appropriate conditions through the boundary.

The working gas used was air having the following properties at 293.15K:
Viscosity = 1.86e-5 kg/m/s
Specific heat = 1883.7 $m^2/s^2/K$
Thermal conductivity = 0.0264 kg-m/s^3/K,
Gas constant = 287.0
Density = 1.2 kg/m^3

The gas was assumed compressible so that the physical sensitivities of pressure and velocity were included in the calculations.

Computational Results.

To ascertain an average velocity across both the inflow and outflow boundary, the magnitude of total velocity was evaluated as an integral over the cross sectional area of each vent.

	Applied Condition	Measured Condition**
IN-FLOW	0.25 m/s	0.2541 m/s
OUT-FLOW	continuative	0.2590 m/s

** Measured data taken 1 grid plane from boundary; this gives a more accurate representation of velocity through the opening instead of at a discrete boundary

Mass flow can then be evaluated using the equation described above: $\dot{m} = \rho A V$.

	Average Mass In-Flow (kg/s)	Average Mass Out-Flow (kg/s)	Difference (%)
Calculated mass flow	0.048787	0.049728	1.89

This variation is within acceptable limits for a compressible flow at steady state.

This is a copy of the Flow-3D input deck used in Case 2:

24 February 2005 - forced ventilation through a 3D room

This is a test deck to evaluate forced ventilation through a closed room.
On one boundary, air is introduced into the room. On another boundary
an open airway of equal dimension is maintained. Using closed form solution
Qin = Qout.

The following assumptions are made. The room is maintained at constant
pressure and temperature. Any changes in the density of the gas should
be local and derived from acceleration.

```
$XPUT

  icmprs  = 1,   remark = 'compressible flow',
  ifrho   = 1,   remark = 'density as function of ff and local T',
  ifenrg  = 2,   remark = 'internal energy, 1st order advection',
  ifvis   = 2,   remark = 'turbulent energy model',
  iorder  = 3,   remark = 'setting iorder = 3 monotonically increasing',
  itb     = 0,   remark = 'no free surfaces',
  nmat    = 2,   remark = 'compressible option requires using 2 mat',
  iwsh    = 0,   remark = 'turn off wall shear',
  ipun    = 1,   remark = 'uniform pressure adjustment',
```

```
   imphtc = 1,     remark = 'fully implicit eval of temp terms',
   ihtc   = 1,     remark = 'turn on heat transfer',

   twfin   = 100.0, remark = 'simulation end, seconds',
   pltdt   = 10.0, remark = 'plotting interval, seconds',
   hpltdt  = 1.0, remark = 'history interval, seconds',
   delt    = 0.1, remark = 'time step, seconds',
   istdy   = 1,   remark = 'accelerate to steady state using non-phys transient',
   autot   = 2.0, remark = 'timestep by stability',
   omega   = 1.7, remark = 'default setting for over-relaxation factor',

   epsadj  = 1.0, remark = 'standard convergence criterion',

   iadix   = 1,   remark = 'pressure iteration options (x,y,z) ADI',
   iadiy   = 1,
   iadiz   = 1,

 $END

 $LIMITS

   itflmx  = 1000000, remark = 'maximum pressure iteration failures allowed',
   itmax   = 100000,    remark = 'allowable inner iteration count',

remark = 'adjust itmax early to quickly step through start-up',
   negtmx  = 100000,  remark = 'negative rhoe resets',

 $END

 $PROPS

   remark  = 'set up properties on fluid 2 to allow for compressibility option',

   mu2     = 1.86e-5, remark = 'viscosity air',
   cv2     = 1883.7,  remark = 'specific heat air',
   thc2    = 0.0264,  remark = 'thermal conductivity air',
   tstar   = 293.15,  remark = 'ref temp for air properties',
   rf2     = 287.0,   remark = 'gas constant air',

 $END

 $SCALAR
   remark = 'none needed for these simulations',
 $END

 $BCDATA
```

```
  remark = 'top wall is continuative (wt) or boundary 6',

  wl    = 6,   remark = 'low x, specified velocity',
  ubc(1) = 0.25,  remark = 'm/s',
  wr    = 2,   remark = 'high x',
  wf    = 2,   remark = 'low y',
  wbk   = 2,   remark = 'high y',
  wb    = 2,   remark = 'low z',
  wt    = 3,   remark = 'high z, continuative',


$END

$MESH

  remark = 'creating simple mesh for test',
  remark = 'simulations run in metric units MKS',

  remark = 'x direction is longest dimension of enclosure corresponding to width',
  nxcelt  = 44,
   px(1)  = -0.20,   nxcell(1)  = 2,   remark = 'inflow boundary',
   px(2)  =  0.00,   nxcell(2)  = 18,  remark = 'interior wall',
   px(3)  =  1.80,   nxcell(3)  = 4,   remark = 'begin outflow vent',
   px(4)  =  2.20,   nxcell(4)  = 18,  remark = 'end outflow vent',
   px(5)  =  4.00,   nxcell(5)  = 2,   remark = 'interior wall',
   px(6)  =  4.20,                     remark = 'wall boundary',

  remark = 'y direction is depth',
  nycelt  = 24,
   py(1)  = -0.20,   nycell(1)  = 2,   remark = 'wall boundary',
   py(2)  =  0.00,   nycell(2)  = 8,   remark = 'interior wall',
   py(3)  =  0.80,   nycell(3)  = 4,   remark = 'begin vent',
   py(4)  =  1.20,   nycell(4)  = 8,   remark = 'end vent',
   py(5)  =  2.00,   nycell(5)  = 2,   remark = 'interior wall',
   py(6)  =  2.20,                     remark = 'wall boundary',

  remark = 'z direction is height',
  nzcelt  = 34,
   pz(1)  = -0.20,   nzcell(1) = 2,    remark = 'wall boundary',
   pz(2)  =  0.00,   nzcell(2) = 4,    remark = 'interior wall',
   pz(3)  =  0.40,   nzcell(3) = 4,    remark = 'begin inflow vent',
   pz(4)  =  0.80,   nzcell(4) = 22,   remark = 'end inflow vent',
   pz(5)  =  3.00,   nzcell(5) = 2,    remark = 'interior wall',
   pz(6)  =  3.20,                     remark = 'continuative boundary',
```

```
$END

$OBS

  nobs = 1,

  remark = 'create the obstacle field',

  remark = 'put in the exterior walls, all 20cm thick insulated',
  remark = 'front and back of box',

  iob(1) = 1, ioh(1) = 1, xl(1) = -0.20, xh(1) = 4.20,
                  yl(1) = -0.20, yh(1) = 0.00,
                  zl(1) = -0.20, zh(1) = 3.20,

  iob(2) = 1, ioh(2) = 1, xl(2) = -0.20, xh(2) = 4.20,
                  yl(2) =  2.00, yh(2) = 2.20,
                  zl(2) = -0.20, zh(2) = 3.20,

  remark = 'left and right side of box',
  iob(3) = 1, ioh(3) = 1, xl(3) = -0.20, xh(3) = 0.00,
                  yl(3) = -0.20, yh(3) = 2.20,
                  zl(3) = -0.20, zh(3) = 3.20,

  iob(4) = 1, ioh(4) = 1, xl(4) =  4.00, xh(4) = 4.20,
                  yl(4) = -0.20, yh(4) = 2.20,
                  zl(4) = -0.20, zh(4) = 3.20,

  remark = 'bottom of box',
  iob(5) = 1, ioh(5) = 1, xl(5) = -0.20, xh(5) = 4.20,
                  yl(5) = -0.20, yh(5) = 2.20,
                  zl(5) = -0.20, zh(5) = 0.00,

  remark = 'top of box',
  iob(6) = 1, ioh(6) = 1, xl(6) = -0.20, xh(6) = 4.20,
                  yl(6) = -0.20, yh(6) = 2.20,
                  zl(6) =  3.00, zh(6) = 3.20,

  remark = 'cut out left vent',
  iob(7) = 1, ioh(7) = 0, xl(7) = -0.20, xh(7) = 0.00,
                  yl(7) =  0.80, yh(7) = 1.20,
                  zl(7) =  0.40, zh(7) = 0.80,

  remark = 'cut out top vent',
  iob(8) = 1, ioh(8) = 0, xl(8) =  1.80, xh(8) = 2.20,
                  yl(8) =  0.80, yh(8) = 1.20,
```

```
                zl(8) =  3.00, zh(8) = 3.20,

$END

$FL
$END

$BF
$END

$TEMP

  remark = 'setting initial temps to 25C to get things started',
  tempi = 300,

$END

$GRAFIC

  icolor = 2,

  remark = 'jobsbk = 10,  jobsf = 14,',

  ncplts = 2,
  contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
  contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,


  remark = 'lay in history points at all thermocouple locations',
  wintl(1) = 'entry way left',
  xloc(1) = 0.0, yloc(1) = 1.0, zloc(1) = 0.60,

  wintl(2) = 'exit way top',
  xloc(2) = 2.0, yloc(2) = 1.0, zloc(2) = 3.00,

  wintl(3) = 'room center',
  xloc(3) = 2.0, yloc(3) = 1.0, zloc(3) = 1.50,

$END

$PARTS
$END
```

Date of Entry: 09 June 2005 Entry By: Mary Ann Clarke
Particle distribution information from Chris Ryder (NRC)

Oxidation of High Burnup Fuels - Inputs to Thermal Calculation

(1) Cladding Size: 9 - 25 mm (BWR, OD); 8 - 15 mm (PWR, OD); 2070 - 4520 mm (length, BWR); 2840 - 5110 mm (length, PWR)

(2) 1 Assembly: 208 rods (PWR); rods (BWR)

(3) Size of Spent Fuel Particle: [0.7 to 3.0] mm, normal distribution

(4) Volume Ratios of Rims to Total Mass including Matrices: 5, 10, 15, 20, 25, 30, 35 (%)

(5) Grain Size - the particulate size after oxidation

Distribution - normal:

Mean - 0.25 micro-m [lower limit 0.05 micro-m] (diameter, rim), 2.5 micro-m [lower limit 0.5 micro -m](diameter, matrix, OCRWM, Codell)

(6) Density - 8.05 g/cm^3 [Belle, U_3O_8]

Received from tma@nrc.gov through Chris Ryder

Notes by MAClarke:
I spoke with Tea (pronounced Tay, spelling? tma@nrc.gov) on 08 June 2005 and he is active in the particle modeling field. He is particularly interested in whether or not commercial CFD packages can discern between a single order of magnitude in terms of particle diameter in distribution. For example, in this data, particle size is bi-modal: at 0.25 micrometers and 2.5 micrometers. To my knowledge, Flow-3d would treat these particles as the same in terms of motion, and only a single particle distribution would be defined, not something bi-modal in nature. I believe the smaller particles are more of a threat to the HVAC system, so it would behoove us to evaluate the particles on this order.

Initial Entry: Pavan Shukla and Sidney Chocron,
Date: 24 June 2005

Title: Technical Development and Evaluation of computational fluid dynamics (CFD) models related to Hi-Star 100 transportation cask thermal calculations as processed through a dry transfer facility (DTF)

Personnel: Pavan Shukla, CNWRA, Division 20, and Sidney Chocron, Southwest Research Institute, Division 18,

Project: This notebook is the continuation of Mary Ann Clarke's work for NRC. Mary Ann prepared a 3-D input deck that was inherited and used as the starting point by Pavan and Sidney. Due to the complexity of the geometry and the data in the input deck it was decided to divide the task in two parts. The first part, performed by Sidney, was to approach the problem from a 2-D perspective. Pavan would continue with the 3-D effort. A copy of all the input decks used during this effort is available in the appendix of this notebook. Geometrical and other details will only be included in this Notebook if they are considered of interest.

Objective to be accomplished
Evaluate the temperature of the assemblies when the lid of the transportation cask is open and left in the transfer facility with and without air conditioning system. The temperature history should range from a few seconds up to 30 days.

Summary of technical approach:
The input deck generated by Mary Ann will be used as the base for the geometry and the constant values. From that input deck two models will be developed: 1) a 2-D approach to the problem to be able to quickly evaluate the influence of some parameters in the model, 2) a 3-D model that would give a better estimate of the temperature in the assembly.

Code specifics:
The code to be used is Flow-3D written by Flow Science, version 9.0. See Flow-3D manual for specifics about this finite diffence code that solves Navier-Stokes equations. The code is being run in an AMD Opteron machine with Suse 9.3 operating system. The directory for the 2-D runs is /homes/schocron/cnwra in machine vader of Division 18. A copy of all the input decks used in this project can be found as an appendix to this document.

Aspects potentially affecting computation reliability:
The only aspect is the grid refinement since time step is automatically computed by the code to remain in the stability region. A run should not be considered final until grid refinement shows no difference in the answer.

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Entry: Sidney Chocron, 24 June 2005

Inherited code from Mary Ann **24 June 2005**

Title of input deck: Development of Hi-Star 100 cask with 24 Basket

In the appendix the reader can find the input deck inherited from Mary Ann before she left the institute to work in the university. The input deck will be used as the base for the development of the 2-D model and to follow on with the 3-D model.

Entry: Sidney Chocron, 1 July 2005

Inherited code from Pavan Shukla **1 July 2005**

Run id: pav02 (input deck can be found in the appendix)

Pavan Shukla was trained by Mary Ann. His first try was to reproduce Holtec study where all the assemblies are put together in the center of an axisymmetric geometry. The runs were being problematic and slow so I am having a look at them. I first try the steady state accelerator of Flow-3D to see if the run proceeds faster, without success.

Entry: Sidney Chocron, 5 July 2005

Mesh Coarsening **5 July 2005**

Run id: pav03

I coarsened the mesh to try to run it faster but with no success. Probably we will need to run it incompressible to accelerate calculations, but right now let's only change one thing at a time. Not much success

---

Entry: Sidney Chocron, 5 July 2005

Error found in gas constant **5 July 2005**

Run id: pav04

Pavan Shukla found an error in the value of the gas constant rf2 (corresponds to the gas constant), which I corrected to 287 J/kg/K. Still the run is too slow and unsatisfactory.

Entry: Sidney Chocron, 10 July 2005

Parallel flow over flat plate **10 July 2005**

Run id: flatplate01

Since the results were pretty unsatisfactory I completely overhauled the input deck by directly using Flow 3D reference manual. Tried in this run to qualitatively match data from the book by Burmeister: "Convective Heat Transfer", Natural Convection Chapter, page 382. This run is only a wall at high temperature that starts the natural convection process. The run was successful enough to begin to build from it, but not relevant enough to include here all the details other than the input deck.

Entry: Sidney Chocron, 10 July 2005

Parallel flow over a flat plate - incompressible **10 July 2005**

Run id: flatplate02

Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady state around 400 s. I added slow velocity (high vel. kills the time step) and I see the boundary layer.

Entry: Sidney Chocron, 10 July 2005

Parallel flow over a flat plate convection **10 July 2005**

Run id: flatplate03

Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge. It takes only around 1 s for steady.

Entry: Sidney Chocron, 12 July 2005

Parallel flow over a flat plate - convection **12 July 2005**

Run id: flatplate04

Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
According to Flow3D manual press iteration problems arise if reversing flows and are not important if the residue and the convergence criterion are close. The flow does reverse in this problem at the bottom. And residues are not far from the convergence criterion.

Entry: Sidney Chocron, 14 July 2005

Parallel flow ov. flat plate – implicit heat transfer **14 July 2005**

Run id: flatplate05

Let's see if with implicit heat transfer it goes faster. It does, from now on all the calculations will be with fully explicit temperature calculation

---

Entry: Sidney Chocron, 14 July 2005

Parallel flow ov. flat plate – pressure boundary **14 July 2005**

Run id: flatplate06

I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes. Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.

Entry: Sidney Chocron, 14 July 2005

Parallel flow over a flat plate – small size **14 July 2005**

Run id: flatplate07

Let's reduce the size of the problem so it runs faster. Then let's compare the following results: 1) discharge with different bndry conditions 2) discharge to open space

---

Entry: Sidney Chocron, 14 July 2005

Parallel flow ov. flat plate – continuative boundary **14 July 2005**

Run id: flatplate08

Continuative bndry at low x.

Entry: Sidney Chocron, 20 July 2005

Parallel flow over a flat plate - open space **20 July 2005**

Run id: flatplate09

Let's do the open space case. This guy runs very fast! And looks great... It seems to confirm that a pressure boundary is a best approach, but we need to run #08 up to completion.

Entry: Sidney Chocron

Natural convect., power source on wall **21 July 2005**

Run id: flatplate10

Some corrections in the mesh and change bndry condition to power. This looks it is working great! Still we are far from the objective which is an assembly with a gap but we are getting there.

Entry: Sidney Chocron

Nat. conv. power source on wall - real size gap **21 July 2005**

Run id: flatplate11

The max. temperature in the previous run was 335 K, which is really encouraging. Now let's go to the real size problem, as far as the air gap goes. Run longer. Now the max temp is 326 K. The run looks very nice although it has some instability which I do not know if it is real or due to the boundary condition. Let's check it in the next run.

Entry: Sidney Chocron

Nat. conv. - real size gap, room added **21 July 2005**

Run id: flatplate12

Let's add a room to check the boundary condition. The max. temp. here is around 350 K, I don't know if we can say this is equivalent to run11. My inclination is to say no... This run took 9 hours.

Entry: Sidney Chocron

Nat. conv. - fine mesh **22 July 2005**

Run id: flatplate13

Let's refine the mesh by a factor of two to see if it makes any difference. Also let's run it longer.

Entry: Sidney Chocron

Run id: flatplate14

Dismissed

Entry: Sidney Chocron

flatplate15: Small reactor, natural convection **26 July 2005**

Run id: flatplate15

Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add a small nuclear reactor (assembly) with it's power as an obstacle and see what happens. Temperature in this run rises up to 500K and does not reach a steady state! Is there something wrong?
I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided by two. Added air gap at extremes

---

Entry: Sidney Chocron

flatplate16: Small reactor, natural convection **01 Aug 2005**

Run id: flatplate16

Steady state happens at around 200 secs, with the max temperature being 415 K. Let's run a coarse mesh and see. The max temperature is now 404 K, so 11 K difference ...

Entry: Sidney Chocron

flatplate17: Small reactor, tobs 600K **02 Aug 2005**

Run id: flatplate17

Let's say that the initial obstacle temperature is 600K and see what happens ... It reaches steady state faster than the cold guy, but the final temperature is the same, as hoped ...

Entry: Sidney Chocron

flatplate18: 2-D assembly with Helium **03 Aug 2005**

Run id: flatplate18

Little excercise to see how long it takes to the helium to leave the gap and be replaced by air. Unfortunately I just realized that Mary Ann got the Cv wrong! I need to check further how that affects the problem.
Relevant result: Helium can be neglected because it goes away very fast.

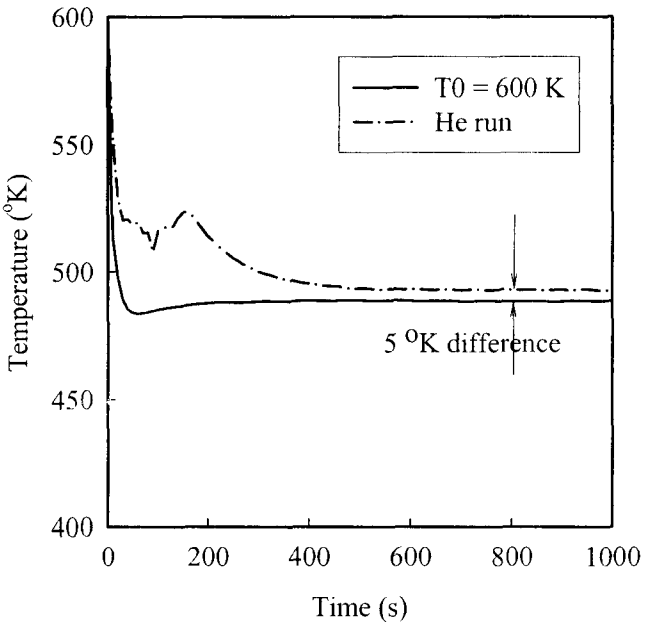

Figure 1: Comparing steady state temperature with and without Helium.

Entry: Sidney Chocron

flatplate19: Cv check, tobs 600K **03 Aug 2005**

Run id: flatplate19

Quick check changing Cv for air since Mary Ann's value seems to be wrong. Please, have a look at the input deck in the appendix.
Ok, this is the first run where it seems interesting to go into some more detail for a notebook.
Figure 2 shows the MPC-24 PWR from the top. This 2-D calculation tries to determine the temperature in the assembly placed in the center of the basket, or assembly 9, as shown in the Figure. Since this is a 2-D run we will only simulate the middle plane of assembly 9, where the temperature is expected to be the highest.

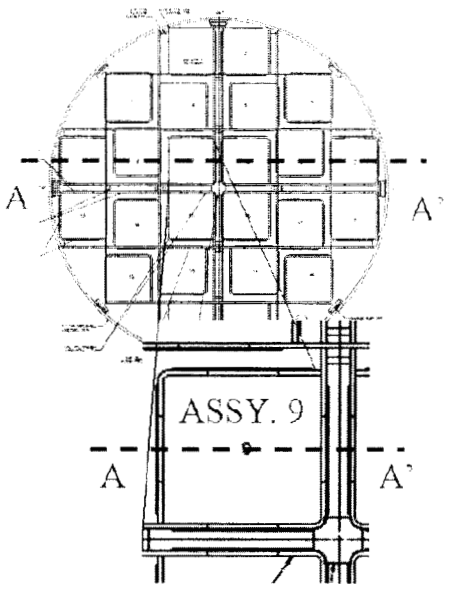

Figure 2: MPC 24 PWR view from above and detail of assembly 9

Figure 3 on the left shows the 'real' assembly, while on the right it shows the 2-D assembly used in the simulations. The symmetry is planar and the dimension of the assembly in the direction perpendicular to the paper is 1 meter with symmetry conditions.

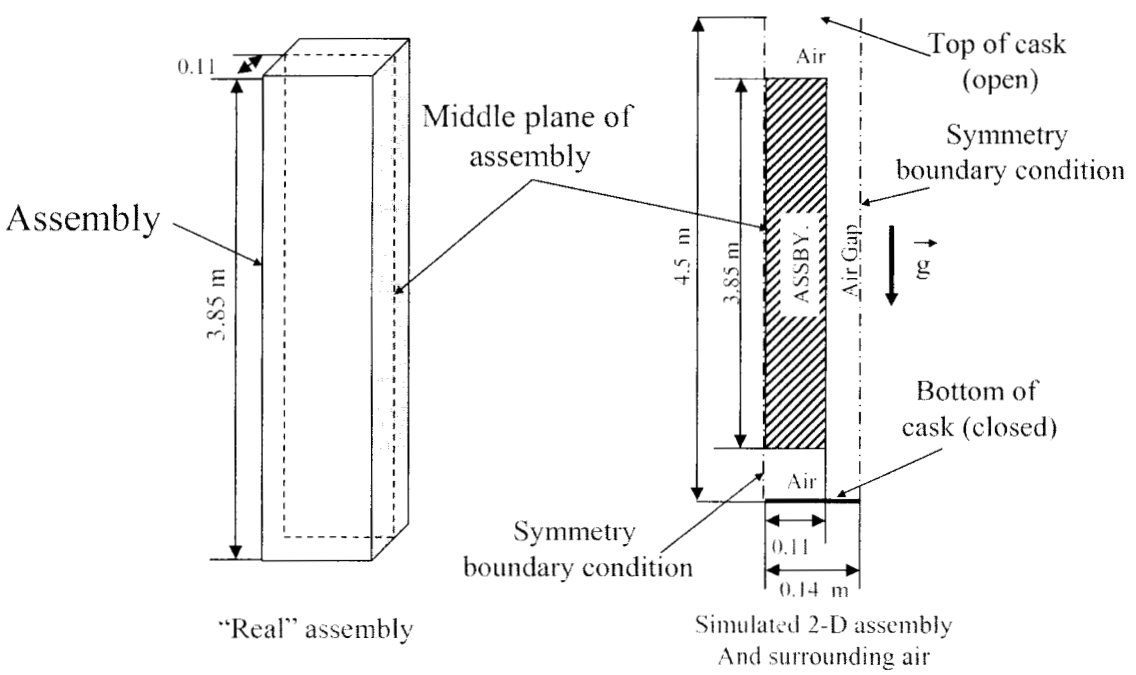

Figure 3: Middle plane approximation followed in the calculations

Because of the left and right symmetry boundary conditions the problem effectively solved with Flow3D will be equivalent to the one shown in Figure 4 where an infinite number of assemblies are placed side by side.

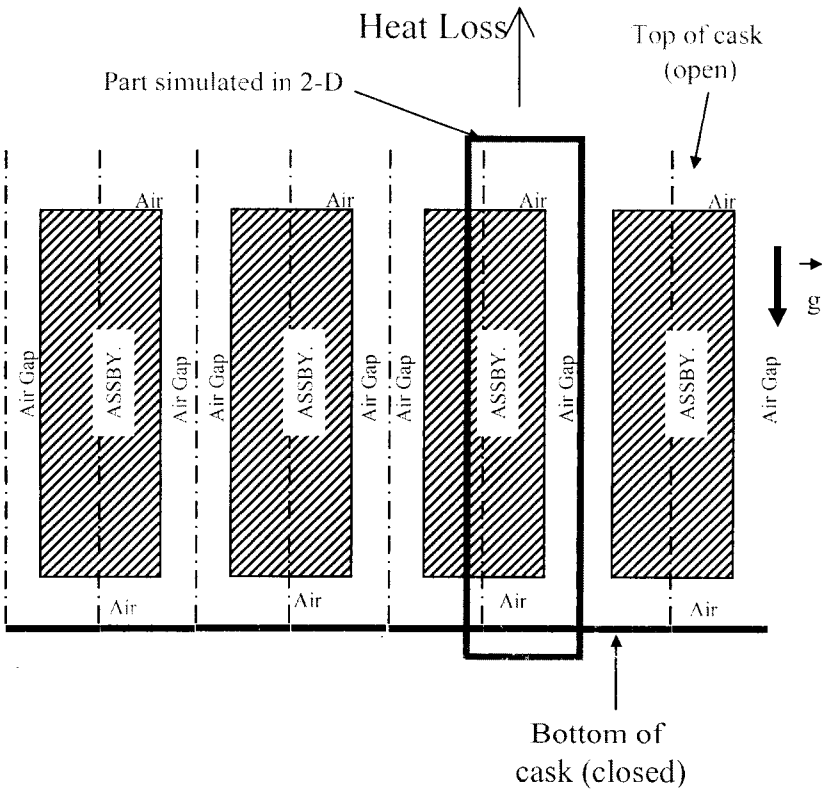

Figure 4: Problem equivalent to the problem solved with Flow-3D

The bottom boundary condition is a wall and the top boundary condition is on pressure. The pressure in the top boundary was set to be whatever the initial pressure value is with hydrostatic pressure distribution, given that the pressure at the bottom of the cask is the reference pressure 101325 Pa. See Figure 5. The initial temperature of the assembly is 600K in this run, the initial temperature of the air is 300K.

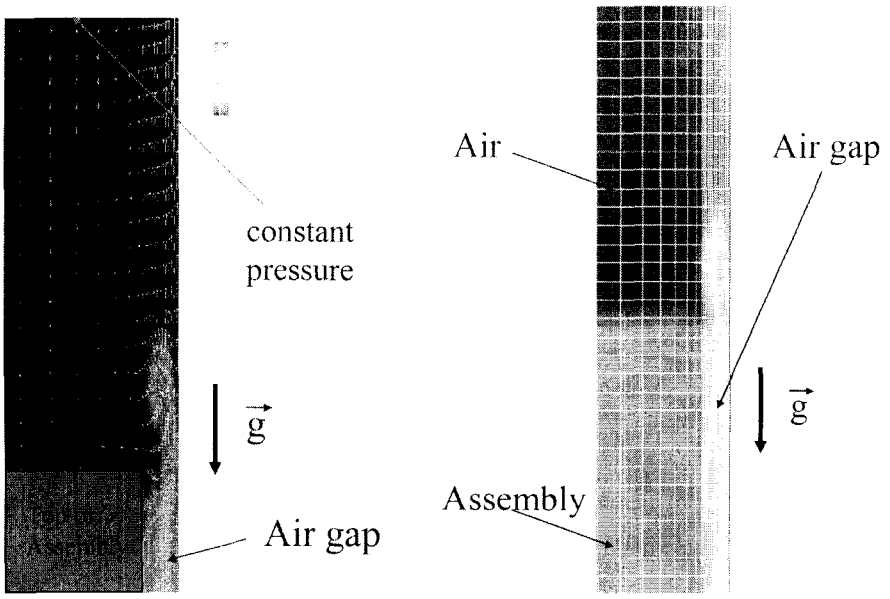

Figure 5: a) Detail of the top of the assembly in the 2-D simulation.. b) Detail of the mesh used

The mesh selected is coarse since these are still preliminary calculations. The mesh has 7 cells across the assembly and 13 cells across the air gap.
Properties for air can be found in, for example, Jacobson, Fundamentals of Atmospheric Modeling or in Wark, Advanced Thermodynamics for Engineers. The thermal expansion coefficient for an ideal gas is 1/T, and the T used was 293 K.
Conductivity of the assembly and rho.Cp for the assembly are taken from Mary Ann input deck right now as a first approach. We might need to change them in the future whenever we double check then. The power need for the 2-D obstacle was calculated to be 436.12 W based on the following logic:
I want the energy that crosses the surface of the real assembly to be the same than the energy that crosses the surface of 2-D assembly, on a per area basis.
Since the real assembly produces 792 W through an area of 3.85x0.2270x4=3.4958 m^3 (I assume top and bottom areas of the assemblies are negligible, 3.85 is the length of the assembly and 0.2270is the side, 4 is the number of faces). The heat per unit area for the real assembly is 792/3.4958= 226.56 W/m^2. For the 2-D simulation the area of the assembly is 3.85x1=3.85 m^2 . So the power of the assembly needs to be 226.56x3.85= 872.25 W to be equivalent. Because of the symmetry I need to divide that power by two: 872.25/2=436.12 W which is the number used (maybe in the future I need to rethink this, do I really need to divide by two?)
Turbulence was assumed to be negligible, I think the flow is going to be laminar, but maybe we should study this in detail later on.

Relevant results from the simulation:

1) Convection pattern around the middle of the assembly, as shown in Figure 6.
2) Final steady state temperature: 488K
3) Detail of convection and temperature at top of cask, see

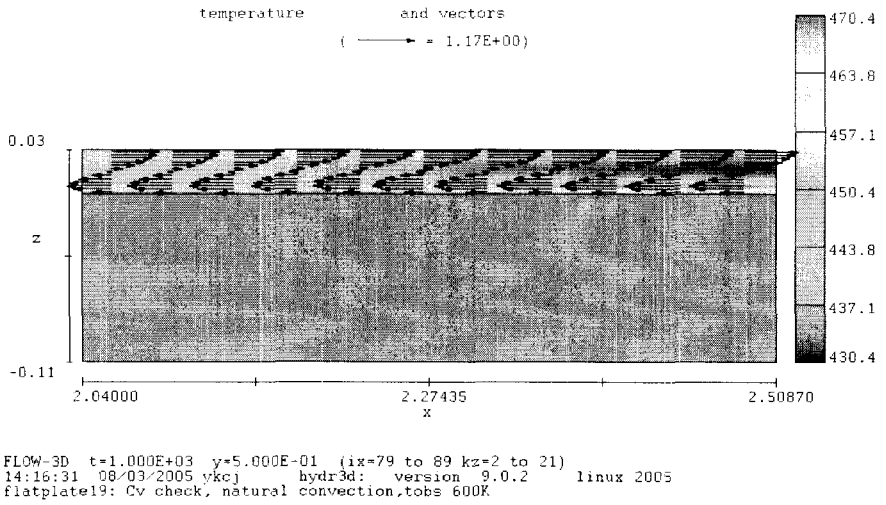

Figure 6: Convection pattern in the middle of the assembly for input deck flatplate19

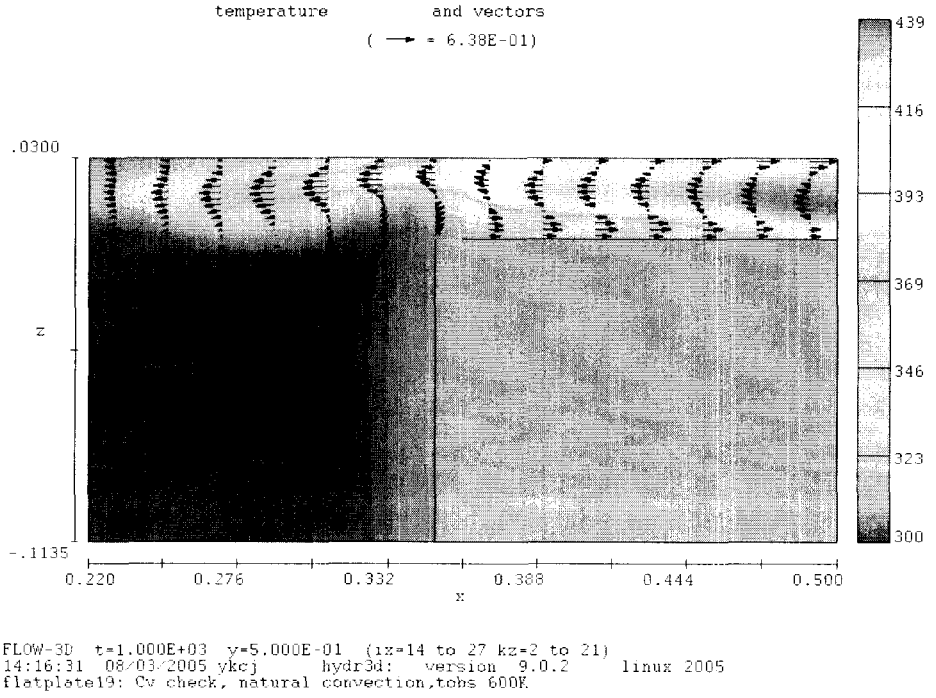

Figure 7: Detail of convection and temperature at top of cask, input deck flatplate19

Entry: Sidney Chocron

flatplate20: compressibility check, tobs 600K **04 Aug 2005**

Run id: flatplate20

I have a new concern today. Maybe the temperature is too high for the incompressible approx.

Entry: Sidney Chocron

flatplate21: 2-D run, T0=300 K **04 Aug 2005**

Run id: flatplate21

Assad wants a run with initial temperature at 300K but the right Cv for air which is 713 J/Kg/K. The comparison of 300 and 600K initial temperature follows:

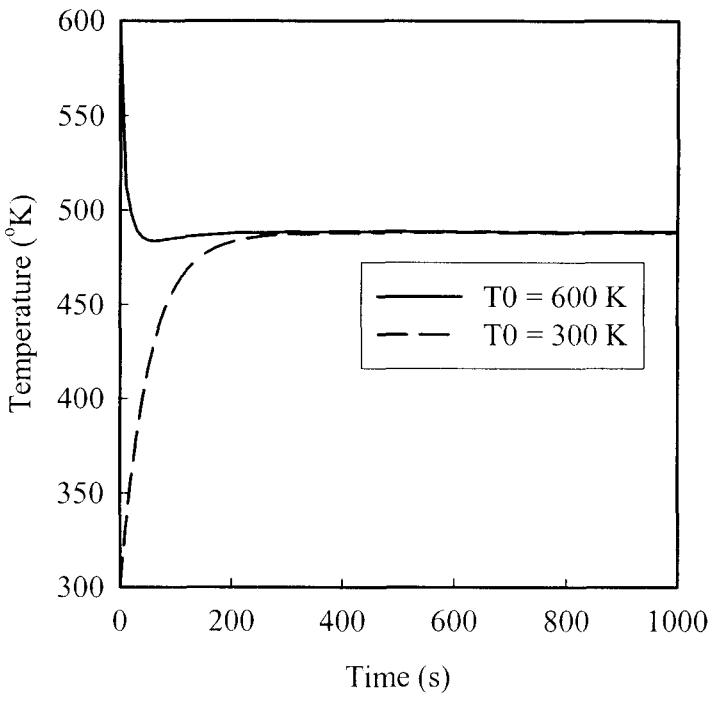

Figure 8: Final steady state temperature for two different initial temperatures of the assembly, input decks flatplate19 and flatplate15.

Entry: Sidney Chocron

flatplate22: Pavan axial symmetry, tobs 600K **09 Aug 2005**

Run id: flatplate22

Trying to reproduce Pavan's results. All the assemblies are lumped together in the center. This seems a very conservative approach that rises the temperature up to thousands of K even with an open lid and a temperature bndry condition. Really bad approach! Dismissed

---

Entry: Sidney Chocron

flatplate23: Room and natural conv., tobs 600K **09 Aug 2005**

Run id: flatplate23

How long does it take for a room to warm up under the heat of an assembly? That is a Bis question. I think the time scale will be impossible and another approx. will be needed, but let's try.

Entry: Sidney Chocron

flatplate24 playing with compressible **14 July 2005**

Run id: flatplate24

I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes. Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.

Entry: Sidney Chocron

flatplate25: Added room to 19, tobs 600K **15 Aug 2005**

Run id: flatplate25

Added the room to justify boundary condition in pressure
Figure 9 shows that the pressure boundary condition is very good.

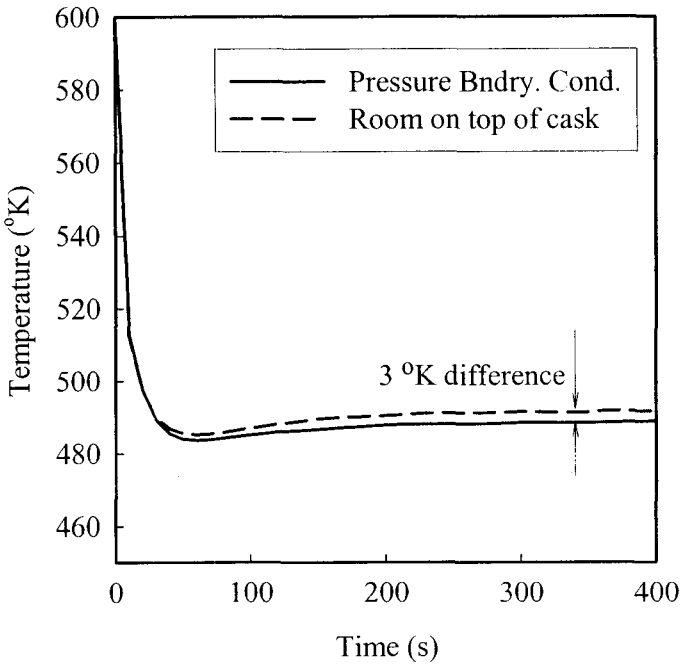

Figure 9: Comparing boundary condition in pressure and room at top of cask

---

Entry: P. Shukla

3DModelquart **17 Aug 2005**

Run id: 3DModelquart

A 3-D model of the transportation cask was simulated. The original code was programmed by MaryAnn Clarke. The input deck was modified to model only quarter of the storage cask and symmetry was imposed on the inner palnes. Some of the model parameters such as pressure at the top of the transportation cask, heat capacity of air and other CFD parameters were modified. The calculation time was exceedingly high and calculations could be run only for 9 seconds. The results are presented in two figures below.

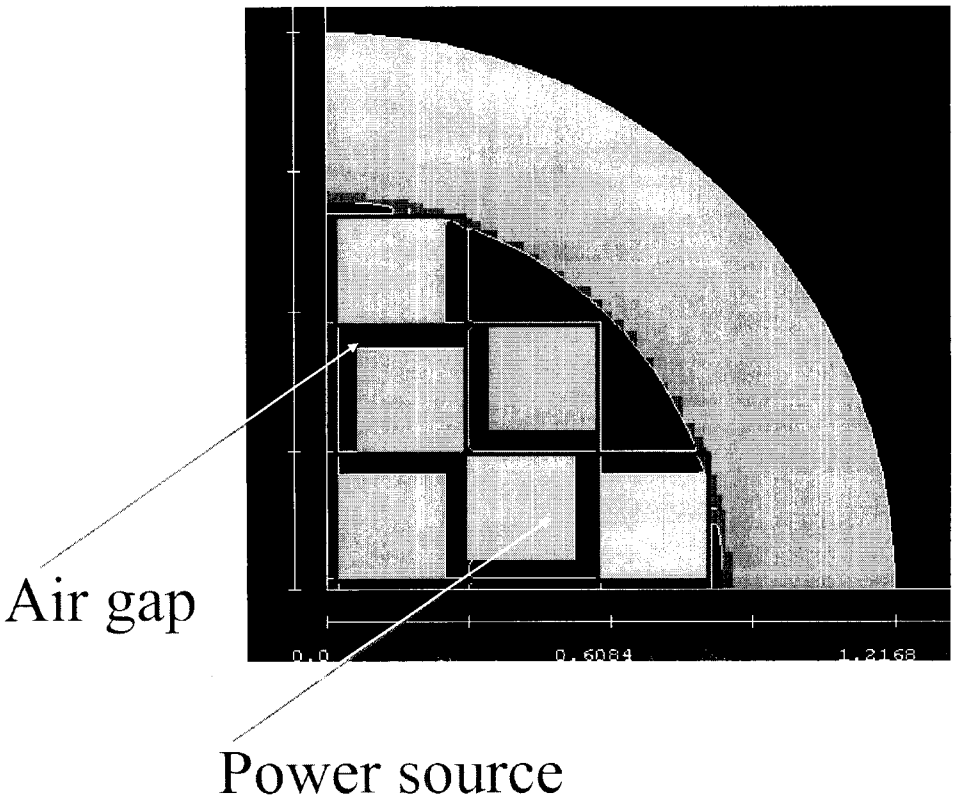

Figure 10: Ninty degree cross section of the transportation cask.

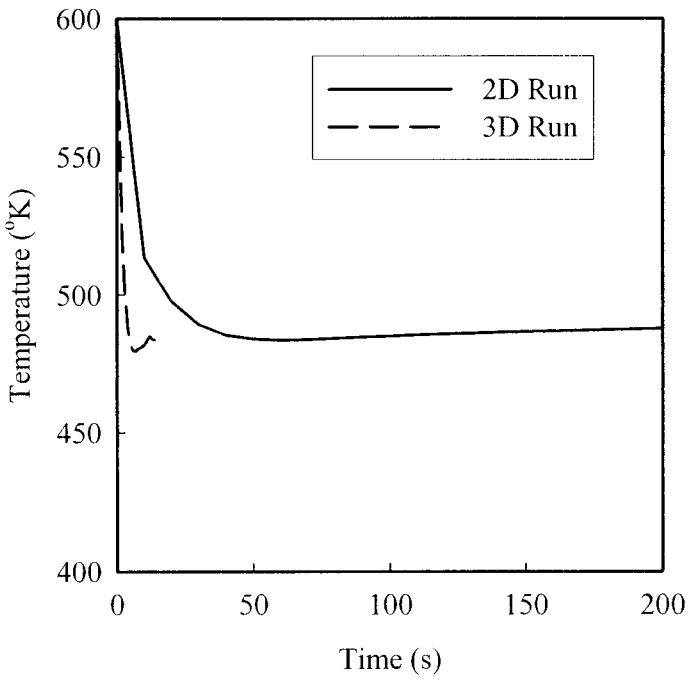

Figure 11: Maxiumu temperature obntained from 2-D and 3-D models.

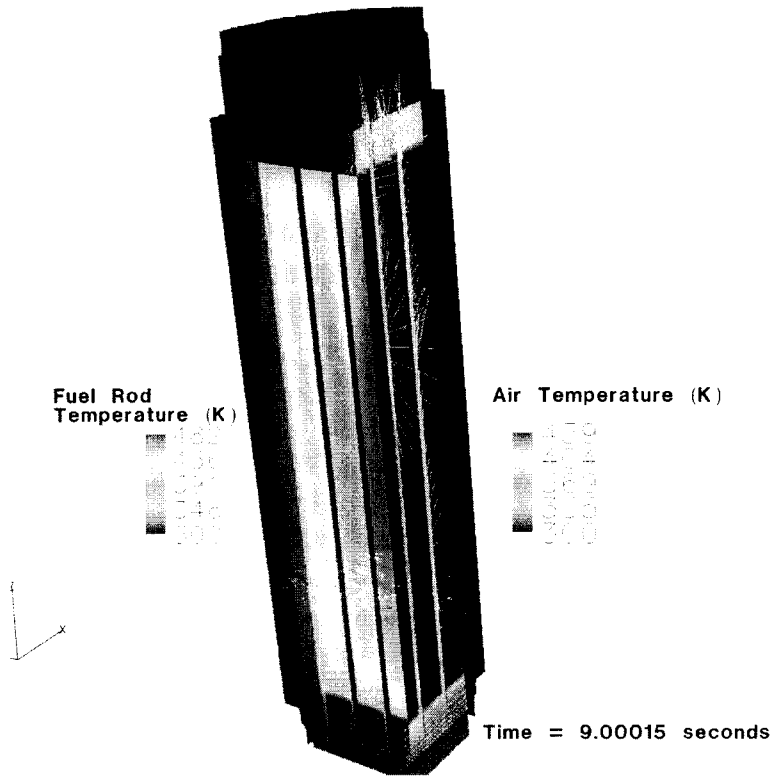

Figure 12: Temperature distribution in the fuel assemblies and in air .

Entry: Sidney Chocron

flatplate26: Room only, long timescale run **17 Aug 2005**

Run id: flatplate26

How fast does the temperature rise in the room for very long times? I changed the orientation to z being vertical! Not solving for obstacle conduction. The run dies after two days, I guess I need to treat the air as compressible ...

Entry: Sidney Chocron

flatplate27: Room only, long time, compressible **18 Aug 2005**

Run id: flatplate27

Compressible run. Explicit coupling (imp=0) kills the run. Changed iadiz to 0. Lots of pressure iteration failures, but stabilizes after 26000 secs. The temperature in the room stabilizes after one day or so. I guess I have leaks of heat through the boundaries, let's correct that.

Entry: Sidney Chocron

flatplate28: Room only, rwall **18 Aug 2005**

Run id: flatplate28

Added RWALL to boundary conditions to see if we stop leaking heat outside.This run stopped early, I do not remember why. RWALL did work to stop the heat leakage

---

Entry: Sidney Chocron

flatplate30: Cv check, tobs 600K, rhocp right **18 Aug 2005**

Run id: flatplate30

Pavan just realized that Rhocp for the assembly is wrong. It looks like Mary Ann only implemented the Cp and not the product. Changed to implicit viscous solution by code recommendation.

Entry: Sidney Chocron

flatplate31: Cv, tobs 600K, rhocp , coarse **18 Aug 2005**

Run id: flatplate31

Since there is not a lot of time let's divide the mesh by two. The final temperature is 600K, like the initial temperature, I am suspicious now ... Let's do a run with a different initial temp.

Entry: Sidney Chocron

flatplate32: Cv check, tobs 600K, RhoCp*10 **19 Aug 2005**

Run id: flatplate32

Study of the influence of RhoCP product here *10

Entry: Sidney Chocron

flatplate33: Cv, RhoCp*10, imp. viscosity **19 Aug 2005**

Run id: flatplate33

Using implicit viscosity to compare. No clear advantage, I stop it.

Entry: Sidney Chocron

flatplate34: Cv check, tobs 600K, RhoCp/10 **19 Aug 2005**

Run id: flatplate34

Now we divide RhoCp by 10 ...

Entry: Sidney Chocron

flatplate35: Cv check, tobs 600K, RhoCp*10 **22 Aug 2005**

Run id: flatplate35

For some unknown reason I stopped run 32. Let's restart here.

Entry: Sidney Chocron

flatplate36: k check, using Helium **22 Aug 2005**

Run id: flatplate36

Pavan wants to be on the safe side and run with k=.2223 W/m/K. The logic behind it is that k for He is 0.129 in English units which is the element with the lowest conductivity in the system. k can be found in Holtec FSAR 4.2.

Entry: P. Shukla

CloseLid2DModel **22 Aug 2005**

Run id: CloseLid2DModel

An axisymmetric 2-D model of the transportation cask with lid being closed was developed. The model is analogous to the one repoeted by HOLTEC Inc. All 24 fuel assemblies were homodenised and were assuemed to exist as a single heat source. The simulations were performed till a steady-state was reached. The maximum predicted temperature was found to be 780 ^{o}K. The program listing is appended at the end.

Entry: Sidney Chocron

flatplate37: k check, using Holtec table **22 Aug 2005**

Run id: flatplate37

We do not know why we are using k=0.696 W/m/s for the assembly. Let's try the number found in Holtec, table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in SI. Final max temp. 497 K.

Entry: Sidney Chocron

flatplate38: Added features to 2-D **29 Sep 2005**

Run id: flatplate38

Pavan thinks we should add the Alloy X and Boral sheets that sourround the assembly. Also we need to change the air gap to accomodate both materials. Changed to implicit viscous calculation. Temperature on the order of thousands ... I erase the results ...

Entry: Sidney Chocron

flatplate39: Turbulence check, Prandtl. **03 Oct 2005**

Run id: flatplate39

One of the concerns of the reviewers is the turbulence model. My thought is that turbulence is not going to make any difference, but let's prove it. Quasi-steady solution at 503 K. Only 6 K difference with the laminar guy, I do not think we should continue with turbulence ...

Entry: Sidney Chocron

flatplate40: Turbulence check, two eqs. k-e **03 Oct 2005**

Run id: flatplate40

Trying now the k-e model. Flow 3-D manual states that turbulence models assume high turbulence in the flow. Clearly this does not look the case in our problem, hopefully we do not see a big difference ... k-e is hundreds of times more slow, impossible to use if we want to apply it to 3-D

Entry: Sidney Chocron

flatplate41: Turbulence check, RNG **03 Oct 2005**

Run id: flatplate41

Now trying RNG. Died because of time step.Conclusion today: The only turbulence model that seems to work is the Prandtl mixing length. Why the others do not work? May be because of using incompressible?

Entry: Sidney Chocron

flatplate42: Room only, compressible, rwall **04 Oct 2005**

Run id: flatplate42

Let's redo this run trying to get to the end (30 days). Tried with 10 iterations in pressure but it does not stabilize. Rerun with 1000.-> Pressure iteration still failing but the residue is small. Temperature is increasing in the room at 150 C per day, a value expected in the analytical prediction. I stopped it after 3.5 days of run or 230000 (2.7 days) cpu time.

Entry: Sidney Chocron

flatplate43: Assembly and air gap, compressible **04 Oct 2005**

Run id: flatplate43

Now we want a run with assembly and air gap, but with compressible air. I noticed there is heat transfer at the bottom of the cask, I need to correct that! 5 seconds of run needed 30 minutes in compressible mode, while 10 seconds of run needed 2 minutes in incompressible mode. So compressible is 30 times slower than incompressible, clearly not affordable for the 3-D. Remember steady state accelerator is on. Final temperature in assembly: 550 K! 55 degrees more than incompressible!

Entry: Sidney Chocron

flatplate44: Porous 2-D assembly **06 Oct 2005**

Run id: flatplate44

Another concern by NRC reviewers was that the assembly should be simulated as a porous material because it is mostly filled with gas. I will assume it is air, although the real guy is He but I will assume He flies away pretty fast. Added OSPOR for heat transfer otherwise temperature goes the thousands. Basically I feel I could get any result I wanted with the three parameters I have at hand... 1.3e4 secs of CPU, same than without porous, something I did not expect!

Entry: Sidney Chocron, 07 Oct 2005

Summary of NRC concerns runs **07 Oct 2005**

Here is a summary I prepared about the last few runs

Runs to clarify NRC concerns

Assembly with compressible gas (run # 43)
One of the reviewers concern was the use of the Boussinesq approximation for air in the 2-D run with the assembly (that was one of our concerns too, we had plans to lift that assumption). Going to ideal gas multiplied by 30 the run time, but indeed changed the result significantly, increasing the maximum temperature in the assembly by 55 K up to 550 K (=530 F or 277 C), see Fig. 1. This run would be unaffordable in 3-D so we need to write some FORTRAN software to link to Flow-3D. The software should allow to still use the incompressible approximation while using an ideal gas equation of state for the air instead the Boussinesq approximation that was being used in the past. This approach would dramatically decrease the computation time.

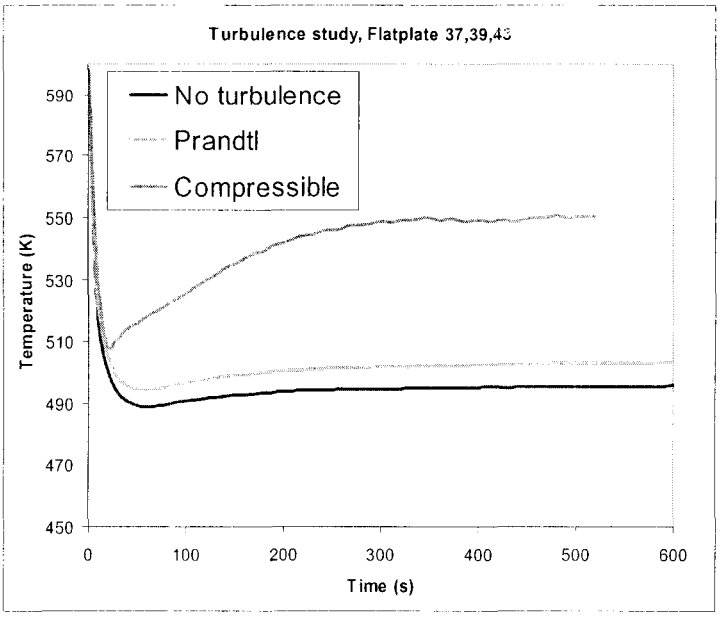

Figure 10: Comparison of the incompressible w/o turbulence run with other models

Turbulence study (incompressible air, 2D assembly, run # 39, 40 and 41)
To address reviewers concerns three different turbulence models (plus a run without turbulence model) were tried: Prandtl, k-ε and RNG. The two last models crashed the runs, the only one that worked was Prandtl Mixing Length model. The result was that the steady state temperature increased by 6 K, see Fig. 1, with respect to the model without turbulence. Although the other models crashed, it is thought that the results would not have been significantly different had they worked fine because the flow is mainly laminar as shown by the Prandtl model.

Porous assembly study (incompressible air, 2D assembly, run #44)
One of the reviewers suggestions was to simulate the assembly as a porous material instead of a solid material. The rationale behind it is that air (or Helium) can indeed flow in between the fuel rods and in fact most of the assembly is void (97% of the volume).
A run was performed with a made up porous material. "Made up" because a porous material has 4 parameters that characterizes it (porosity, two Darcy coefficients and surface per unit of volume). With the available data only one or two of the coefficients can be determined realistically, it would help to find out the diameter of the fuel rods. The results are encouraging in the sense that the temperature drops significantly, as expected, in the cask. This preliminary run gave a maximum temperature of 350 K in the assembly. The gas flowing in the assembly was assumed to be air. Boussinesq should be a good approximation here since the temperature variation is small. The feeling is that playing with the porous material characteristics any temperature could be obtained.

Transfer Room alone, compressible gas (run # 42)
A room with the size of the transfer room was simulated having inside a 19 kW heater. The room was adiabatic. As expected with the simple analytical model the room warmed up at a rate of 156 K/day (model predicted 140 /day). The calculation was a very simple, 2-D, and coarse (only 330 cells!) but still took 3 days of CPU to complete 3.5 days of run, still pretty far from the 30 days that is the objective. This is due to the compressibility of the gas. With these computation times it impossible to predict in a reasonable time what will happen after 30 days in a more complex geometry with walls, etc … As explained in the first paragraph we need to talk to Flow-3D (or Steve Green) to ask them how to implement ideal gas while still keeping the run incompressible. Steve Green suggested this idea which would imply to write some FORTRAN code and link it to Flow-3D.

Conclusions

1) Turbulence does not seem to be an issue, it is thought it can be ignored in future runs, although more work should be done to reinforce this point of view.
2) It is important to implement the ideal gas, incompressible approximation as an additional model for Flow-3D through writing a subroutine.
3) Porous media could be pursued, but it is unlikely meaningful parameters will be available for the porous material, since experiments would be needed to obtain them.

Entry by: P. Shukla 07 Oct. 2005

Effective thermal conductivity of MPC shell and air gap between overpack and MPC:
In the original design of transportation cask, there is a space between MPC wall and overpack. The gap is too narraow to be modeled in the CFD calculations, therefore, for computational convenience, the region of air gap plus MPC wall is replaced by a solid region with an effective thermal conductivity. The effective conductivity K_{eff} for two adjoining medium in the cylindrical geometry is given by

$$K_{eff} = \frac{\log\left(\frac{r_3}{r_1}\right)}{\left[\frac{\log\left(\frac{r_2}{r_1}\right)}{K_1} + \frac{\log\left(\frac{r_3}{r_2}\right)}{K_2}\right]}$$

where r_1 and r_2 are the inner and outer radius of the first medium (MPC shell)with thermal conductivity K_1, and r_2 and r_3 are the inner and outer radius of the second medium, i.e. air, with thermal conductivity K_2. The calculated values of K_{eff} using the above expression is given below in the Table.

Temperature	r_1 (inch)	r_2 (inch)	r_3 (inch)	K_1 (Btu/ft-hr-°F)	K_2 (Btu/ft-hr-°F)	Keff (W/s-°K)
200 °F	33.6875	34.1875	34.375	8.4	0.0173	0.1099
450 °F	33.6875	34.1875	34.375	9.8	0.0225	0.1429
700 °F	33.6875	34.1875	34.375	11	0.0272	0.1727

Values of K_1 and K_2 were obtained from Table 4.4.2 (HI START -100 FSAR)

Effective thermal conductivity of gamma shield and four outer shell layers of overpack:
Gamma shield shell layer and four outer shell layers of overpack were modeled as one medium. The effective thermal conductivity of this composite sheel layer can be detemoned by the following expression

$$K_{eff} = r_0 \log\left(\frac{r_5}{r_0}\right)\left[\sum_{i=1}^{5} \frac{\delta}{K_{air}} \frac{r_0}{r_i} + \frac{r_0 \log \frac{r_5}{r_0}}{K_{cst}}\right]$$

where

K_{eff} = Effective intermediate shell region thermal conductivity
r_0 = inside radius of the gamma shield
r_i = outer reaidus of ith intermediate shell
δ = interfacial air gap (2000 μ-inch)
K_{air} = air thermal conductivity
K_{cst} = carbon steel thermal conductivity

Values of r_0, r_1, r_2, r_3, r_4, r_5 are

r_0 (inch)	r_1 (inch)	r_2 (inch)	r_3 (inch)	r_4 (inch)	r_5 (inch)
36.875	38.375	39.375	40.375	41.375	42.375

and values of Keff, Kair, and Kcst as a function of temperature are given by below.

Temperature	K_2 (Btu/ft-hr-°F)	K_1 (Btu/ft-hr-°F)	Keff (W/s-°K)
200 °F	0.0173	24.4	12.0115
450 °F	0.0225	23.9	14.2896
700 °F	0.0272	22.4	15.7024

APPENDIX

Following the reader can find all the input decks used during this work. The input decks are separated by the symbols !*********, so a search by that symbol will take the reader from one input deck to the next. All of them are identified by a run number and title at the beginning.

```
!*****************************************************************************************
**********
Development of Hi-Star 100 cask with 24 Basket
**********************************************
20 June 2005
Updated informational fields

24 May 2005
Turning off air flow and allowing thermal progression only

11 May 2005  Chris Ryder asked that I look at the 24 Basket with different fuel.
Resetting obstacle field with this basket and fuel source.  Basic parameters will be
the same.  Grid will need to be slightly reworked to accomodate new fuel spacing.

  $XPUT

      icmprs  = 1,    remark = 'compressible flow',
      iorder  = 3,    remark = 'setting iorder = 3 monotonically increasing',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 2,    remark = '1 compressible mat',
      iwsh    = 0,    remark = 'turn off wall shear',

      remark = 'switch to remark out when flow on',
      remark = 'ihonly = 0',     remark = 'solve all conservation equations',
      ihonly = 2,     remark = 'turn off material flow, heat transfer only',
      imphtc = 0,     remark = 'fully explicit eval of temp terms',
      remark = 'ihtc   = 0',     remark = 'turn off heat transfer',
      ihtc   = 2,     remark = 'turn on heat conduction through obstacles',
      ifrho  = 1,     remark = 'allows local variation in density',
      ifenrg = 2,     remark = 'fluid energy transport on',
      gz = -9.81,     remark = 'gravity',


      twfin   =  100.0,  remark = 'simulation end, seconds',
      pltdt   =  1.0,   remark = 'plotting interval, seconds',
      hpltdt  =  1.0,    remark = 'history interval, seconds',
      delt    =  1.0e-5, remark = 'time step, seconds',
      remark = 'istdy   =  0',      remark = 'accelerate to steady state using non-phys
transient',
                         remark = 'minimum timestep',
      dtmax   =  100,    remark = 'maximum timestep',

      autot   =  2.0, remark = 'timestep by stability',
      omega   =  1.7, remark = 'default setting for over-relaxation factor',

      epsadj  =  1.0, remark = 'standard convergence criterion',

      igmres = 1,

      remark = 'iadix   =  1',   remark = 'pressure iteration options (x,y,z) ADI',
      remark = 'iadiy   =  1',
      remark = 'iadiz   =  1',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  10,    remark = 'allowable inner iteration count',
      itdtmx  =  100,
                        remark = 'adjust itmax early to quickly step through start-up',
      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
```

```
      rhof2     = 1.2,
      mu2      = 1.86e-5, remark = 'viscosity air',
      cv2      = 1883.7,  remark = 'specific heat air',
      thc2     = 0.0264,  remark = 'thermal conductivity air',
      thexf2   = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar    = 293.15,  remark = 'ref temp for air properties',

  $END

  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      remark = 'top wall is continuative (wt) or boundary 6',
      remark = 'set up as no ventilation',
      remark = 'made all bc continuative to start so cask is set in infinite air',

      wl      = 3,     remark = 'low x, continuative',
      wr      = 3,     remark = 'high x',
      wf      = 3,     remark = 'low y',
      wbk     = 3,     remark = 'high y',
      wb      = 3,     remark = 'low z',
      wt      = 3,     remark = 'high z, continuative',
      remark = 'eventually add cross-velocity at top of cask if necessary',

      tbcd = 300.0,

      remark = 'f boundaries are automatically 0 (mat 2)',

  $END

     nxcelt = 100,
       px(1) = -2.4336375,  nxcell(1) = 100,
       px(2) =  2.4336375,

     nycelt = 100,
       py(1) = -2.4336375,  nycell(1) = 100,
       py(2) =  2.4336375,

     nzcelt = 100,
       pz(1) = -0.2159000,  nzcell(1) = 100,
       pz(2) =  6.0,

  $MESH

      remark = 'full Cartesian mesh',
      nxcelt    = 180,
        px(1)   = -2.4336375,  nxcell(1)   = 10, remark = '4ft air gap beyond cask',
        px(2)   = -1.2144375,  nxcell(2)   = 10, remark = 'overpack neutron shielding outside
diameter',
        px(3)   = -1.0890250,  nxcell(3)   = 3, remark = 'overpack multilayer shell outside
diameter',
        px(4)   = -1.0572750,  nxcell(4)   = 10, remark = 'overpack baseplate diameter',
        px(5)   = -0.9366250,  nxcell(5)   = 6, remark = 'overpack inner shell outside diameter',
        px(6)   = -0.8731250,  nxcell(6)   = 1, remark = 'overpack inner shell inside diameter',
        px(7)   = -0.8683650,  nxcell(7)   = 1, remark = 'MPC base plate outside diameter',
        px(8)   = -0.8540750,  nxcell(8)   = 1, remark = 'outside MPC shell diameter',
        px(9)   = -0.8477250,  nxcell(9)   = 2, remark = 'inside MPC shell diameter',
        px(10)  = -0.8216900,  nxcell(10)  = 2, remark = 'being fuel basket',
        px(11)  = -0.8137525,  nxcell(11)  = 10, remark = 'end basket, left edge in assemblies
7,13',
        px(12)  = -0.5842000,  nxcell(12)  = 2, remark = 'begin basket, right edge in assemblies
7,13',
        px(13)  = -0.5762625,  nxcell(13)  = 3, remark = 'end basket, left edge in assemblies
3,19',
        px(14)  = -0.5288280,  nxcell(14)  = 7, remark = 'left edge in assemblies 8,14',
        px(15)  = -0.3496945,  nxcell(15)  = 3, remark = 'right edge in assemblies 3,19',
        px(16)  = -0.3022600,  nxcell(16)  = 2, remark = 'begin basket, right edge in assemblies
8,14',
```

```
        px(17) = -0.2943225,  nxcell(17) = 3, remark = 'end basket, left edge in assemblies
4,20',
        px(18) = -0.2517902,  nxcell(18) = 7, remark = 'left edge in assemblies 1,9,15,23',
        px(19) = -0.0677545,  nxcell(19) = 3, remark = 'right edge in assemblies 4,20',
        px(20) = -0.0252222,  nxcell(20) = 2, remark = 'right edge in assemblies 1,9,15,23 -
begin basket',
        px(21) = -0.0172847,  nxcell(21) = 2, remark = 'end basket,  start air',
        px(22) =  0.0000000,  nxcell(22) = 2, remark = 'air',
        px(23) =  0.0172847,  nxcell(23) = 2, remark = 'end air, begin basket',
        px(24) =  0.0252222,  nxcell(24) = 3, remark = 'end basket, left edge in assemblies
2,10,16,24',
        px(25) =  0.0677545,  nxcell(25) = 7, remark = 'left edge in assemblies 5,21',
        px(26) =  0.2517902,  nxcell(26) = 3, remark = 'right edge in assemblies 2,10,16,24',
        px(27) =  0.2943225,  nxcell(27) = 2, remark = 'right edge in assemblies 5,21, begin
basket',
        px(28) =  0.3022600,  nxcell(28) = 3, remark = 'end basket, left edge in assemblies
11,17',
        px(29) =  0.3496945,  nxcell(29) = 7, remark = 'left edge in assemblies 6,22',
        px(30) =  0.5288280,  nxcell(30) = 3, remark = 'right edge in assemblies 11,17',
        px(31) =  0.5762625,  nxcell(31) = 2, remark = 'right edge in assemblies 6,22, begin
basket',
        px(32) =  0.5842000,  nxcell(32) = 10, remark = 'end basket, left edge assemblies 12,18',
        px(33) =  0.8137525,  nxcell(33) = 2, remark = 'right edge assemblies 12,18, begin
basket',
        px(34) =  0.8216900,  nxcell(34) = 2, remark = 'end fuel basket',
        px(35) =  0.8477250,  nxcell(35) = 1, remark = 'inside MPC shell diameter',
        px(36) =  0.8540750,  nxcell(36) = 1, remark = 'outside MPC shell diameter',
        px(37) =  0.8683650,  nxcell(37) = 1, remark = 'MPC base plate outside diameter',
        px(38) =  0.8731250,  nxcell(38) = 6, remark = 'overpack inner shell inside diameter',
        px(39) =  0.9366250,  nxcell(39) = 10, remark = 'overpack inner shell outside diameter',
        px(40) =  1.0572750,  nxcell(40) = 3, remark = 'overpack baseplate diameter',
        px(41) =  1.0890250,  nxcell(41) = 10, remark = 'overpack multilayer shell outside
diameter',
        px(42) =  1.2144375,  nxcell(42) = 10, remark = 'overpack neutron shielding outside
diameter',
        px(43) =  2.4336375,                  remark = '4ft air gap beyond cask',

      nycelt   = 180,
        py(1)  = -2.4336375,  nycell(1)  = 10, remark = '4ft air gap beyond cask',
        py(2)  = -1.2144375,  nycell(2)  = 10, remark = 'overpack neutron shielding outside
diameter',
        py(3)  = -1.0890250,  nycell(3)  = 3, remark = 'overpack multilayer shell outside
diameter',
        py(4)  = -1.0572750,  nycell(4)  = 10, remark = 'overpack baseplate diameter',
        py(5)  = -0.9366250,  nycell(5)  = 6, remark = 'overpack inner shell outside diameter',
        py(6)  = -0.8731250,  nycell(6)  = 1, remark = 'overpack inner shell inside diameter',
        py(7)  = -0.8683650,  nycell(7)  = 1, remark = 'MPC base plate outside diameter',
        py(8)  = -0.8540750,  nycell(8)  = 1, remark = 'outside MPC shell diameter',
        py(9)  = -0.8477250,  nycell(9)  = 2, remark = 'inside MPC shell diameter',
        py(10) = -0.8216900,  nycell(10) = 2, remark = 'end fuel basket',
        py(11) = -0.8137525,  nycell(11) = 10, remark = 'bottom edge assemblies 23, 24, begin
basket',
        py(12) = -0.5842000,  nycell(12) = 2, remark = 'end basket, top edge assemblies 23,24',
        py(13) = -0.5762625,  nycell(13) = 3, remark = 'bottom edge assemblies 19,22, begin
basket',
        py(14) = -0.5288280,  nycell(14) = 7, remark = 'bottom edge assemblies 20,21',
        py(15) = -0.3496945,  nycell(15) = 3, remark = 'top edge assemblies 19,22',
        py(16) = -0.3022600,  nycell(16) = 2, remark = 'end basket, top edge assemblies 20,21',
        py(17) = -0.2943225,  nycell(17) = 3, remark = 'bottom edge assemblies 14,17, begin
basket',
        py(18) = -0.2517902,  nycell(18) = 7, remark = 'bottom edge assemblies 13,15,16,18',
        py(19) = -0.0677545,  nycell(19) = 3, remark = 'top edge assemblies 14,17',
        py(20) = -0.0252222,  nycell(20) = 2, remark = 'begin basket, top edge assemblies
13,15,16,18',
        py(21) = -0.0172847,  nycell(21) = 2, remark = 'begin air, end basket',
        py(22) =  0.0000000,  nycell(22) = 2, remark = 'air',
        py(23) =  0.0172847,  nycell(23) = 2, remark = 'end air, begin basket',
        py(24) =  0.0252222,  nycell(24) = 3, remark = 'end basket, bottom edge assemblies
7,9,10,12',
        py(25) =  0.0677545,  nycell(25) = 7, remark = 'bottom edge assemblies 8,11',
        py(26) =  0.2517902,  nycell(26) = 3, remark = 'top edge assemblies 7,9,10,12',
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        py(27) =  0.2943225,  nycell(27) = 2, remark = 'top edge assemblies 8, 11, begin basket',
        py(28) =  0.3022600,  nycell(28) = 3, remark = 'end basket, bottom edge assemblies 4,5',
        py(29) =  0.3496945,  nycell(29) = 7, remark = 'bottom edge assemblies 3,6',
        py(30) =  0.5288280,  nycell(30) = 3, remark = 'top edge assemblies 4,5',
        py(31) =  0.5762625,  nycell(31) = 2, remark = 'top edge assemblies 3,6, begin basket',
        py(32) =  0.5842000,  nycell(32) = 10, remark = 'end basket, bottom edge assemblies 1,2',
        py(33) =  0.8137525,  nycell(33) = 2, remark = 'top edge assemblies 1,2',
        py(34) =  0.8216900,  nycell(34) = 2, remark = 'end fuel basket',
        py(35) =  0.847725,   nycell(35) = 1, remark = 'inside MPC shell diameter',
        py(36) =  0.854075,   nycell(36) = 1, remark = 'outside MPC shell diameter',
        py(37) =  0.868365,   nycell(37) = 1, remark = 'MPC base plate outside diameter',
        py(38) =  0.873125,   nycell(38) = 6, remark = 'overpack inner shell inside diameter',
        py(39) =  0.936625,   nycell(39) = 10, remark = 'overpack inner shell outside diameter',
        py(40) =  1.057275,   nycell(40) = 3, remark = 'overpack base plate outside diameter',
        py(41) =  1.089025,   nycell(41) = 10, remark = 'overpack multilayer shell outside
diameter',
        py(42) =  1.2144375,  nycell(42) = 10, remark = 'overpack neutron shielding outside
diameter',
        py(43) =  2.4336375,                 remark = '4ft air gap beyond cask'


     nzcelt     = 99,
        pz(1)  = -0.2159000,  nzcell(1)  = 5, remark = 'bottom overpack base plate',
        pz(2)  = -0.0635000,  nzcell(2)  = 2, remark = 'top overpack base plate',
        pz(3)  =  0.0000000,  nzcell(3)  = 2, remark = 'bottom of fuel basket/bottom of MPC
shell',
        pz(4)  =  0.0635000,  nzcell(4)  = 5, remark = 'bottom overpack neutron shielding',
        pz(5)  =  0.3052800,  nzcell(5)  = 47, remark = 'begin fuel',
        pz(6)  =  4.1651200,  nzcell(6)  = 5, remark = 'top fuel',
        pz(7)  =  4.4037250,  nzcell(7)  = 2, remark = 'top overpack neutron shielding',
        pz(8)  =  4.4704000,  nzcell(8)  = 2, remark = 'top of fuel basket',
        pz(9)  =  4.5212000,  nzcell(9)  = 9, remark = 'top of MPC shell',
        pz(10) =  4.7910750,  nzcell(10) = 5, remark = 'top overpack layering system',
        pz(11) =  4.9434750,  nzcell(11) = 15, remark = 'top overpack idealized lid edge',
        pz(12) =  6.0,                       remark = '3+ feet higher than cask',

  $END

  $OBS

     nobs = 32,

     remark = 'create the obstacle field',
     remark = 'begin with fuel basket:  MPC-24, Holtec drawing 3926, sheet 2, rev 2',

     remark = 'thermal conductivity given in J/m-s-K at 400C',
     remark = 'data from Hi-Star FSAR Report HI-201260, chapter4',
     remark = 'see table 4.4.5 for PWR thermal conductivity',

     remark = 'general characteristics',
     remark = '24 locations for spent fuel of similar geometric config',

     remark = 'lay in x-cut plates first, left to right',

     remark = 'thermal conductivity = kobs unit:   Watt/m/K = kg-m/s3/K',
     remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
     remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',

     remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
     remark = 'Report HI-2012610',
     remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
     remark = 'thermal conductivity values from Table 4.4.7: generalized',
     remark = 'thermal conductivity vs. temperature',
     remark = 'choosing values at 400C',
     remark = 'rcobs = specific heat',

     remark = '24 Basket',
     remark = 'A',
     iob(1) = 1, ioh(1) = 1, xl(1) = -0.3022600, xh(1) =  0.3022600,
                             yl(1) =  0.8137525, yh(1) =  0.8216900,
                             zl(1) =  0.0000000, zh(1) =  4.4831000,
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                        kobs(1) = 2.286,
                        rcobs(1) = 544.28,

remark = 'B',
iob(2) = 1, ioh(2) = 1, xl(2) = -0.5842000, xh(2) =  0.5842000,
                        yl(2) =  0.5762625, yh(2) =  0.5842000,
                        zl(2) =  0.0000000, zh(2) =  4.4831000,

remark = 'C',
iob(3) = 1, ioh(3) = 1, xl(3) = -0.8216900, xh(3) =  0.8216900,
                        yl(3) =  0.2943225, yh(3) =  0.3022600,
                        zl(3) =  0.0000000, zh(3) =  4.4831000,

remark = 'D',
iob(4) = 1, ioh(4) = 1, xl(4) = -0.8216900, xh(4) =  0.8216900,
                        yl(4) =  0.0172847, yh(4) =  0.0252222,
                        zl(4) =  0.0000000, zh(4) =  4.4831000,

remark = 'A2',
iob(5) = 1, ioh(5) = 1, xl(5) = -0.3022600, xh(5) =  0.3022600,
                        yl(5) = -0.8216900, yh(5) = -0.8137525,
                        zl(5) =  0.0000000, zh(5) =  4.4831000,

remark = 'B2',
iob(6) = 1, ioh(6) = 1, xl(6) = -0.5842000, xh(6) =  0.5842000,
                        yl(6) = -0.5842000, yh(6) = -0.5762625,
                        zl(6) =  0.0000000, zh(6) =  4.4831000,

remark = 'C2',
iob(7) = 1, ioh(7) = 1, xl(7) = -0.8216900, xh(7) =  0.8216900,
                        yl(7) = -0.3022600, yh(7) = -0.2943225,
                        zl(7) =  0.0000000, zh(7) =  4.4831000,

remark = 'D2',
iob(8) = 1, ioh(8) = 1, xl(8) = -0.8216900, xh(8) =  0.8216900,
                        yl(8) = -0.0252222, yh(8) = -0.0172847,
                        zl(8) =  0.0000000, zh(8) =  4.4831000,

remark = 'A3',
iob(9) = 1, ioh(9) = 1, xl(9) =  0.8137525, xh(9) =  0.8216900,
                        yl(9) = -0.3022600, yh(9) =  0.3022600,
                        zl(9) =  0.0000000, zh(9) =  4.4831000,

remark = 'B3',
iob(10) = 1, ioh(10) = 1, xl(10) =  0.5762625, xh(10) = 0.5842000,
                          yl(10) = -0.5842000, yh(10) = 0.5842000,
                          zl(10) =  0.0000000, zh(10) = 4.4831000,

remark = 'C3',
iob(11) = 1, ioh(11) = 1, xl(11) =  0.2943225, xh(11) = 0.3026600,
                          yl(11) = -0.8216900, yh(11) = 0.8216900,
                          zl(11) =  0.0000000, zh(11) = 4.4831000,

remark = 'D3',
iob(12) = 1, ioh(12) = 1, xl(12) =  0.0172847, xh(12) = 0.0252222,
                          yl(12) = -0.8216900, yh(12) = 0.8216900,
                          zl(12) =  0.0000000, zh(12) = 4.4831000,

remark = 'A4',
iob(13) = 1, ioh(13) = 1, xl(13) = -0.8216900, xh(13) = -0.8137525,
                          yl(13) = -0.3022600, yh(13) =  0.3022600,
                          zl(13) =  0.0000000, zh(13) =  4.4831000,

remark = 'B4',
iob(14) = 1, ioh(14) = 1, xl(14) = -0.5842000, xh(14) = -0.5762625,
                          yl(14) = -0.5842000, yh(14) =  0.5842000,
                          zl(14) =  0.0000000, zh(14) =  4.4831000,

remark = 'C4',
iob(15) = 1, ioh(15) = 1, xl(15) = -0.3022600, xh(15) = -0.2943225,
                          yl(15) = -0.8216900, yh(15) =  0.8216900,
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                          zl(15) =  0.0000000, zh(15) =  4.4831000,

remark = 'D4',
iob(16) = 1, ioh(16) = 1, xl(16) = -0.0252222, xh(16) = -0.0172847,
                          yl(16) = -0.8216900, yh(16) =  0.8216900,
                          zl(16) =  0.0000000, zh(16) =  4.4831000,


remark = 'lay in 1/2in thick MPC shell at phi67.25in',
remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
remark = 'pages 3 and 4',
iob(23) = 2, ioh(23) = 1, ral(23) =  0.8477250, rah(23) = 0.8731250,
remark = 'actual spacing - eliminated b/c of grid resolution rah(23) =  0.854075,',
                          zl(23)  =  0.0000000, zh(23)  =  4.5212000,
                          kobs(2) = 0.0478,
                          rcobs(2) = 502.41,

remark = 'lay in MPC base plate 2.5in thick',
remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
remark = 'page 2(thickness), page 3(diameter)',
iob(24) = 3, ioh(24) = 1, ral(24) =  0.0000000, rah(24) = 0.8731250, remark = '0.8683625',
                          zl(24)  = -0.0635000, zh(24)  = 0.0000000,
                          kobs(3) = 0.0478,
                          rcobs(3) = 502.41,

remark = 'not including MPC lid - am assuming system is open',
remark = 'not including drain sump or fuel basket support rails',

remark = 'lay in overpack components',
remark = 'Holtec print 3913:  Hi-Star 100 Overpack Elevation View',
remark = 'base plate, page 2',
remark = '6in thick, 83.5in outside diameter',
iob(25) = 4, ioh(25) = 1, ral(25) =  0.0000000, rah(25) =  1.0572750,
                          zl(25)  = -0.21590000, zh(25) = -0.0635000,
                          kobs(4) = 30.3456,
                          rcobs(4) = 418.67,

remark = 'overpack inner shell, page 2',
remark = 'simplified to incorporate the full cask wall',
remark = '68.75in inside diameter, 73.75in outside diameter',
remark = '191.125in height from cask base plate',
iob(26) = 5, ioh(26) = 1, ral(26) =  0.8731250, rah(26) =  0.9366250,
                          zl(26)  = -0.0635000, zh(26)  =  4.7910750,
                          kobs(5) = 2.8117,
                          rcobs(5) = 502.41,

remark = 'overpack multilayered shells',
remark = 'simplified to incorporate the full cask wall',
remark = '73.75in inside diameter, 6 in thick 4x1.25 gamma layers + 1in shell',
iob(27) = 6, ioh(27) = 1, ral(27) =  0.9366250, rah(27) =  1.0890250,
                          zl(27)  = -0.0635000, zh(27)  =  4.7910750,
                          kobs(6) = 2.8117,
                          rcobs(6) = 502.41,

remark = 'overpack neutron shielding',
remark = 'simplified to incorporate neutron shield and radial channels that form the shell',
remark = 'details from page 6',
remark = 'thickness of neutron shield = 4-7/16in + thickness of channel 1/2in = 4-15/16in',
remark = 'idealized inside diameter = 85.75in, outside diameter = 95.625in',
remark = 'height runs from 8-3/4in off cask base to 173-1/8in',
iob(28) = 7, ioh(28) = 1, ral(28) =  1.0890250, rah(28) =  1.2144375,
                          zl(28)  =  0.0635000, zh(28)  =  4.4037250,
                          kobs(7) = 2.8117,
                          rcobs(7) = 1632.85,

remark = 'overpack - approximation of outside rim around lid',
remark = 'idealized inside diameter = 68.75in, outside diameter = 83.25in',
remark = '6in thick',
remark = 'approximating from page 2, print 3913',
iob(29) = 8, ioh(29) = 1, ral(29) =  0.8731250, rah(29) =  1.0572750,
                          zl(29)  =  4.7910750, zh(29)  =  4.9434750,
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                          kobs(8) = 2.8117,
                          rcobs(8) = 1632.85,

remark = 'ready to lay in the PWRs and heat source information',
remark = 'supposition:  PWR completely fill open area in MPC basket formation',
remark = 'doing this until better geometry provided',
remark = 'shortening PWR units by 12in on each end (centered)'
remark = 'based on info from PA Cox - check with Amit/Bis - ok',

remark = 'thermal conductivity is based on design specifications of Table 4.4.5',
remark = 'trend line created from data shown then conservatively extrapolated',
remark = 'to 400C;  values implemented at 232.22C from table',

remark = 'power values based on worst case scenario; 19008 total Watts, from',
remark = 'Table 4.4.18:  MPC-24 Basket Peak Fuel Claddings Temp as Function...',
tobs(1) = 0.0,


remark = 'lay in new 24 assembly',
remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',
iob(30) = 9, ioh(30) = 1, xl(30) = -0.2517902, xh(30) = -0.0252222,
                          yl(30) =  0.5842000, yh(30) =  0.8137525,
                          zl(30) =  0.3052800, zh(30) =  4.1651200,
                          kobs(9) = 0.696,
                          rcobs(9) = 234.46,
                          pobs(1,9) = 792,

remark = 'Slot 2',
iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                           yl(31) =  0.5842000, yh(31) =  0.8137525,
                           zl(31) =  0.3052800, zh(31) =  4.1651200,
                           kobs(10) = 0.696,
                           rcobs(10) = 234.46,
                           pobs(1,10) = 792,

remark = 'Slot 3',
iob(32) = 11, ioh(32) = 1, xl(32) = -0.5762625, xh(32) = -0.3496945,
                           yl(32) =  0.3496945, yh(32) =  0.5762625,
                           zl(32) =  0.3052800, zh(32) =  4.1651200,
                           kobs(11) = 0.696,
                           rcobs(11) = 234.46,
                           pobs(1,11) = 792,

remark = 'Slot 4',
iob(33) = 12, ioh(33) = 1, xl(33) = -0.2943225, xh(33) = -0.0677545,
                           yl(33) =  0.3022600, yh(33) =  0.5288280,
                           zl(33) =  0.3052800, zh(33) =  4.1651200,
                           kobs(12) = 0.696,
                           rcobs(12) = 234.46,
                           pobs(1,12) = 792,

remark = 'Slot 5',
iob(34) = 13, ioh(34) = 1, xl(34) =  0.0677545, xh(34) = 0.2943225,
                           yl(34) =  0.3022600, yh(34) = 0.5288280,
                           zl(34) =  0.3052800, zh(34) = 4.1651200,
                           kobs(13) = 0.696,
                           rcobs(13) = 234.46,
                           pobs(1,13) = 792,

remark = 'Slot 6',
iob(35) = 14, ioh(35) = 1, xl(35) =  0.3496945, xh(35) = 0.5762625,
                           yl(35) =  0.3496945, yh(35) = 0.5762625,
                           zl(35) =  0.3052800, zh(35) = 4.1651200,
                           kobs(14) = 0.696,
                           rcobs(14) = 234.46,
                           pobs(1,14) = 792,

remark = 'Slot 7',
iob(36) = 15, ioh(36) = 1, xl(36) = -0.8137525, xh(36) = -0.5842000,
                           yl(36) =  0.0252222, yh(36) =  0.2517902,
                           zl(36) =  0.3052800, zh(36) =  4.1651200,
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                              kobs(15) = 0.696,
                              rcobs(15) = 234.46,
                              pobs(1,15) = 792,

remark = 'Slot 8',
iob(37) = 16, ioh(37) = 1, xl(37) = -0.5288280,  xh(37) = -0.3022600,
                              yl(37) =  0.0677545,  yh(37) =  0.2942590,
                              zl(37) =  0.3052800,  zh(37) =  4.1651200,
                              kobs(16) = 0.696,
                              rcobs(16) = 234.46,
                              pobs(1,16) = 792,

remark = 'Slot 9',
iob(38) = 17, ioh(38) = 1, xl(38) = -0.2517902, xh(38) = -0.0252222,
                              yl(38) =  0.0252222, yh(38) =  0.2517902,
                              zl(38) =  0.3052800, zh(38) =  4.1651200,
                              kobs(17) = 0.696,
                              rcobs(17) = 234.46,
                              pobs(1,17) = 792,

remark = 'Slot 10',
iob(39) = 18, ioh(39) = 1, xl(39) =  0.0252222, xh(39) = 0.2517902,
                              yl(39) =  0.0252222, yh(39) = 0.2517902,
                              zl(39) =  0.3052800, zh(39) = 4.1651200,
                              kobs(18) = 0.696,
                              rcobs(18) = 234.46,
                              pobs(1,18) = 792,

remark = 'Slot 11',
iob(40) = 19, ioh(40) = 1, xl(40) =  0.3022600, xh(40) =  0.5288280,
                              yl(40) =  0.0677545, yh(40) =  0.2942590,
                              zl(40) =  0.3052800, zh(40) =  4.1651200,
                              kobs(19) = 0.696,
                              rcobs(19) = 234.46,
                              pobs(1,19) = 792,

remark = 'Slot 12',
iob(41) = 20, ioh(41) = 1, xl(41) =  0.5842000, xh(41) = 0.8137525,
                              yl(41) =  0.0252222, yh(41) = 0.2517902,
                              zl(41) =  0.3052800, zh(41) = 4.1651200,
                              kobs(20) = 0.696,
                              rcobs(20) = 234.46,
                              pobs(1,20) = 792,

remark = 'Slot 13',
iob(42) = 21, ioh(42) = 1, xl(42) = -0.8137525, xh(42) = -0.5842000,
                              yl(42) = -0.2517902, yh(42) = -0.0252222,
                              zl(42) =  0.3052800, zh(42) =  4.1651200,
                              kobs(21) = 0.696,
                              rcobs(21) = 234.46,
                              pobs(1,21) = 792,

remark = 'Slot 14',
iob(43) = 22, ioh(43) = 1, xl(43) = -0.5288280,  xh(43) = -0.3022600,
                              yl(43) = -0.2942590,  yh(43) = -0.0677545,
                              zl(43) =  0.3052800,  zh(43) =  4.1651200,
                              kobs(22) = 0.696,
                              rcobs(22) = 234.46,
                              pobs(1,22) = 792,

remark = 'Slot 15',
iob(44) = 23, ioh(44) = 1, xl(44) = -0.2517902, xh(44) = -0.0252222,
                              yl(44) = -0.2517902, yh(44) = -0.0252222,
                              zl(44) =  0.3052800, zh(44) =  4.1651200,
                              kobs(23) = 0.696,
                              rcobs(23) = 234.46,
                              pobs(1,23) = 792,

remark = 'Slot 16',
iob(45) = 24, ioh(45) = 1, xl(45) =  0.0252222,  xh(45) =  0.2517902,
                              yl(45) = -0.2517902,  yh(45) = -0.0252222,
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                                zl(45) =  0.3052800,  zh(45) =  4.1651200,
                                kobs(24)= 0.696,
                                rcobs(24) = 234.46,
                                pobs(1,24) = 792,

 remark = 'Slot 17',
 iob(46) = 25, ioh(46) = 1, xl(46) =  0.3022600,  xh(46) =  0.5288280,
                                yl(46) = -0.2942590,  yh(46) = -0.0677545,
                                zl(46) =  0.3052800,  zh(46) =  4.1651200,
                                kobs(25) = 0.696,
                                rcobs(25) = 234.46,
                                pobs(1,25) = 792,

 remark = 'Slot 18',
 iob(47) = 26, ioh(47) = 1, xl(47) =  0.5842000,  xh(47) =  0.8137525,
                                yl(47) = -0.2517902,  yh(47) = -0.0252222,
                                zl(47) =  0.3052800,  zh(47) =  4.1651200,
                                kobs(26) = 0.696,
                                rcobs(26) = 234.46,
                                pobs(1,26) = 792,

 remark = 'Slot 19',
 iob(48) = 27, ioh(48) = 1, xl(48) = -0.5762625, xh(48) = -0.3496945,
                                yl(48) = -0.5762625, yh(48) = -0.3496945,
                                zl(48) =  0.3052800, zh(48) =  4.1651200,
                                kobs(27) = 0.696,
                                rcobs(27) = 234.46,
                                pobs(1,27) = 792,

 remark = 'Slot 20',
 iob(49) = 28, ioh(49) = 1, xl(49) = -0.2943225, xh(49) = -0.0677545,
                                yl(49) = -0.5288280, yh(49) = -0.3022600
                                zl(49) =  0.3052800, zh(49) =  4.1651200,
                                kobs(28) = 0.696,
                                rcobs(28) = 234.46,
                                pobs(1,28) = 792,

 remark = 'Slot 21',
 iob(50) = 29, ioh(50) = 1, xl(50) =  0.0677545,  xh(50) =  0.2943225,
                                yl(50) = -0.5288280,  yh(50) = -0.3022600,
                                zl(50) =  0.3052800,  zh(50) =  4.1651200,
                                kobs(29) = 0.696,
                                rcobs(29) = 234.46,
                                pobs(1,29) = 792,

 remark = 'Slot 22',
 iob(51) = 30, ioh(51) = 1, xl(51) =  0.3496945,  xh(51) =  0.5762625,
                                yl(51) = -0.5762625,  yh(51) = -0.3496945,
                                zl(51) =  0.3052800,  zh(51) =  4.1651200,
                                kobs(30) = 0.696,
                                rcobs(30) = 234.46,
                                pobs(1,30) = 792,

 remark = 'Slot 23',
 iob(52) = 31, ioh(52) = 1, xl(52) = -0.2517902, xh(52) = -0.0252222,
                                yl(52) = -0.8137525, yh(52) = -0.5842000,
                                zl(52) =  0.3052800, zh(52) =  4.1651200,
                                kobs(31) = 0.696,
                                rcobs(31) = 234.46,
                                pobs(1,31) = 792,

 remark = 'Slot 24',
 iob(53) = 32, ioh(53) = 1, xl(53) =  0.0252222, xh(53) =  0.2517902,
                                yl(53) = -0.8137525, yh(53) = -0.5842000,
                                zl(53) =  0.3052800, zh(53) =  4.1651200,
                                kobs(32) = 0.696,
                                rcobs(32) = 234.46,
                                pobs(1,32) = 792,

$END
```

```
  $FL

      remark = 'setting 1atm in Pa',
      presi = 101325.0,

  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END

!*****************************************************************************************
**********
Development of 2D Model for CASK 24.
**********************************
01 July 2005  pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT

      icmprs  = 1,    remark = 'compressible flow',
      iorder  = 3,    remark = 'setting iorder = 3 monotonically increasing',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 2,    remark = '1 compressible mat',
      iwsh    = 0,    remark = 'turn off wall shear',

      remark = 'switch to remark out when flow on',
      ihonly = 2,     remark = 'turn off material flow, heat transfer only',
      imphtc = 0,     remark = 'fully explicit eval of temp terms',
      ihtc   = 2,     remark = 'turn on heat conduction through obstacles',
      ifrho  = 1,     remark = 'allows local variation in density',
      ifenrg = 2,     remark = 'fluid energy transport on',
      gz = -9.81,     remark = 'gravity',


      remark = 'trest    =  1.43e-4,',
      twfin   =  1000.0,  remark = 'simulation end, seconds',
      pltdt   =  10,      remark = 'plotting interval, seconds',
      hpltdt  =  100.0,    remark = 'history interval, seconds',
      delt    =  1.0e-5, remark = 'time step, seconds',
      istdy   =  1,      remark = 'accelerate to steady state using non-phys transient',
                         remark = 'minimum timestep',
      dtmax   =  100,    remark = 'maximum timestep',

      autot   =  2.0, remark = 'timestep by stability',
```

```
    omega   =  1.7, remark = 'default setting for over-relaxation factor',

    epsadj  =  1.0, remark = 'standard convergence criterion',

    igmres = 1,

    remark = 'iadix   =  1',   remark = 'pressure iteration options (x,y,z) ADI',
    remark = 'iadiy   =  1',
    remark = 'iadiz   =  1',

$END

$LIMITS

    itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
    itmax   =  10,    remark = 'allowable inner iteration count',
    itdtmx  =  100,
                      remark = 'adjust itmax early to quickly step through start-up',
    negtmx  =  100000,  remark = 'negative rhoe resets',
    ncflmx  =  1000,    remark = 'convection failures allowed',

$END

$PROPS

    remark  = 'set up properties on fluid 2 to allow for compressibility option',

    units   = 'si',
    rhof2    = 1.2,
    mu2     = 1.86e-5, remark = 'viscosity air',
    cv2     = 1883.7,  remark = 'specific heat air',
    thc2    = 0.0264,  remark = 'thermal conductivity air',
    thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
    tstar   = 293.15,  remark = 'ref temp for air properties',

$END

$SCALAR
    remark = 'none needed for these simulations',
$END

$BCDATA

    remark = 'top wall is continuative (wt) or boundary 6',
    remark = 'set up as no ventilation',
    remark = 'made all bc continuative to start so cask is set in infinite air',

    wl      = 1,  remark = 'low x, continuative',
    wr      = 2,  remark = 'high x',
    wf      = 1,   remark = 'low y',
    wbk     = 1,  remark = 'high y',
    wb      = 2,    remark = 'low z',
    wt      = 3,    remark = 'high z, continuative',
    tbc(2)  = 300.0,
    tbc(5)  = 300.0,
    remark = 'pobc(2)= 0',
    remark = 'pobc(5)= 0',
    tbc(6)  = 300,  remark = 'boundary condition at top of the cask'
    remark = 'eventually add cross-velocity at top of cask',

$END


$MESH

    remark = 'cylindrical mesh',
    icyl     = 1,
    nxcelt   = 20,
      px(1)  =  0.000000000,  nxcell(1)  = 10, remark = 'origin of the coordinate system',
       px(2)  =  0.127827306,  nxcell(2)  = 10,  remark = 'end point of the edge of the power
source',
```

```
      px(3)   =  0.162396706,

    nycelt    = 1,
      pya(1)=0.0,  nycell(1)=1, remark='cylindrical mesh...',
      pya(2)=10,   remark='azimuthal angle...',

   nzcelt     = 40,
      pz(1)   =  0.0000000,  nzcell(1)  = 10, remark = 'bottom overpack base plate',
      pz(2)   =  0.3052800,  nzcell(2)  = 20, remark = 'starting point of the fuel rod',
      pz(3)   =  4.1651200,  nzcell(3)  = 10, remark = 'top of the fuel rod',
      pz(4)   =  4.9434750,                   remark = 'head space',
$END

$OBS

   nobs = 1,
   remark = 'create the obstacle field',
   remark = 'general characteristics',
   remark = 'thermal conductivity = kobs unit:'
   remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
   remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',
   remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
   remark = 'Report HI-2012610',
   remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
   remark = 'thermal conductivity values from Table 4.4.7: generalized',
   remark = 'thermal conductivity vs. temperature',
   remark = 'choosing values at 400C based on instruction from C Ryder',
   remark = 'rcobs = specific heat',
   remark = '24 Basket',
   remark = 'A',
   remark = 'lay in 1/2in thick MPC shell at phi67.25in',
   remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
   remark = 'pages 3 and 4',
   remark = 'lay in MPC base plate 2.5in thick',
   remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
   remark = 'page 2(thickness), page 3(diameter)',
   remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',

   iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

$END

$FL

    remark = 'setting 1atm in Pa',
    presi = 101325.0,

$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',
```

```
      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*********************************************************************************************
**********
Development of 2D Model for CASK 24.
***********************************
05 July 2005 pav03  Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also
think that we do not
                    need compresibility, but right now let's only care about the mesh. The result
in the obstacle is the same,
                    but in the fluid that does not happen. Let's stay now with low resolution to
play with it.
01 July 2005 pav02  Inherited from Pavan, steady state accelerator.
                    Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT

      icmprs  = 1,    remark = 'compressible flow',
      iorder  = 3,    remark = 'setting iorder = 3 monotonically increasing',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 2,    remark = '1 compressible mat',
      iwsh    = 0,    remark = 'turn off wall shear',

      remark = 'switch to remark out when flow on',
      ihonly = 2,     remark = 'turn off material flow, heat transfer only',
      imphtc = 0,     remark = 'fully explicit eval of temp terms',
      ihtc   = 2,     remark = 'turn on heat conduction through obstacles',
      ifrho  = 1,     remark = 'allows local variation in density',
      ifenrg = 2,     remark = 'fluid energy transport on',
      gz = -9.81,     remark = 'gravity',


      remark = 'trest   =  1.43e-4,',
      twfin   =  1000.0,  remark = 'simulation end, seconds',
      pltdt   =  10,      remark = 'plotting interval, seconds',
      hpltdt  =  100.0,    remark = 'history interval, seconds',
      delt    =  1.0e-5, remark = 'time step, seconds',
      istdy   =  1,      remark = 'accelerate to steady state using non-phys transient',
                         remark = 'minimum timestep',
      dtmax   =  100,    remark = 'maximum timestep',

      autot   =  2.0, remark = 'timestep by stability',
      omega   =  1.7, remark = 'default setting for over-relaxation factor',

      epsadj  =  1.0, remark = 'standard convergence criterion',

      igmres = 1,

      remark = 'iadix   =  1',   remark = 'pressure iteration options (x,y,z) ADI',
      remark = 'iadiy   =  1',
      remark = 'iadiz   =  1',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  10,    remark = 'allowable inner iteration count',
      itdtmx  =  100,
                        remark = 'adjust itmax early to quickly step through start-up',
      negtmx  =  100000,  remark = 'negative rhoe resets',
```

```
    ncflmx  =  1000,    remark = 'convection failures allowed',

$END

$PROPS

    remark  = 'set up properties on fluid 2 to allow for compressibility option',

    units   = 'si',
    rhof2    = 1.2,
    mu2     = 1.86e-5, remark = 'viscosity air',
    cv2     = 1883.7,  remark = 'specific heat air',
    thc2    = 0.0264,  remark = 'thermal conductivity air',
    thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
    tstar   = 293.15,  remark = 'ref temp for air properties',
$END

$SCALAR
    remark = 'none needed for these simulations',
$END

$BCDATA

    remark = 'top wall is continuative (wt) or boundary 6',
    remark = 'set up as no ventilation',
    remark = 'made all bc continuative to start so cask is set in infinite air',

    wl     = 1,  remark = 'low x, continuative',
    wr     = 2,  remark = 'high x',
    wf     = 1,   remark = 'low y',
    wbk    = 1,  remark = 'high y',
    wb     = 2,    remark = 'low z',
    wt     = 3,    remark = 'high z, continuative',
    tbc(2) = 300.0,
    tbc(5) = 300.0,
    remark = 'pobc(2)= 0',
    remark = 'pobc(5)= 0',
    tbc(6) = 300,  remark = 'boundary condition at top of the cask'
    remark = 'eventually add cross-velocity at top of cask',

$END


$MESH

    remark = 'cylindrical mesh',
    icyl     = 1,
    nxcelt   = 20,
      px(1)  =  0.000000000,  nxcell(1)  = 5, remark = 'origin of the coordinate system',
       px(2)  =  0.127827306,  nxcell(2)  = 5,  remark = 'end point of the edge of the power
source',
       px(3)  =  0.162396706,

    nycelt   = 1,
      pya(1)=0.0,  nycell(1)=1, remark='cylindrical mesh...',
      pya(2)=10,   remark='azimuthal angle...',

   nzcelt    = 40,
      pz(1)  =  0.0000000,  nzcell(1)  = 5, remark = 'bottom overpack base plate',
      pz(2)  =  0.3052800,  nzcell(2)  = 10, remark = 'starting point of the fuel rod',
      pz(3)  =  4.1651200,  nzcell(3)  = 5, remark = 'top of the fuel rod',
      pz(4)  =  4.9434750,                  remark = 'head space',
$END

$OBS

   nobs = 1,
   remark = 'create the obstacle field',
   remark = 'general characteristics',
   remark = 'thermal conductivity = kobs unit:'
   remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
```

```
    remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',
    remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
    remark = 'Report HI-2012610',
    remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
    remark = 'thermal conductivity values from Table 4.4.7: generalized',
    remark = 'thermal conductivity vs. temperature',
    remark = 'choosing values at 400C based on instruction from C Ryder',
    remark = 'rcobs = specific heat',
    remark = '24 Basket',
    remark = 'A',
    remark = 'lay in 1/2in thick MPC shell at phi67.25in',
    remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
    remark = 'pages 3 and 4',
    remark = 'lay in MPC base plate 2.5in thick',
    remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
    remark = 'page 2(thickness), page 3(diameter)',
    remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',

    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                               yl(1) =  0.0000000,  yh(1) = 10.000000000,
                               zl(1) =  0.3052800,  zh(1) =  4.1651200,
                              tobs(1)  = 0,
                              kobs(1)  = 0.476,
                              rcobs(1) = 234.46,
                              pobs(1,1)= 22,

  $END

  $FL

      remark = 'setting 1atm in Pa',
      presi = 101325.0,

  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
Development of 2D Model for CASK 24.
***********************************

05 July 2005 pav04  Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03  Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also
think that we do not
```

```
                    need compresibility, but right now let's only care about the mesh. The result
in the obstacle is the same,
                    but in the fluid that does not happen. Let's stay now with low resolution to
play with it.
01 July 2005 pav02  Inherited from Pavan, steady state accelerator.
                    Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT

      icmprs  = 1,    remark = 'compressible flow',
      iorder  = 3,    remark = 'setting iorder = 3 monotonically increasing',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 2,    remark = '1 compressible mat',
      iwsh    = 0,    remark = 'turn off wall shear',

      remark = 'switch to remark out when flow on',
      ihonly = 2,     remark = 'turn off material flow, heat transfer only',
      imphtc = 0,     remark = 'fully explicit eval of temp terms',
      ihtc   = 2,     remark = 'turn on heat conduction through obstacles',
      ifrho  = 1,     remark = 'allows local variation in density',
      ifenrg = 2,     remark = 'fluid energy transport on',
      gz = -9.81,     remark = 'gravity',


      remark = 'trest   =  1.43e-4,',
      twfin   =  1000.0,  remark = 'simulation end, seconds',
      pltdt   =  10,      remark = 'plotting interval, seconds',
      hpltdt  =  100.0,    remark = 'history interval, seconds',
      delt    =  1.0e-5, remark = 'time step, seconds',
      istdy   =  1,      remark = 'accelerate to steady state using non-phys transient',
                         remark = 'minimum timestep',
      dtmax   =  100,    remark = 'maximum timestep',

      autot   =  2.0, remark = 'timestep by stability',
      omega   =  1.7, remark = 'default setting for over-relaxation factor',

      epsadj  =  1.0, remark = 'standard convergence criterion',

      igmres = 1,

      remark = 'iadix   =  1',   remark = 'pressure iteration options (x,y,z) ADI',
      remark = 'iadiy   =  1',
      remark = 'iadiz   =  1',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  10,    remark = 'allowable inner iteration count',
      itdtmx  =  100,
                        remark = 'adjust itmax early to quickly step through start-up',
      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof2    = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.
  $END
```

```
$SCALAR
    remark = 'none needed for these simulations',
$END

$BCDATA

    remark = 'top wall is continuative (wt) or boundary 6',
    remark = 'set up as no ventilation',
    remark = 'made all bc continuative to start so cask is set in infinite air',

    wl     = 1,  remark = 'low x, continuative',
    wr     = 2,  remark = 'high x',
    wf     = 1,   remark = 'low y',
    wbk    = 1,  remark = 'high y',
    wb     = 2,    remark = 'low z',
    wt     = 3,    remark = 'high z, continuative',
    tbc(2) = 300.0,
    tbc(5) = 300.0,
    remark = 'pobc(2)= 0',
    remark = 'pobc(5)= 0',
    tbc(6) = 300,  remark = 'boundary condition at top of the cask'
    remark = 'eventually add cross-velocity at top of cask',

$END


$MESH

    remark = 'cylindrical mesh',
    icyl     = 1,
    nxcelt   = 20,
      px(1)  =  0.000000000,  nxcell(1)  = 5, remark = 'origin of the coordinate system',
      px(2)  =  0.127827306,  nxcell(2)  = 5,  remark = 'end point of the edge of the power
source',
      px(3)  =  0.162396706,

    nycelt   = 1,
      pya(1)=0.0,  nycell(1)=1, remark='cylindrical mesh...',
      pya(2)=10,   remark='azimuthal angle...',

   nzcelt    = 40,
      pz(1)  =  0.0000000,  nzcell(1)  = 5, remark = 'bottom overpack base plate',
      pz(2)  =  0.3052800,  nzcell(2)  = 10, remark = 'starting point of the fuel rod',
      pz(3)  =  4.1651200,  nzcell(3)  = 5, remark = 'top of the fuel rod',
      pz(4)  =  4.9434750,                  remark = 'head space',
$END

$OBS

   nobs = 1,
   remark = 'create the obstacle field',
   remark = 'general characteristics',
   remark = 'thermal conductivity = kobs unit:'
   remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
   remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',
   remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
   remark = 'Report HI-2012610',
   remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
   remark = 'thermal conductivity values from Table 4.4.7: generalized',
   remark = 'thermal conductivity vs. temperature',
   remark = 'choosing values at 400C based on instruction from C Ryder',
   remark = 'rcobs = specific heat',
   remark = '24 Basket',
   remark = 'A',
   remark = 'lay in 1/2in thick MPC shell at phi67.25in',
   remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
   remark = 'pages 3 and 4',
   remark = 'lay in MPC base plate 2.5in thick',
   remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
   remark = 'page 2(thickness), page 3(diameter)',
```

```
    remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',

    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                               yl(1) =  0.0000000,  yh(1) = 10.000000000,
                               zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

  $END

  $FL

      remark = 'setting 1atm in Pa',
      presi = 101325.0,

  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END

!*****************************************************************************************
**********
flatplate01
*****************
Parallel flow over a flat plate - temperature distribution
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 2,    remark = 'allows local variation in density,option 2 solves transport eq',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',
```

```
   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 0,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 1,    remark = 'compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 2,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = 0., remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 0,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct., =3 y direct',
    remark='      trest   = 0.',   remark = ' restart time'.

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,   remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear, =1 on',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100.,remark = 'history interval, seconds',
      lpr=10,

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Termination Control',
      twfin   =  1000.0,  remark = 'simulation end, seconds',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,    remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,    remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
```

```
      ithtmx  =  50,       remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.
  $END

  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl     = 6,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 3,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 2,  remark = 'low z',
      wt     = 3,  remark = 'high z, continuative',

      tbc(1) = 300.0,
      tbc(5) = 400.0,

      ubc(1) = 10., remark = ' velocity at boundary',
  $END


  $MESH

      nxcelt   = 10,
        px(1)  =  0.0,  nxcell(1) = 10,
        px(2)  =  10. ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 10,
        pz(1)  =  0.0,  nzcell(1)  = 10,
        pz(2)  =  1.,
  $END

  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                 yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                 zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
```

```
                              pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      ui     = 10. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate02
*****************
Parallel flow over a flat plate - temperature distribution - incompressible

10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',
```

```
   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 0,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = 0., remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 0,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
    remark='      trest   = 0.',   remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  1., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 20.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,    remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,    remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',
```

```
      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl     = 6,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 3,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 2,  remark = 'low z',
      wt     = 3,  remark = 'high z, continuative',


      tbc(5) = 350.0,

      ubc(1) = .1, remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt   = 10,
        px(1)  =  0.0,  nxcell(1) = 10,
        px(2)  =  .1 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 100,
        pz(1)  =  0.0,  nzcell(1)  = 100,
        pz(2)  = .1,
  $END

  $OBS


  $END
```

```
  obstacle text ignored for later on...
    nobs = 1,
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

 $FL

    remark = 'setting 1atm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = .1 ,
 $END

 $BF
 $END

 $TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

 $END

 $GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

 $END


 $PARTS
 $END
!*****************************************************************************************
**********
flatplate03
*****************
Parallel flow over a flat plate - temperature distribution - incompressible

10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
```

```
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 0,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 0,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.,   remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 2.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',
```

```
   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,    remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  100000,    remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl     = 3,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 3,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 2,  remark = 'low z',
      wt     = 3,  remark = 'high z, continuative',


      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt   = 10,
       px(1)  =  0.0,  nxcell(1) = 10,
        px(2)  =  .1 ,
```

```
    nycelt    = 1,
      py(1)=0.0,  nycell(1)=1,
      py(2)=1.,

   nzcelt     = 50,
      pz(1)   =  0.0,  nzcell(1)   = 50,
      pz(2)   = .03,
$END

$OBS


$END

  obstacle text ignored for later on...
    nobs = 1,
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

$FL

    remark = 'setting 1atm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*****************************************************************************************
**********
flatplate04
*****************
Parallel flow over a flat plate - temperature distribution - incompressible
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
```

```
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 0,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
```

```
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
```

```
      thexfl   = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar    = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2    = 1.2,
      mu2      = 1.86e-5, remark = 'viscosity air',
      cv2      = 1883.7,  remark = 'specific heat air',
      thc2     = 0.0264,  remark = 'thermal conductivity air',
      thexf2   = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar    = 293.15,  remark = 'ref temp for air properties',
      rf2      = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl      = 3,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',


      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt    = 1000,
        px(1)   =  0.0,  nxcell(1) = 1000,
        px(2)   =  3.81 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 25,
        pz(1)   =  0.0,  nzcell(1)  = 25,
        pz(2)   = .03,
  $END

  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
                               pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
```

```
    ui      = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate05
*****************
Parallel flow over a flat plate - temperature distribution - incompressible
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
```

```
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
```

```
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl      = 3,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',
```

```
    tbc(5) = 350.0,

    ubc(1) = 0., remark = ' velocity at boundary',
$END
    tbc(1) = 300.0,

$MESH

    nxcelt   = 1000,
      px(1)  =  0.0,  nxcell(1) = 1000,
      px(2)  =  3.81 ,

    nycelt   = 1,
      py(1)=0.0,  nycell(1)=1,
      py(2)=1.,

   nzcelt    = 25,
      pz(1)  =  0.0,  nzcell(1)  = 25,
      pz(2)  = .03,
$END

$OBS


$END

  obstacle text ignored for later on...
    nobs = 1,
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

$FL

    remark = 'setting 1atm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
```

```
  $END
!*****************************************************************************************
**********
flatplate06
*****************
Parallel flow over a flat plate - temperature distribution - incompressible

14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,     remark = 'solve internal energy',
```

```
      ifrho    = 1,     remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder   = 1,     remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj   =  1.0, remark = 'multiplier for pressure iteration',
      epshtc   =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly   = 0,     remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc     = 1,     remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc   = 1,     remark = '=0 explicit eval of temp, =1 fully implicit',
      imp      = 0,     remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis   = 0,     remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs   = 0,     remark = '0=incompr., 1=compressible flow',
      itb      = 0,     remark = 'no free surfaces',
      nmat     = 1,     remark = '1 compressible mat',

   remark  = ' Gravity',
      gx       = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis    = 2,     remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest    = 0.0   ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp    = 1,     remark = ' mentor help',
      istdy    = 0,     remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght   = 2.,    remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh     = 1,     remark = '=0 turn off wall shear',
      ifvis    = 0,     remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish    = 0,     remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt    =  .1, remark = 'plotting interval, seconds',
      hpltdt   =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin    = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix    = 0,     remark=' =0 SOR, =1 ADI',
      iadiy    = 0,     remark=' =0 SOR, =1 ADI',
      iadiz    = 0,     remark=' =0 SOR, =1 ADI',
      omega    = 1.7,   remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt     =  1.0e-5, remark = 'initial time step, seconds',
      dtmax    =  100.,   remark = 'maximum timestep',
      autot    =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx   =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax    =  1000,      remark = 'max press iter per time step',
```

```
      itdtmx  =  100,      remark = ' max # of press iterations before time step reduced',
      idtht   =  20,       remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,       remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,   remark = 'negative rhoe resets',
      ncflmx  =  1000,     remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.30,
      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt   = 1000,
        px(1)  =  0.0,  nxcell(1) = 1000,
        px(2)  =  3.81 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 25,
        pz(1)  =  0.0,  nzcell(1)  = 25,
        pz(2)  = .03,
  $END

  $OBS
```

```
  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
                               pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate07
****************
Parallel flow over a flat plate - temperature distribution - incompressible

14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
```

```
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',
```

```
   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 1883.7,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
```

```
      tstar    = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2    = 1.2,
      mu2      = 1.86e-5, remark = 'viscosity air',
      cv2      = 1883.7,  remark = 'specific heat air',
      thc2     = 0.0264,  remark = 'thermal conductivity air',
      thexf2   = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar    = 293.15,  remark = 'ref temp for air properties',
      rf2      = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101321.50,
      tbc(1) = 300.,
      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt    = 100,
        px(1)   =  0.0,  nxcell(1) = 100,
        px(2)   =  .3 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 25,
        pz(1)   =  0.0,  nzcell(1)  = 25,
        pz(2)   = .03,
  $END

  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                 yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                 zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
                               pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
```

```
    ui      = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate08
*****************
Parallel flow over a flat plate - temperature distribution - incompressible

14 July 2005 flatplate08  Continuative bndry at low x.
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with different bndry conditions 2) discharge to open space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
```

```
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',
```

```
   remark  = ' Physical model options',
      iwsh    = 1,     remark = '=0 turn off wall shear',
      ifvis   = 0,     remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,     remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,     remark=' =0 SOR, =1 ADI',
      iadiy   = 0,     remark=' =0 SOR, =1 ADI',
      iadiz   = 0,     remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA
```

```
      wl      = 3,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt    = 100,
        px(1)   =  0.0,  nxcell(1) = 100,
        px(2)   =  .3 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 25,
        pz(1)   =  0.0,  nzcell(1)  = 25,
        pz(2)   = .03,
  $END

  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
                               pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
```

```
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate09
*****************
Parallel flow over a flat plate - temperature distribution - incompressible - open space

20 July 2005 flatplate09  Let's do the open space case. This guy run very fast! And looks
great... It seems to confirm that
                          a pressure boundary is a best approach, but we need to run #08 up to
completion.
14 July 2005 flatplate08  Continuative bndry at low x. Part of the air recirculates back warming
it up in the gap. A continuative
                          boundary does not look a good option .... Specified pressure, as in run
07 looks much better.
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with different bndry conditions 2) discharge to open space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
```

```
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
```

```
      twfin    = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix    = 0,     remark=' =0 SOR, =1 ADI',
      iadiy    = 0,     remark=' =0 SOR, =1 ADI',
      iadiz    = 1,     remark=' =0 SOR, =1 ADI',
      omega    = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt     =  1.0e-5, remark = 'initial time step, seconds',
      dtmax    =  100.,   remark = 'maximum timestep',
      autot    =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl      = 3,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
```

```
    tbc(1) = 300.0,

$MESH

    nxcelt   = 100,
      px(1)  =  0.0,  nxcell(1) = 100,
      px(2)  =  .3 ,

    nycelt   = 1,
      py(1)=0.0,  nycell(1)=1,
      py(2)=1.,

   nzcelt    = 25,
      pz(1)  =  0.0,  nzcell(1)  = 25,
      pz(2)  = .03,
$END

Second mesh for the open space, much coarser.

$BCDATA

    wl     = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
    wr     = 3,  remark = 'high x',
    wf     = 1,  remark = 'low y',
    wbk    = 1,  remark = 'high y',
    wb     = 2,  remark = 'low z',
    wt     = 2,  remark = 'high z, continuative',

$END

$MESH

    nxcelt   = 28,
      px(1)  =  -.3,  nxcell(1) = 16,
      px(2)  =  -.2,  nxcell(2) =  8,
      px(3)  =  -.1,  nxcell(3) =  4,
      px(4)  =   .0,


    nycelt   = 1,
      py(1)=0.0,  nycell(1)=1,
      py(2)=1.,

   nzcelt    = 77,
      pz(1)  =  0.00, nzcell(1)  = 25,
      pz(2)  =  0.03, nzcell(2)  = 30,
      pz(3)  =  0.1,  nzcell(3)  = 15,
      pz(4)  =  0.2,  nzcell(4)  =  7,
      pz(5)  =   .3,
$END


$OBS


$END

  obstacle text ignored for later on...
    nobs = 1,
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

$FL

    remark = 'setting latm in Pa',
```

```
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*****************************************************************************************
**********
Flatplate10. Natural convection with power source on wall

21 July 2005 flatplate10  Some corrections in the mesh and change bndry condition to power. This
looks it is working great!
20 July 2005 flatplate09  Let's do the open space case. This guy run very fast! And looks
great... It seems to confirm that
                          a pressure boundary is a best approach, but we need to run #08 up to
completion. Done ... Confirmed that
                          the air recirculates into the cavity warming it up so continuative
boundary is not a good approx. to
                          simulate an open space.
14 July 2005 flatplate08  Continuative bndry at low x. Part of the air recirculates back warming
it up in the gap. A continuative
                          boundary does not look a good option .... Specified pressure, as in run
07 looks much better.
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with different bndry conditions 2) discharge to open space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
```

```
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',
```

```
   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
```

```
      cv2      = 1883.7,  remark = 'specific heat air',
      thc2     = 0.0264,  remark = 'thermal conductivity air',
      thexf2   = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar    = 293.15,  remark = 'ref temp for air properties',
      rf2      = 287.


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter. The gap here is 0.3 m
     so the power should be 61.55 W
  $BCDATA

      wl      = 3,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,
      wf      = 1,
      wbk     = 1,
      wb      = 2,
      wt      = 1,   remark='This saves us the other half of the gap',

      pobc(5)=61.55,
      ubc(1) = 0., remark = ' velocity at boundary',
  $END


  $MESH

      nxcelt    = 100,
        px(1)   =  0.0,  nxcell(1) = 100,
        px(2)   =  .3 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 25,
        pz(1)   =  0.0,  nzcell(1)  = 25,
        pz(2)   = .03,
  $END

  Second mesh for the open space, much coarser.

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 3,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 2,  remark = 'high z, continuative',

  $END

  $MESH

      nxcelt    = 28,
        px(1)   =  -.3,  nxcell(1) =  4,
        px(2)   =  -.2,  nxcell(2) =  8,
        px(3)   =  -.1,  nxcell(3) = 16,
        px(4)   =   .0,


      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,
```

```
   nzcelt     = 77,
      pz(1)   =  0.00, nzcell(1)  = 25,
      pz(2)   =  0.03, nzcell(2)  = 30,
      pz(3)   =  0.1,  nzcell(3)  = 15,
      pz(4)   =  0.2,  nzcell(4)  =  7,
      pz(5)   =   .3,
$END


$OBS


$END

  obstacle text ignored for later on...
    nobs = 1,
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

$FL

    remark = 'setting 1atm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*********************************************************************************************
**********
Flatplate11. Natural convection with power source on wall - real size gap

21 July 2005 flatplate11  The max. temperature in the previous run was 335 K, which is really
encouraging. Now let's go to
                          the real size problem. Run longer. Now the max temp is 326 K. The run
looks very nice althoug it has some
                          instability which I do not know if it is real or due to the boundary
condition. Let's check it
                          in the next run.
```

21 July 2005 flatplate10 Some corrections in the mesh and change bndry condition to power. This looks it is working great!
The program does not properly compute the hydrostatic pressure in the second mesh. Let's ignore
that now, but we should ask Flow 3D how to do it...
20 July 2005 flatplate09 Let's do the open space case. This guy run very fast! And looks great... It seems to confirm that
a pressure boundary is a best approach, but we need to run #08 up to completion. Done ... Confirmed that
the air recirculates into the cavity warming it up so continuative boundary is not a good approx. to
simulate an open space.
14 July 2005 flatplate08 Continuative bndry at low x. Part of the air recirculates back warming it up in the gap. A continuative
boundary does not look a good option .... Specified pressure, as in run 07 looks much better.
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with different bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not

```
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  1., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 100.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',
```

```
   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,
      wf      = 1,
      wbk     = 1,
      wb      = 2,
      wt      = 1,   remark='This saves us the other half of the gap',

      pobc(5)=198.,
      pbctyp=0.,
      pbc(1) =101280.,
      tbc(1) =300.,
  $END
      pbctyp=0.,
      pbc(1) =101318.,

  $MESH
```

```
      nxcelt    = 300,
        px(1)   =  0.0,  nxcell(1) = 100,
        px(2)   =  1.0,  nxcell(2) =  50,
        px(3)   =  2.0,  nxcell(3) =  50,
        px(4)   =  3.0,  nxcell(4) = 100,
         px(5)  =  3.86 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 25,
        pz(1)   =  0.0,  nzcell(1)  = 25,
        pz(2)   = .03,
  $END


  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
                               pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
Flatplate12. Natural convection with power source on wall - real size gap
```

21 July 2005 flatplate12 Let's add a room to check the boundary condition. The max. temp. here is around 350 K, I don't know if
we can say this is equivalent to run11. My inclination is to say no... This run took 9 hours.
21 July 2005 flatplate11 The max. temperature in the previous run was 335 K, which is really encouraging. Now let's go to
the real size problem. Run longer. Now the max temp is 326 K. The run looks very nice although it has some
instability which I do not know if it is real or due to the boundary condition. Let's check it
in the next run.
21 July 2005 flatplate10 Some corrections in the mesh and change bndry condition to power. This looks it is working great!
The program does not properly compute the hydrostatic pressure in the second mesh. Let's ignore
that now, but we should ask Flow 3D how to do it...
20 July 2005 flatplate09 Let's do the open space case. This guy run very fast! And looks great... It seems to confirm that
a pressure boundary is a best approach, but we need to run #08 up to completion. Done ... Confirmed that
the air recirculates into the cavity warming it up so continuative boundary is not a good approx. to
simulate an open space.
14 July 2005 flatplate08 Continuative bndry at low x. Part of the air recirculates back warming it up in the gap. A continuative
boundary does not look a good option .... Specified pressure, as in run 07 looks much better.
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with different bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce

```
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  1., remark = 'plotting interval, seconds',
```

```
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 100.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 9,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,
      wf      = 1,
      wbk     = 1,
```

```
      wb      = 2,
      wt      = 1,   remark='This saves us the other half of the gap',

      pobc(5)=198.,      remark=' this is the power',
      pbctyp=0.,
      pbc(1) =101280.,
      tbc(1) =300.,
  $END
      pbctyp=0.,
      pbc(1) =101280.,
      tbc(1) =300.,

  $MESH

      nxcelt    = 300,
        px(1)   =  0.0,  nxcell(1) = 100,
        px(2)   =  1.0,  nxcell(2) =  50,
        px(3)   =  2.0,  nxcell(3) =  50,
        px(4)   =  3.0,  nxcell(4) = 100,
         px(5)   =  3.86 ,

      nycelt    = 1,
         py(1)=0.0,  nycell(1)=1,
         py(2)=1.,

     nzcelt     = 25,
         pz(1)   =  0.0,  nzcell(1)   = 25,
         pz(2)   = .03,
  $END

Second mesh!

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 9,
      wf      = 1,
      wbk     = 1,
      wb      = 2,
      wt      = 1,   remark='This saves us the other half of the gap',

  $END

  $MESH

      nxcelt    = 95,
        px(1)   = -4.0,  nxcell(1) =   7,
        px(2)   = -3.0,  nxcell(2) =  13,
        px(3)   = -2.0,  nxcell(3) =  25,
        px(4)   = -1.0,  nxcell(4) =  50,
         px(5)   =  0. ,

      nycelt    = 1,
         py(1)=0.0,  nycell(1)=1,
         py(2)=1.,

     nzcelt     = 120,
        pz(1)   = -4.0,  nzcell(1) =   7,
        pz(2)   = -3.0,  nzcell(2) =  13,
        pz(3)   = -2.0,  nzcell(3) =  25,
        pz(4)   = -1.0,  nzcell(4) =  50,
         pz(5)   =  0.0,  nzcell(5) =  25,
         pz(6)   = .03,
  $END



  $OBS
```

```
$END

  obstacle text ignored for later on...
    nobs = 1,
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

$FL

    remark = 'setting 1atm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*****************************************************************************************
**********
Flatplate13. Natural convection with power source on wall and room - real size gap - fine mesh

22 July 2005 flatplate13  Let's refine the mesh by a factor of two to see if it makes any
difference. Also let's run it longer.
21 July 2005 flatplate12  Let's add a room to check the boundary condition. The max. temp. here
is around 350 K, I don't know if
                          we can say this is equivalent to run11. My inclination is to say no...
This run took 9 hours.
21 July 2005 flatplate11  The max. temperature in the previous run was 335 K, which is really
encouraging. Now let's go to
                          the real size problem. Run longer. Now the max temp is 326 K. The run
looks very nice although it has some
                          instability which I do not know if it is real or due to the boundary
condition. Let's check it
                          in the next run.
21 July 2005 flatplate10  Some corrections in the mesh and change bndry condition to power. This
looks it is working great!
                          The program does not properly compute the hydrostatic pressure in the
second mesh. Let's ignore
                          that now, but we should ask Flow 3D how to do it...
```

20 July 2005 flatplate09 Let's do the open space case. This guy run very fast! And looks great... It seems to confirm that
a pressure boundary is a best approach, but we need to run #08 up to completion. Done ... Confirmed that
the air recirculates into the cavity warming it up so continuative boundary is not a good approx. to
simulate an open space.
14 July 2005 flatplate08 Continuative bndry at low x. Part of the air recirculates back warming it up in the gap. A continuative
boundary does not look a good option .... Specified pressure, as in run 07 looks much better.
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with different bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.

Goal is estimate the thermal contribution of one reactor.

24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  1., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 100.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',
```

```
  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.



  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 9,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,
      wf      = 1,
      wbk     = 1,
      wb      = 2,
      wt      = 1,   remark='This saves us the other half of the gap',

      pobc(5)=198.,     remark=' this is the power',
      pbctyp=0.,
      pbc(1) =101280.,
      tbc(1) =300.,
  $END
      pbctyp=0.,
      pbc(1) =101280.,
      tbc(1) =300.,

  $MESH

      nxcelt   = 600,
       px(1)  =  0.0,  nxcell(1) = 200,
       px(2)  =  1.0,  nxcell(2) = 100,
```

```
      px(3)   =  2.0,  nxcell(3) = 100,
      px(4)   =  3.0,  nxcell(4) = 200,
       px(5)   =  3.86 ,

     nycelt    = 1,
       py(1)=0.0,  nycell(1)=1,
       py(2)=1.,

    nzcelt     = 50,
       pz(1)   =  0.0,  nzcell(1)   = 50,
       pz(2)   = .03,
  $END

Second mesh!

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 9,
      wf      = 1,
      wbk     = 1,
      wb      = 2,
      wt      = 1,   remark='This saves us the other half of the gap',

  $END

  $MESH

     nxcelt    = 190,
      px(1)   = -4.0,  nxcell(1) =  14,
      px(2)   = -3.0,  nxcell(2) =  26,
      px(3)   = -2.0,  nxcell(3) =  50,
      px(4)   = -1.0,  nxcell(4) = 100,
       px(5)   =  0. ,

     nycelt    = 1,
       py(1)=0.0,  nycell(1)=1,
       py(2)=1.,

    nzcelt     = 240,
      pz(1)   = -4.0,  nzcell(1) =  14,
      pz(2)   = -3.0,  nzcell(2) =  26,
      pz(3)   = -2.0,  nzcell(3) =  50,
      pz(4)   = -1.0,  nzcell(4) = 100,
       pz(5)   =  0.0,  nzcell(5) =  50,
       pz(6)   = .03,
  $END



  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
      iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                                yl(1) =  0.0000000,  yh(1) = 10.000000000,
                                zl(1) =  0.3052800,  zh(1) =  4.1651200,
                               tobs(1)  = 0,
                               kobs(1)  = 0.476,
                               rcobs(1) = 234.46,
                               pobs(1,1)= 22,

  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
```

```
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*****************************************************************************************
**********
!*****************************************************************************************
**********
flatplate15: Small reactor, natural convection

26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
```

```
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',
```

```
   remark  = ' Initialization and Restart',
      ipdis   = 2,     remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,     remark = ' mentor help',
      istdy   = 0,     remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,    remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,     remark = '=0 turn off wall shear',
      ifvis   = 0,     remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,     remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 100.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,     remark=' =0 SOR, =1 ADI',
      iadiy   = 0,     remark=' =0 SOR, =1 ADI',
      iadiz   = 1,     remark=' =0 SOR, =1 ADI',
      omega   = 1.7,   remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

```
    Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
    we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 300,
        px(1)  =  0.0,  nxcell(1) = 100,
        px(2)  =  1.0,  nxcell(2) =  50,
        px(3)  =  2.0,  nxcell(3) =  50,
        px(4)  =  3.0,  nxcell(4) = 100,
        px(5)  =  4.50 ,

      nycelt   = 1.
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 38,
        pz(1)  = -0.1135,nzcell(1)  = 13,
        pz(2)  =  0.0,   nzcell(2)  = 25,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 300.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END
```

```
$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*****************************************************************************************
**********
flatplate15: Small reactor, natural convection

01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
```

```
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong  I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
```

```
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per meter per face. In this example

```
    we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 150,
        px(1)   =  0.0,  nxcell(1) =  50,
        px(2)   =  1.0,  nxcell(2) =  25,
        px(3)   =  2.0,  nxcell(3) =  25,
        px(4)   =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.

     nzcelt     = 20,
        pz(1)   = -0.1135,nzcell(1)   =  7,
        pz(2)   =  0.0,   nzcell(2)   = 13,
        pz(3)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 300.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting latm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP
```

```
      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate17: Small reactor, natural convection,tobs 600K

02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
```

```
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',
```

```
   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

```
     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 150,
        px(1)   =  0.0,  nxcell(1) =  50,
        px(2)   =  1.0,  nxcell(2) =  25,
        px(3)   =  2.0,  nxcell(3) =  25,
        px(4)   =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 20,
        pz(1)   = -0.1135,nzcell(1)   =  7,
        pz(2)   =  0.0,   nzcell(2)   = 13,
        pz(3)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END
```

```
  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate18. 2-D assembly with Helium

03 Aug  2005 flatplate18  Little excercise to see how long it takes to the helium to leave the
gap and be replaced by air.
                          Unfortunately I just realized that Mary Ann got the Cv wrong! I need to
check further how that affects
                          the problem.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
```

12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      ifvof   = 2,    remark = 'flag for advection,0= no adv,2=second order adv,3=VOF interface
track,4=VOF +donor,5=Semi-Lag',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',
```

```
   remark  = ' File Control Options',
      idlinp  = 0,    remark = '=0 do not delete hd3in.dat',
      idlrst  = 0,    remark = '=0 do not delete hd3rstr.dat',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 1,    remark = '0=no free surfaces,1=free surf or sharp interface',
      nmat    = 2,    remark = '2 incompressible mat',
      ifvelp  = 0,    remark = '0= solve all fluid transport equations,1= same as ihonly=1,2=same
as ihonly=2',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      fclean  = 0.05, remark = ' fluid fraction cleanup',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',


   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS
```

```
      units    = 'si',
      rhof     = 1.225,
      mu1      = 1.86e-5, remark = 'viscosity air',
      cv1      = 713.,    remark = 'Mary Ann had here 1883.7, who knows why',
      thc1     = 0.0264,  remark = 'thermal conductivity air',
      thexf1   = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar    = 293.15,  remark = 'ref temp for air properties',

      rhof2    = 0.178,
      mu2      = 1.90e-5, remark = 'viscosity Helium from my Apuntes de Termodinamica',
      cv2      = 2077.5 , remark = 'R gas constant for He: 8.31 J/mol/K / 4e-3 kg/mol=2077.5
J/kg/K, Cv=Cp-R=3114.5 J/kg/K',
      thc2     = 0.142  , remark = 'thermal conductivity He',
      thexf2   = 3.48e-3, remark = 'in fact beta=-1/V*(dV/dT) and for an ideal gas beta=1/T so for
293K -> beta~3.41e-3 K-1, similar to Batchelor',

  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 9,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',


  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 150,
        px(1)   =  0.0,  nxcell(1) =  50,
        px(2)   =  1.0,  nxcell(2) =  25,
        px(3)   =  2.0,  nxcell(3) =  25,
        px(4)   =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 20,
        pz(1)   = -0.1135,nzcell(1)   =  7,
        pz(2)   =  0.0,   nzcell(2)   = 13,
        pz(3)   = .03,
  $END

  Let's add a room full of air

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 9,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 2,  remark = 'high z, continuative',
```

```
  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 60,
        px(1)   = -9.0,  nxcell(1) =  50,
        px(2)   = -0.5,  nxcell(2) =  10,
        px(3)   =  0.0,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 70,
        pz(1)   = -9.0,    nzcell(1)   = 50,
        pz(2)   = -0.1135,nzcell(2)   =  7,
        pz(3)   =  0.0,    nzcell(3)   = 13,
        pz(4)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46
                             pobs(1,1) -436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      nfls = 2 ,   remark='number of fluid regions',

      remark=' Helium in the gap',
        freg(1)=0.,
        fxh(1) = 100., fxl(1) = 0., fyh(1) = 100., fyl(1)=-100.,fzh(1)=100.,fzl(1)=-100.,

      remark=' Air in room',
        freg(2)=1.,
        fxh(2) = 0., fxl(2) =-100., fyh(2) = 100., fyl(2)=-100.,fzh(2)=100.,fzl(2)=-100.,

      remark = 'setting 1atm in Pa',
        presi  = 101325.0,
        pvoid  = 101325.0,
        ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END
```

```
  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate19: Cv check, natural convection,tobs 600K

03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
```

more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compressibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',
```

```
   remark  = ' Numerical options',
      ihelp   = 1,     remark = ' mentor help',
      istdy   = 0,     remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,    remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,     remark = '=0 turn off wall shear',
      ifvis   = 0,     remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,     remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,     remark=' =0 SOR, =1 ADI',
      iadiy   = 0,     remark=' =0 SOR, =1 ADI',
      iadiz   = 1,     remark=' =0 SOR, =1 ADI',
      omega   = 1.7,   remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA
```

```
      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting latm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,
```

```
  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate20: compressibility check, natural convection,tobs 600K

04 Aug  2005 flatplate20  I have a new concern today. Maybe the temperature is too high for the
incompressible approx.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
```

11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 1,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',
```

```
   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

```
    Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
    we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END
```

```
  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate21: 2-D run, natural convection, T0=300 K

04 Augu 2005 flatplate21  Assad wants a run with initial temperature at 300K but the right Cv for
air which is 713 J/Kg/K.
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
```

```
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',
```

```
   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

```
     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
        px(5)  =  4.50 ,

      nycelt   = 1.
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 300.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting latm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END
```

```
$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*************************************************************************************************
**********
flatplate22: Pavan axial symmetry, natural convection,tobs 600K

09 Aug  2005 flatplate22  Trying to  reproduce Pavan's results. All the assemblies are lumped
together in the center. This seems a
                          very conservative approach that rises the temperature up to thousands
of K even with an open lid and a
                          temperature bndry condition. Really bad approach! Dismiss!!
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
```

```
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',
```

```
   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = -9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 1,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
```

```
      tstar    = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 1,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 5,  remark = 'high z, continuative',

      pbc(6)  = 101280.,
      tbc(6)  = 300.,
      tbc(2)  = 300.,
  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH

      icyl      = 1,
      nxcelt    = 25,
        px(1)   =  .0 ,  nxcell(1) =  15,
        px(2)   =  .63,  nxcell(2) =  10,
        px(3)   =  .84,


      nycelt    = 1,
        pya(1)=0.0,  nycell(1)=1,
        pya(2)=10.,

     nzcelt     = 50,
        pz(1)   =  0. ,   nzcell(1)  =  50,
        pz(2)   =  4.5,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.  , xh(1) =   .63,
                             yl(1) =   0.  , yh(1) = 10.0 ,
                             zl(1) =   .35 , zh(1)=   4.20,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =19008,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

  $FL

      remark = 'setting latm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END
```

```
  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate23: Room and natural convection.tobs 600K

09 Aug  2005 flatplate23  How long does it take for a room to warm up under the heat of an
assembly? That is a Bis question.
                          I think the time scale will be impossible and another approx. will be
needed, but let's try.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
```

12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
```

```
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  3600., remark = 'plotting interval, seconds, every hour',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 3.e6,  remark = 'simulation end, seconds, around a month ...',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END
```

```
$SCALAR
    remark = 'none needed for these simulations',
$END

$BCDATA

    wl     = 9,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
    wr     = 2,  remark = 'high x',
    wf     = 1,  remark = 'low y',
    wbk    = 1,  remark = 'high y',
    wb     = 1,  remark = 'low z',
    wt     = 1,  remark = 'high z ',


$END
    pbc(1) = 101280.,
    tbc(1) = 300.,
    tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
$MESH
    nxcelt   =  74,
      px(1)  =  0.0,  nxcell(1) =  25,
      px(2)  =  1.0,  nxcell(2) =  12,
      px(3)  =  2.0,  nxcell(3) =  12,
      px(4)  =  3.0,  nxcell(4) =  25,
      px(5)  =  4.50 ,

    nycelt   = 1,
      py(1)=0.0,  nycell(1)=1,
      py(2)=1.,

   nzcelt    = 11,
      pz(1)  = -0.1135,nzcell(1)  =  4,
      pz(2)  =  0.0,   nzcell(2)  =  7,
      pz(3)  = .03,
$END

ROOM MESH

Let's add the room with dimensions: Length=14.6 m, Height= 21.3 m, Width= 1 m. These come from
the fact that I am simulating 55% of the
assembly (in terms of power) and there are 24 assemblies in the real case so the volume of the
room needs to be scaled by .55/24. The
room that Chris Ryder provided is 70 ft x 190 ft x 36 ft, he said the dimensions are wrong, by
the way, so 21.3 m x 57.9 m x 10.98 m.
A few multiplications should give the 14.6 x 21.3 x 1 m3 mentioned, look at the notebook.

$BCDATA

    wl     = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
    wr     = 9,  remark = 'high x',
    wf     = 1,  remark = 'low y',
    wbk    = 1,  remark = 'high y',
    wb     = 2,  remark = 'low z',
    wt     = 2,  remark = 'high z, continuative',


$END

$MESH
    nxcelt   =  35,
      px(1)  =-21.3,  nxcell(1) =  25,
      px(2)  = -1.0,  nxcell(2) =  10,
      px(3)  =   .0,

    nycelt   = 1,
      py(1)=0.0,  nycell(1)=1,
```

```
      py(2)=1.,

    nzcelt     = 26,
       pz(1)   =-14.6    ,nzcell(1)   = 15,
       pz(2)   = -0.1135,nzcell(2)   =  4,
       pz(3)   =  0.0,    nzcell(3)   =  7,
       pz(4)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12, remark=' Remember there is symmetry so only half
the power is here...',
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
```

flatplate24 playing with compressible

14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
```

```
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  .1, remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 10.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
```

```
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 1883.7,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END

* for later use**
      rhof2   = 1.2,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 1883.7,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
      rf2     = 287.


  $SCALAR
      remark = 'none needed for these simulations',
  $END

  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 2,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.30,
      tbc(5) = 350.0,

      ubc(1) = 0., remark = ' velocity at boundary',
  $END
      tbc(1) = 300.0,

  $MESH

      nxcelt   = 1000,
        px(1)  =  0.0,  nxcell(1) = 1000,
        px(2)  =  3.81 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 25,
        pz(1)  =  0.0,  nzcell(1)  = 25,
        pz(2)  = .03,
  $END

  $OBS


  $END

    obstacle text ignored for later on...
      nobs = 1,
```

```
    iob(1) = 1, ioh(1) = 1,   ral(1) =  0.0000000, rah(1) =  0.127827306,
                              yl(1) =  0.0000000,  yh(1) = 10.000000000,
                              zl(1) =  0.3052800,  zh(1) =  4.1651200,
                             tobs(1)  = 0,
                             kobs(1)  = 0.476,
                             rcobs(1) = 234.46,
                             pobs(1,1)= 22,

  $FL

    remark = 'setting 1atm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

  $END

  $GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate25: Added room to 19, natural convection,tobs 600K

15 Aug  2005 flatplate25  Added the room to justify boundary condition in pressure
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
```

1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
```

```
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
```

```
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  Let's add a room full of air

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 9,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 2,  remark = 'high z, continuative',
```

```
  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 60,
        px(1)  = -9.0,  nxcell(1) =  50,
        px(2)  = -0.5,  nxcell(2) =  10,
        px(3)  =  0.0,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 70,
        pz(1)  = -9.0,   nzcell(1)  = 50,
        pz(2)  = -0.1135,nzcell(2)  =  7,
        pz(3)  =  0.0,   nzcell(3)  = 13,
        pz(4)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
```

```
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate26: Room only, long timescale run

17 Aug  2005 flatplate26  How fast does the temperature rise in the room for very long times? I
changed the orientation to z being
                          vertical! Not solving for obstacle conduction. The run dies after two
days, I guess I need to treat
                          the air as compressible ...
15 Aug  2005 flatplate25  Added the room to justify boundary condition in pressure
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
```

The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = -9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
```

```
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  43200., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 2592000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

  Only the room will be here

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 1,  remark = 'high x',
```

```
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 2,  remark = 'high z, continuative',


  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 15,
        px(1)   =    .0,  nxcell(1) =  15,
        px(2)   = 14.6,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 22,
        pz(1)   =  0. ,   nzcell(1)  = 22,
        pz(2)   = 21.6,
  $END

  Power is corrected to have the same output with the new geometry. Volume of the obstacle was
.437 m3 in run 25, now the volume
  is 1 m3. Now that I think about it, it does not matter as long as the room is the right size
  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =  13.6 , xh(1) =  14.6,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =   0.  , zh(1)=   1.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,
```

```
  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate27: Room only, long timescale run, compressible

18 Aug  2005 flatplate27  Compressible run. Explicit coupling (imp=0) kills the run. Changed
iadiz to 0. Lots of pressure iteration
                          failures, but stabilizes after 26000 secs. The temperature in the room
stabilizes after one day or so. I
                          guess I have leaks of heat through the boundaries, let's correct that.
17 Aug  2005 flatplate26  How fast does the temperature rise in the room for very long times? I
changed the orientation to z being
                          vertical! Not solving for obstacle conduction. The run dies after two
days, I guess I need to treat
                          the air as compressible ...
15 Aug  2005 flatplate25  Added the room to justify boundary condition in pressure
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
```

more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 2,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 1,    remark = '=0 explicit press-vel incompatible  with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 1,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = -9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 1,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',
```

```
   remark  = ' Numerical options',
      ihelp   = 1,     remark = ' mentor help',
      istdy   = 1,     remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,    remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,     remark = '=0 turn off wall shear',
      ifvis   = 0,     remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,     remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  43200., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 2592000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,     remark=' =0 SOR, =1 ADI',
      iadiy   = 0,     remark=' =0 SOR, =1 ADI',
      iadiz   = 0,     remark=' =0 SOR, =1 ADI',
      omega   = 1.7,   remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,    remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',

      rhof2    = 1.225,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 713.  ,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      rf2     = 287.   , remark = 'Gas constant for air',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
```

```
$END

Only the room will be here

$BCDATA

     wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
     wr      = 1,  remark = 'high x',
     wf      = 1,  remark = 'low y',
     wbk     = 1,  remark = 'high y',
     wb      = 2,  remark = 'low z',
     wt      = 2,  remark = 'high z, continuative',

     fbc(1)=1.,fbc(2)=1.,fbc(3)=1.,fbc(4)=1.,fbc(5)=1.,fbc(6)=1.,


$END
     tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
$MESH
     nxcelt    = 15,
       px(1)   =    .0,  nxcell(1) =  15,
       px(2)   = 14.6,

     nycelt    = 1,
       py(1)=0.0,  nycell(1)=1,
       py(2)=1.,

    nzcelt     = 22,
       pz(1)   =  0. ,   nzcell(1)   = 22,
       pz(2)   = 21.6,
$END

Power is corrected to have the same output with the new geometry. Volume of the obstacle was
.437 m3 in run 25, now the volume
is 1 m3. Now that I think about it, it does not matter as long as the room is the right size
$OBS
   nobs=1,
   iob(1) = 1, ioh(1) = 1, xl(1) =  13.6 , xh(1) =  14.6,
                           yl(1) =   0.  , yh(1) =  1.0,
                           zl(1) =   0.  , zh(1)=   1.0,
                           kobs(1) = 0.696,
                           rcobs(1) = 234.46,
                           pobs(1,1) =436.12,
                           twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                           tobs(1)  =0.,


$END

Next defaults to all compressible fluid when icmprs=1.

$FL

     remark = 'setting 1atm in Pa',
     presi  = 101325.0,
     pvoid  = 101325.0,
     ui     = 0. ,
$END

$BF
$END

$TEMP

     remark = 'setting initial temps to 25C to get things started',
     tempi = 300.0,

$END
```

```
$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*****************************************************************************************
**********
flatplate28: Room only, long timescale run, compressible, rwall

18 Aug  2005 flatplate28  Added RWALL to boundary conditions to see if we stop leaking heat
outside.This run stopped early, I
                          do not remember why. RWALL did work to stop the heat leakage
18 Aug  2005 flatplate27  Compressible run. Explicit coupling (imp=0) kills the run. Changed
iadiz to 0. Lots of pressure iteration
                          failures, but stabilizes after 26000 secs. The temperature in the room
stabilizes after one day or so. I
                          guess I have leaks of heat through the boundaries, let's correct that.
17 Aug  2005 flatplate26  How fast does the temperature rise in the room for very long times? I
changed the orientation to z being
                          vertical! Not solving for obstacle conduction. The run dies after two
days, I guess I need to treat
                          the air as compressible ...
15 Aug  2005 flatplate25  Added the room to justify boundary condition in pressure
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
```

```
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 2,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 1,    remark = '=0 explicit press-vel incompatible  with incompress, =1 implicit
coupling, =2 ADI',
```

```
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 1,    remark = '0=inccmpr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = -9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 1,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 1,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  43200., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 2592000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,    remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
```

```
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',

      rhof2    = 1.225,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 713.  ,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      rf2     = 287.   , remark = 'Gas constant for air',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

  Only the room will be here

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 1,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 2,  remark = 'high z, continuative',

      fbc(1)=1.,fbc(2)=1.,fbc(3)=1.,fbc(4)=1.,fbc(5)=1.,fbc(6)=1., remark='fluid 2 boundary
condition',
      rwall(1)=0.,rwall(2)=0.,rwall(3)=0.,rwall(4)=0.,rwall(5)=0.,rwall(6)=0., remark='No heat
transfer boundary condition',


  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 15,
        px(1)   =    .0,  nxcell(1) =  15,
        px(2)   = 14.6,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 22,
        pz(1)   =  0. ,   nzcell(1)   = 22,
        pz(2)   = 21.6,
  $END

  Power is corrected to have the same output with the new geometry. Volume of the obstacle was
.437 m3 in run 25, now the volume
  is 1 m3. Now that I think about it, it does not matter as long as the room is the right size
  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =  13.6 , xh(1) =  14.6,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =   0.  , zh(1)=   1.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END

  Next defaults to all compressible fluid when icmprs=1.
```

```
$FL

    remark = 'setting latm in Pa',
    presi  = 101325.0,
    pvoid  = 101325.0,
    ui     = 0. ,
$END

$BF
$END

$TEMP

    remark = 'setting initial temps to 25C to get things started',
    tempi = 300.0,

$END

$GRAFIC

    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END


$PARTS
$END
!*************************************************************************************************
**********
!*************************************************************************************************
**********
flatplate30: Cv check, natural convection,tobs 600K, rhocp right

18 Aug  2005 flatplate30  Pavan just realized that Rhocp for the assembly is wrong. It looks like
Mary Ann only implemented
                          the Cp and not the product. Changed to implicit viscous solution by
code recommendation.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
```

Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compressibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
```

```
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 1,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END
```

```
$PROPS

    remark  = 'set up properties on fluid 2 to allow for compressibility option',

    units   = 'si',
    rhof    = 1.225,
    mul     = 1.86e-5, remark = 'viscosity air',
    cvl     = 713.  ,  remark = 'specific heat air',
    thcl    = 0.0264,  remark = 'thermal conductivity air',
    thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
    tstar   = 293.15,  remark = 'ref temp for air properties',
$END


$SCALAR
    remark = 'none needed for these simulations',
$END

    Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
    we have the full length so P=792/4=198 W.
$BCDATA

    wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
    wr     = 2,  remark = 'high x',
    wf     = 1,  remark = 'low y',
    wbk    = 1,  remark = 'high y',
    wb     = 1,  remark = 'low z',
    wt     = 1,  remark = 'high z, continuative',

    pbc(1) = 101280.,
    tbc(1) = 300.,

$END
    tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
$MESH
    nxcelt   = 150,
      px(1)  =  0.0,  nxcell(1) =  50,
      px(2)  =  1.0,  nxcell(2) =  25,
      px(3)  =  2.0,  nxcell(3) =  25,
      px(4)  =  3.0,  nxcell(4) =  50,
       px(5)  =  4.50 ,

    nycelt   = 1,
      py(1)=0.0,  nycell(1)=1,
      py(2)=1.,

   nzcelt    = 20,
      pz(1)  = -0.1135,nzcell(1)  =  7,
      pz(2)  =  0.0,   nzcell(2)  = 13,
      pz(3)  = .03,
$END

$OBS
   nobs=1,
   iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                           yl(1) =   0.  , yh(1) =  1.0,
                           zl(1) =  -.1135,zh(1)=  0.0,
                           kobs(1) = 0.696,
                           rcobs(1) = 2568743.8, remark=' Mary Ann had 234.46, but density
U=10956 and Cp=234.46, according to her notebook',
                           pobs(1,1) =436.12,
                           twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                           tobs(1)  =0.,


$END
```

```
    iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                               yl(31) =  0.5842000, yh(31) =  0.8137525,
                               zl(31) =  0.3052800, zh(31) =  4.1651200,
                               kobs(10) = 0.696,
                               rcobs(10) = 234.46,
                               pobs(1,10) = 792,


  $FL

      remark = 'setting latm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
*********
flatplate31: Cv check, natural convection,tobs 600K, rhocp right,coarse

18 Aug  2005 flatplate31  Since there is not a lot of time let's divide the mesh by two. The
final temperature is 600K, like the
                          initial temperature, I am suspicious now ... Let's do a run with a
different initial temp.
18 Aug  2005 flatplate30  Pavan just realized that Rhocp for the assembly is wrong. It looks like
Mary Ann only implemented
                          the Cp and not the product. Changed to implicit viscous solution by
code recommendation.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
```

25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
$XPUT
 remark  = ' Advection Options',
```

```
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 1,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
```

```
      itmax   =  1000,       remark = 'max press iter per time step',
      itdtmx  =  100,      remark = ' max # of press iterations before time step reduced',
      idtht   =  20,       remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,       remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,     remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 74,
        px(1)  =  0.0,  nxcell(1) =  25,
        px(2)  =  1.0,  nxcell(2) =  12,
        px(3)  =  2.0,  nxcell(3) =  12,
        px(4)  =  3.0,  nxcell(4) =  25,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  4,
        pz(2)  =  0.0,   nzcell(2)  =  7,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
```

```
                              kobs(1) = 0.696,
                              rcobs(1) = 2568743.8, remark=' Mary Ann had 234.46, but density
U=10956 and Cp=234.46, according to her notebook',
                              pobs(1,1) =436.12,
                              twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                              tobs(1)  =0.,


  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate32: Cv check, natural convection,tobs 600K, RhoCp*10

19 Aug  2005 flatplate32  Study of the influence of RhoCP product here *10
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
```

let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.

24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END
```

```
  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
```

```
    nobs=1,
    iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                            yl(1) =   0.  , yh(1) =  1.0,
                            zl(1) =  -.1135,zh(1)=  0.0,
                            kobs(1) = 0.696,
                            rcobs(1) = 2344.6, remark='multiplied by 10 from original',
                            pobs(1,1) =436.12,
                            twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                            tobs(1)  =0.,


  $END

    iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                               yl(31) =  0.5842000, yh(31) =  0.8137525,
                               zl(31) =  0.3052800, zh(31) =  4.1651200,
                               kobs(10) = 0.696,
                               rcobs(10) = 234.46,
                               pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate33: Cv check, natural convection,tobs 600K, RhoCp*10, implicit viscosity

19 Aug  2005 flatplate33  Using implicit viscosity to compare.No clear advantage, I stop it.
19 Aug  2005 flatplate32  Study of the influence of RhoCP product here *10
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
```

01 Augu 2005 flatplate16 Steady state happens at around 200 secs, with the max temperature being 415 K. Let's run a coarse mesh
and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I restart this guy from zero and
let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not

```
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 1,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',
```

```
   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
```

```
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 2344.6, remark='multiplied by 10 from original',
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate34: Cv check, natural convection,tobs 600K, RhoCp/10

19 Aug  2005 flatplate34  Now we divide RhoCp by 10 ...
19 Aug  2005 flatplate32  Study of the influence of RhoCP product here *10
```

03 Aug 2005 flatplate19 Quick check changing Cv for air since Mary Ann's value seems to be wrong.
02 Aug 2005 flatplate17 Let's say that the initial obstacle temperature is 600K and see what happens ... It reaches steady state
faster than the cold guy, but the final temperature is the same, as hoped ...
01 Augu 2005 flatplate16 Steady state happens at around 200 secs, with the max temperature being 415 K. Let's run a coarse mesh
and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I restart this guy from zero and
let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!

```
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',
```

```
   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
       px(1)  =  0.0,  nxcell(1) =  50,
       px(2)  =  1.0,  nxcell(2) =  25,
       px(3)  =  2.0,  nxcell(3) =  25,
       px(4)  =  3.0,  nxcell(4) =  50,
        px(5)  =  4.50 ,
```

```
     nycelt    = 1,
       py(1)=0.0,  nycell(1)=1,
       py(2)=1.,

    nzcelt     = 20,
       pz(1)   = -0.1135,nzcell(1)   =  7,
       pz(2)   =  0.0,   nzcell(2)   = 13,
       pz(3)   = .03,
 $END

 $OBS
    nobs=1,
    iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                            yl(1) =   0.  , yh(1) =  1.0,
                            zl(1) =  -.1135,zh(1)=  0.0,
                            kobs(1) = 0.696,
                            rcobs(1) = 23.446, remark='divided by 10 from original',
                            pobs(1,1) =436.12,
                            twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                            tobs(1)  =0.,


 $END

    iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                               yl(31) =  0.5842000, yh(31) =  0.8137525,
                               zl(31) =  0.3052800, zh(31) =  4.1651200,
                               kobs(10) = 0.696,
                               rcobs(10) = 234.46,
                               pobs(1,10) = 792,


 $FL

     remark = 'setting 1atm in Pa',
     presi  = 101325.0,
     pvoid  = 101325.0,
     ui     = 0. ,
 $END

 $BF
 $END

 $TEMP

     remark = 'setting initial temps to 25C to get things started',
     tempi = 300.0,

 $END

 $GRAFIC

     icolor = 2,

     remark = 'jobsbk = 10,  jobsf = 14,',

     ncplts = 4,
     contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
     contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
     contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
     contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

 $END


 $PARTS
 $END
```

```
!*****************************************************************************************
**********
flatplate35: Cv check, natural convection,tobs 600K, RhoCp*10

22 Aug  2005 flatplate35  For some unknown reason I stopped run 32. Let's restart here.
19 Aug  2005 flatplate32  Study of the influence of RhoCP product here *10
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
```

```
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
```

```
      hpltdt   =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,     remark=' =0 SOR, =1 ADI',
      iadiy   = 0,     remark=' =0 SOR, =1 ADI',
      iadiz   = 1,     remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
```

```
     nxcelt    = 150,
       px(1)   =  0.0,  nxcell(1) =  50,
       px(2)   =  1.0,  nxcell(2) =  25,
       px(3)   =  2.0,  nxcell(3) =  25,
       px(4)   =  3.0,  nxcell(4) =  50,
        px(5)  =  4.50 ,

     nycelt    = 1,
       py(1)=0.0,  nycell(1)=1,
       py(2)=1.,

    nzcelt     = 20,
       pz(1)   = -0.1135,nzcell(1)  =  7,
       pz(2)   =  0.0,   nzcell(2)  = 13,
       pz(3)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 2344.6, remark='multiplied by 10 from original',
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,
```

```
  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate36: k check, using Helium

22 Aug  2005 flatplate36  Pavan wants to be on the safe side and run with k=.2223 W/m/K. The
logic behind it is that k for He is
                          0.129 in English units which is the element with the lowest
conductivity in the system. k can be found
                          in Holtec FSAR 4.2.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
```

```
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
```

```
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',
```

```
      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1. xl(1) =   0.35. xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.223, remark='Helium conductivity, conservative',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',
```

```
      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate37: k check, using Holtec table

22 Aug  2005 flatplate37  We do not know why we are using k=0.696 W/m/s for the assembly. Let's
try the number found in Holtec,
                          table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in
SI. Final max temp. 497 K.
22 Aug  2005 flatplate36  Pavan wants to be on the safe side and run with k=.2223 W/m/K. The
logic behind it is that k for He is
                          0.129 in English units which is the element with the lowest
conductivity in the system. k can be found
                          in Holtec FSAR 4.2. Final temperature 522 K.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
```

```
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
                          more realistic dimensions. So summarizing: 1) long field, 2) Constant
Temp bound, 3) Symmetry in z.
                          The run is going very slow,probably because of the pressure iteration
stuff (I am using 100000, and never
                          getting the pressure iteration convergence problem). Let's limit it to
300 as Pavan's brother suggests.
                          Maybe the pressure iteration problems come from not having initial
hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03  Now let's try natural convection with gravity along x-axis. The fluid
is initially at rest. Steady state
                          is very fast. I see again the boundary layer. I need a very high number
of pressure iterations to converge.
                          It takes only around 1 s for steady.
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',
```

```
   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

```
     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
        px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.476, remark='Holtec value, table 4.4.5',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END
```

```
  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate38: Added features to 2-D

29 Sep  2005 flatplate38  Pavan thinks we should add the Alloy X and Boral sheets that sourround
the assembly. Also we need to
                          change the air gap to accomodate both materials. Changed to implicit
viscous calculation. Temperature
                          on the order of thousands ... I erase the results ...
22 Aug  2005 flatplate37  We do not know why we are using k=0.696 W/m/s for the assembly. Let's
try the number found in Holtec,
                          table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in
SI. Final max temp. 497 K.
22 Aug  2005 flatplate36  Pavan wants to be on the safe side and run with k=.2223 W/m/K. The
logic behind it is that k for He is
                          0.129 in English units which is the element with the lowest
conductivity in the system. k can be found
                          in Holtec FSAR 4.2. Final temperature 522 K.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
```

14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
```

```
      ihtc     = 2,     remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,     remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,     remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 1,     remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,     remark = '0=incompr., 1=compressible flow',
      itb     = 0,     remark = 'no free surfaces',
      nmat    = 1,     remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,     remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,     remark = ' mentor help',
      istdy   = 0,     remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,    remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,     remark = '=0 turn off wall shear',
      ifvis   = 0,     remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,     remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,     remark=' =0 SOR, =1 ADI',
      iadiy   = 0,     remark=' =0 SOR, =1 ADI',
      iadiz   = 1,     remark=' =0 SOR, =1 ADI',
      omega   = 1.7,   remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS
```

```
      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mul     = 1.86e-5, remark = 'viscosity air',
      cvl     = 713.  ,  remark = 'specific heat air',
      thcl    = 0.0264,  remark = 'thermal conductivity air',
      thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 28,
        pz(1)  = -0.1233     ,nzcell(1)  =  7,
        pz(2)  = -0.0098425 ,nzcell(2)  =  4,
        pz(3)  =  0.0        ,nzcell(3)  = 10,
        pz(4)  =   .0153797 ,
  $END

  $OBS
     nobs=2,

     remark = ' Assembly',
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1233,zh(1)=  -0.0098425,
                             kobs(1) = 0.16931, remark='Pavans value effective conductivity using
parallel formula',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,

     remark = ' Alloy X plate and Boral',
     iob(2) = 2, ioh(2) = 1, xl(2) =   0.35, xh(2) =  4.20,
```

```
                              yl(2) =   0.  , yh(2) =  1.0,
                              zl(2) =  -0.0098425, zh(2) =  0.,
                              kobs(2) = 11.02238, remark=' Pavan calculated this number',
                              rcobs(2) = 234.46,
                              twobs(1,2) = 600.,   remark=' this is the initial temperature of the
obstacle',


  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate39: Turbulence check, Prandtl.

03 Oct  2005 flatplate39  One of the concerns of the reviewers is the turbulence model. My
thought is that turbulence is not going
                          to make any difference, but let's prove it. Quasi-steady solution at
503 K. Only 6 K difference with the
                          laminar guy, I do not think we should continue with turbulence ...
22 Aug  2005 flatplate37  We do not know why we are using k=0.696 W/m/s for the assembly. Let's
try the number found in Holtec,
                          table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in
SI. Final max temp. 497 K.
22 Aug  2005 flatplate36  Pavan wants to be on the safe side and run with k=.2223 W/m/K. The
logic behind it is that k for He is
                          0.129 in English units which is the element with the lowest
conductivity in the system. k can be found
                          in Holtec FSAR 4.2. Final temperature 522 K.
```

03 Aug 2005 flatplate19 Quick check changing Cv for air since Mary Ann's value seems to be wrong.
02 Aug 2005 flatplate17 Let's say that the initial obstacle temperature is 600K and see what happens ... It reaches steady state
faster than the cold guy, but the final temperature is the same, as hoped ...
01 Augu 2005 flatplate16 Steady state happens at around 200 secs, with the max temperature being 415 K. Let's run a coarse mesh
and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I restart this guy from zero and
let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow, probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!

```
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 1,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',
```

```
   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,
```

```
     nycelt    = 1,
       py(1)=0.0,  nycell(1)=1,
       py(2)=1.,

    nzcelt     = 20,
       pz(1)   = -0.1135,nzcell(1)   =  7,
       pz(2)   =  0.0,   nzcell(2)   = 13,
       pz(3)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.476, remark='Holtec value, table 4.4.5',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1. xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
```

```
!*****************************************************************************************
**********
flatplate40: Turbulence check, two eqs. k-e

03 Oct  2005 flatplate40  Trying now the k-e model. Flow 3-D manual states that turbulence models
assume high turbulence in the flow.
                          Clearly this does not look the case in our problem, hopefully we do not
see a big difference ...
                          k-e is hundreds of times more slow, impossible to use if we want to
apply it to 3-D
03 Oct  2005 flatplate39  One of the concerns of the reviewers is the turbulence model. My
thought is that turbulence is not going
                          to make any difference, but let's prove it.
22 Aug  2005 flatplate37  We do not know why we are using k=0.696 W/m/s for the assembly. Let's
try the number found in Holtec,
                          table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in
SI. Final max temp. 497 K.
22 Aug  2005 flatplate36  Pavan wants to be on the safe side and run with k=.2223 W/m/K. The
logic behind it is that k for He is
                          0.129 in English units which is the element with the lowest
conductivity in the system. k can be found
                          in Holtec FSAR 4.2. Final temperature 522 K.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens  .. It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04  Ok, I think that even with the pressure iteration complaints this is
working fine. Although it is slow.
12 July 2005 flatplate04  According to Flow3D manual press iteration problems arise if reversing
flows and are not important if the
                          residue and the convergence criterior are close. The flow does reverse
in this problem at the bottom.
                          And residues are not far from the convergence criterion.
                          Back to iadix=0 and large iterations (1000). 14 hours to complete the
run. Very long!
12 July 2005 flatplate04  Hydrostatic distribution does not help with pressure iterations, but I
think it is a nice idea.
                          Nevertheless the results looks very nice with the center of the gap
with negative velocity and convection
                          happening on the wall. Let's restart it to see if we get rid of press
iteration problems. Nope.
                          Now trying iadi.
11 July 2005 flatplate04  Natural convection was working great for a constant temperature wall.
Let's use now a constant power
                          wall with similar dimensions to the ones in the reactor. Afterwards
let's incorporate the gap. First
```

more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',
```

```
   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 3,    remark = 'Turbulence model:=0 local viscos, =1 Prandtl, =2 turb energ, 3=
k-eps, 4=RNG, =-1 large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA
```

```
      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 150,
        px(1)   =  0.0,  nxcell(1) =  50,
        px(2)   =  1.0,  nxcell(2) =  25,
        px(3)   =  2.0,  nxcell(3) =  25,
        px(4)   =  3.0,  nxcell(4) =  50,
         px(5)   =  4.50 ,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

      nzcelt    = 20,
        pz(1)   = -0.1135,nzcell(1)   =  7
        pz(2)   =  0.0,   nzcell(2)   = 13,
        pz(3)   = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.476, remark='Holtec value, table 4.4.5',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,
```

```
  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*********************************************************************************************
**********
flatplate41: Turbulence check, RNG

03 Oct  2005 flatplate41  Now trying RNG. Died because of time step.Conclusion today: The only
turbulence model that seems to work
                          is the Prandtl mixing length. Why the others do not work? May be
because of using incompressible?
03 Oct  2005 flatplate39  One of the concerns of the reviewers is the turbulence model. My
thought is that turbulence is not going
                          to make any difference, but let's prove it. Quasi-steady solution at
503 K. Only 6 K difference with the
                          laminar guy, I do not think we should continue with turbulence ...
22 Aug  2005 flatplate37  We do not know why we are using k=0.696 W/m/s for the assembly. Let's
try the number found in Holtec,
                          table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in
SI. Final max temp. 497 K.
22 Aug  2005 flatplate36  Pavan wants to be on the safe side and run with k=.2223 W/m/K. The
logic behind it is that k for He is
                          0.129 in English units which is the element with the lowest
conductivity in the system. k can be found
                          in Holtec FSAR 4.2. Final temperature 522 K.
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
                          let it run up to 1000 s.
26 July 2005 flatplate15  I rerun it, did not realize that I chose symmetry on the lower boundary
so power should be divided
                          by two. Added air gap at extremes
25 July 2005 flatplate15  Runs 08 thru 13 have been a success. Let's now solve conduction +
convection problem. So we add the
                          nuclear reactor with it's power as an obstacle and see what happens.
Temperature in this run rises
                          up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07  Let's reduce the size of the problem so it runs faster. Then let's
compare the following results:
                          1) discharge with differente bndry conditions 2) discharge to open
space
14 July 2005 flatplate06  I think a pressure boundary condition in the upper part (x=0) is more
realistic as far as the cask goes.
                          Will it be a big problem? It does not look like a problem, but let's do
a more realistic condition.
14 July 2005 flatplate05  Let's see if with implicit heat transfer it goes faster.
```

14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.
24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 1,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
```

```
      ihtc     = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 0,    remark = '=0 explicit press-vel incomp with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 0,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 0,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 4,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  10., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 1,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS
```

```
      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl     = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr     = 2,  remark = 'high x',
      wf     = 1,  remark = 'low y',
      wbk    = 1,  remark = 'high y',
      wb     = 1,  remark = 'low z',
      wt     = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.476, remark='Holtec value, table 4.4.5',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
```

```
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting 1atm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,

      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*****************************************************************************************
**********
flatplate42: Room only, long timescale run, compressible, rwall

04 Oct  2005 flatplate42  Let's redo this run trying to get to the end (30 days).
18 Aug  2005 flatplate28  Added RWALL to boundary conditions to see if we stop leaking heat
outside.This run stopped early, I
                          do not remember why. RWALL did work to stop the heat leakage
18 Aug  2005 flatplate27  Compressible run. Explicit coupling (imp=0) kills the run. Changed
iadiz to 0. Lots of pressure iteration
                          failures, but stabilizes after 26000 secs. The temperature in the room
stabilizes after one day or so. I
                          guess I have leaks of heat through the boundaries, let's correct that.
17 Aug  2005 flatplate26  How fast does the temperature rise in the room for very long times? I
changed the orientation to z being
                          vertical! Not solving for obstacle conduction. The run dies after two
days, I guess I need to treat
                          the air as compressible ...
15 Aug  2005 flatplate25  Added the room to justify boundary condition in pressure
03 Aug  2005 flatplate19  Quick check changing Cv for air since Mary Ann's value seems to be
wrong.
02 Aug  2005 flatplate17  Let's say that the initial obstacle temperature is 600K and see what
happens ... It reaches steady state
                          faster than the cold guy, but the final temperature is the same, as
hoped ...
01 Augu 2005 flatplate16  Steady state happens at around 200 secs, with the max temperature being
415 K. Let's run a coarse mesh
                          and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I
restart this guy from zero and
```

let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations. but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not
need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,
but in the fluid that does not happen. Let's stay now with low resolution to play with it.
01 July 2005 pav02 Inherited from Pavan, steady state accelerator.
Goal is estimate the thermal contribution of one reactor.

24 June 2005

```
  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 2,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 1,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 1,    remark = '=0 explicit press-vel incompatible  with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 1,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gz      = -9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 1,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 1,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',

   remark  = ' Plot output',
      pltdt   =  43200., remark = 'plotting interval, seconds',
      hpltdt  =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin   = 2592000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix   = 0,    remark=' =0 SOR, =1 ADI',
      iadiy   = 0,    remark=' =0 SOR, =1 ADI',
      iadiz   = 0,    remark=' =0 SOR, =1 ADI',
      omega   = 1.7,  remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt    =  1.0e-5, remark = 'initial time step, seconds',
      dtmax   =  100.,   remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',

  $END
```

```
  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  10,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',

      rhof2    = 1.225,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 713.  ,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      rf2     = 287.   , remark = 'Gas constant for air',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

  Only the room will be here

  $BCDATA

      wl      = 2,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 1,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 2,  remark = 'low z',
      wt      = 2,  remark = 'high z, continuative',

      fbc(1)=1.,fbc(2)=1.,fbc(3)=1.,fbc(4)=1.,fbc(5)=1.,fbc(6)=1., remark='fluid 2 boundary
condition',
      rwall(1)=0.,rwall(2)=0.,rwall(3)=0.,rwall(4)=0.,rwall(5)=0.,rwall(6)=0., remark='No heat
transfer boundary condition',


  $END
      tbcd    = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt    = 15,
        px(1)   =    .0,  nxcell(1) =  15,
        px(2)   = 14.6,

      nycelt    = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt     = 22,
```

```
      pz(1)  =  0. ,   nzcell(1)  = 22,
      pz(2)  = 21.6,
  $END

  Power is corrected to have the same output with the new geometry. Volume of the obstacle was
.437 m3 in run 25, now the volume
  is 1 m3. Now that I think about it, it does not matter as long as the room is the right size
  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =  13.6 , xh(1) =  14.6,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =   0.  , zh(1)=   1.0,
                             kobs(1) = 0.696,
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,


  $END

  Next defaults to all compressible fluid when icmprs=1.

  $FL

     remark = 'setting 1atm in Pa',
     presi  = 101325.0,
     pvoid  = 101325.0,
     ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

     remark = 'setting initial temps to 25C to get things started',
     tempi = 300.0,

  $END

  $GRAFIC

     icolor = 2,

     remark = 'jobsbk = 10,  jobsf = 14,',

     ncplts = 4,
     contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
     contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
     contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
     contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
!*************************************************************************************************
**********
flatplate43: Assembly and air gap, compressible

04 Oct  2005 flatplate43  Now we want a run with assembly and air gap, but with compressible air.
I noticed there is heat transfer
                          at the bottom of the cask, I need to correct that! 5 seconds of run
needed 30 minutes in compressible
                          mode, while 10 seconds of run needed 2 minutes in incompressible mode.
So compressible is 30 times slower
                          than incompressible, clearly not affordable for the 3-D. Remember
steady state accelerator is on.
```

22 Aug 2005 flatplate37 We do not know why we are using k=0.696 W/m/s for the assembly. Let's try the number found in Holtec,
table 4.4.5 at 450 deg F which is 0.275 in English or 0.476 W/m/K in SI. Final max temp. 497 K.
22 Aug 2005 flatplate36 Pavan wants to be on the safe side and run with k=.2223 W/m/K. The logic behind it is that k for He is
0.129 in English units which is the element with the lowest conductivity in the system. k can be found
in Holtec FSAR 4.2. Final temperature 522 K.
03 Aug 2005 flatplate19 Quick check changing Cv for air since Mary Ann's value seems to be wrong.
02 Aug 2005 flatplate17 Let's say that the initial obstacle temperature is 600K and see what happens ... It reaches steady state
faster than the cold guy, but the final temperature is the same, as hoped ...
01 Augu 2005 flatplate16 Steady state happens at around 200 secs, with the max temperature being 415 K. Let's run a coarse mesh
and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I restart this guy from zero and
let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.
12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.

```
10 July 2005 flatplate02  Incompressible, conduction only works fine, but time scale is enormous,
1e6 for 1 meter, let's reduce
                          the size of the field. For a 1 cm height mesh it works fine with heat
transfer only. Timescale to steady
                          state around 400 s. I added slow velocity (high vel kills the time
step) and I see the boundary layer
                          developing and heat transfer happening from the boundary. Steady state
decreased to 2 s with the velocity!!
                          Also the characteristic distance where T drops from 350 to 329 is very
small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01  Trying to reproduce book analytical data
05 July 2005 pav04        Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03        Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I
also think that we do not
                          need compresibility, but right now let's only care about the mesh. The
result in the obstacle is the same,
                          but in the fluid that does not happen. Let's stay now with low
resolution to play with it.
01 July 2005 pav02        Inherited from Pavan, steady state accelerator.
                          Goal is estimate the thermal contribution of one reactor.
24 June 2005

  $XPUT
   remark  = ' Advection Options',
      ifenrg  = 2,    remark = 'solve internal energy',
      ifrho   = 2,    remark = '=0 const dens, =1 density function of T, =2 solve transport, =3
second order',
      iorder  = 1,    remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

   remark  = ' Convergence Criteria',
      epsadj  =  1.0, remark = 'multiplier for pressure iteration',
      epshtc  =  1.0, remark = 'multiplier for temp iteration',

   remark  = ' Heat Transfer Options',
      ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in
obstacles only',
      ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve
obs conduction',

   remark  = ' Explicit/Implicit Options',
      imphtc  = 1,    remark = '=0 explicit eval of temp, =1 fully implicit',
      imp     = 1,    remark = '=0 explicit press-vel incompatible  with incompress, =1 implicit
coupling, =2 ADI',
      impvis  = 0,    remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

   remark  = ' Flow mode options',
      icmprs  = 1,    remark = '0=incompr., 1=compressible flow',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',

   remark  = ' Gravity',
      gx      = 9.81, remark = 'gravity -9,81',

   remark  = ' Initialization and Restart',
      ipdis   = 2,    remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x
direct, =3 y direct',
      trest   = 0.0  ,remark = ' restart time',

   remark  = ' Numerical options',
      ihelp   = 1,    remark = ' mentor help',
      istdy   = 1,    remark = ' =0 normal transients, =1 steady state accelerator for compress
flow',
      omeght  = 2.,   remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

   remark  = ' Physical model options',
      iwsh    = 1,    remark = '=0 turn off wall shear',
      ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
      ivish   = 0,    remark = ' no viscous heating, =1 include visc heat',
```

```
   remark  = ' Plot output',
      pltdt    =  10., remark = 'plotting interval, seconds',
      hpltdt   =  100000.,remark = 'history interval, seconds',


   remark  = ' Termination Control',
      twfin    = 1000.0,  remark = 'simulation end, seconds',

   remark  = ' Pressure interation options',
      iadix    = 0,     remark=' =0 SOR, =1 ADI',
      iadiy    = 0,     remark=' =0 SOR, =1 ADI',
      iadiz    = 1,     remark=' =0 SOR, =1 ADI',
      omega    = 1.7,   remark = 'default setting for over-relaxation factor',

   remark  = ' Time Step Control',
      delt     =  1.0e-5, remark = 'initial time step, seconds',
      dtmax    =  100.,   remark = 'maximum timestep',
      autot    =  2.0, remark = 'timestep by stability',

  $END

  $LIMITS

      itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
      itmax   =  1000,      remark = 'max press iter per time step',
      itdtmx  =  100,     remark = ' max # of press iterations before time step reduced',
      idtht   =  20,      remark = ' max # of temp iter before dt reduced',
      ithtmx  =  50,      remark = ' only when implicit heat transf., max # of temp iter per
cycle',

      negtmx  =  100000,  remark = 'negative rhoe resets',
      ncflmx  =  1000,    remark = 'convection failures allowed',

  $END

  $PROPS

      remark  = 'set up properties on fluid 2 to allow for compressibility option',

      units   = 'si',
      rhof    = 1.225,
      mu1     = 1.86e-5, remark = 'viscosity air',
      cv1     = 713.  ,  remark = 'specific heat air',
      thc1    = 0.0264,  remark = 'thermal conductivity air',
      thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      tstar   = 293.15,  remark = 'ref temp for air properties',

      rhof2    = 1.225,
      mu2     = 1.86e-5, remark = 'viscosity air',
      cv2     = 713.  ,  remark = 'specific heat air',
      thc2    = 0.0264,  remark = 'thermal conductivity air',
      thexf2  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
      rf2     = 287.   , remark = 'Gas constant for air',
  $END


  $SCALAR
      remark = 'none needed for these simulations',
  $END

     Release of power in Mary Ann's code is 792 W for a 3.86 m long power generator. So 205 W per
meter per face. In this example
     we have the full length so P=792/4=198 W.
  $BCDATA

      wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
      wr      = 2,  remark = 'high x',
      wf      = 1,  remark = 'low y',
      wbk     = 1,  remark = 'high y',
      wb      = 1,  remark = 'low z',
```

```
      wt      = 1,  remark = 'high z, continuative',

      pbc(1) = 101280.,
      tbc(1) = 300.,

  $END
      tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
  $MESH
      nxcelt   = 150,
        px(1)  =  0.0,  nxcell(1) =  50,
        px(2)  =  1.0,  nxcell(2) =  25,
        px(3)  =  2.0,  nxcell(3) =  25,
        px(4)  =  3.0,  nxcell(4) =  50,
         px(5)  =  4.50 ,

      nycelt   = 1,
        py(1)=0.0,  nycell(1)=1,
        py(2)=1.,

     nzcelt    = 20,
        pz(1)  = -0.1135,nzcell(1)  =  7,
        pz(2)  =  0.0,   nzcell(2)  = 13,
        pz(3)  = .03,
  $END

  $OBS
     nobs=1,
     iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                             yl(1) =   0.  , yh(1) =  1.0,
                             zl(1) =  -.1135,zh(1)=  0.0,
                             kobs(1) = 0.476, remark='Holtec value, table 4.4.5',
                             rcobs(1) = 234.46,
                             pobs(1,1) =436.12,
                             twobs(1,1) = 600.,   remark=' this is the initial temperature of the
obstacle',
                             tobs(1)  =0.,



  $END

     iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                                yl(31) =  0.5842000, yh(31) =  0.8137525,
                                zl(31) =  0.3052800, zh(31) =  4.1651200,
                                kobs(10) = 0.696,
                                rcobs(10) = 234.46,
                                pobs(1,10) = 792,


  $FL

      remark = 'setting latm in Pa',
      presi  = 101325.0,
      pvoid  = 101325.0,
      ui     = 0. ,
  $END

  $BF
  $END

  $TEMP

      remark = 'setting initial temps to 25C to get things started',
      tempi = 300.0,

  $END

  $GRAFIC

      icolor = 2,
```

```
      remark = 'jobsbk = 10,  jobsf = 14,',

      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

  $END


  $PARTS
  $END
```

3DModelquart

```
Development of Hi-Star 100 cask with 24 Basket
16 August  2005 Changing fluid propoeties and boundary condition.
03 August 2005  Changing the Cv= 713.50 J/Kg/K for air and settimg the power obstacle
                initial temperature to 600 K.
22 July 2005    nmat is set equal to 1, pressure at the top of the cask is 101254.368 Pa.
                Hydrostatic pressure in z direction.
05 July 2005    Default value of gas constant R was in wrong units. Corrected here.

20 June 2005
Updated informational fields

24 May 2005
Turning off air flow and allowing thermal progression only

11 May 2005  Chris Ryder asked that I look at the 24 Basket with different fuel.
Resetting obstacle field with this basket and fuel source.  Basic parameters will be
the same.  Grid will need to be slightly reworked to accomodate new fuel spacing.

  $XPUT

      icmprs  = 0,    remark = 'incompressible flow',
      iorder  = 3,    remark = 'setting iorder = 3 monotonically increasing',
      itb     = 0,    remark = 'no free surfaces',
      nmat    = 1,    remark = '1 compressible mat',
      iwsh    = 0,    remark = 'turn off wall shear',

      remark = 'switch to remark out when flow on',
      remark = 'ihonly = 0',     remark = 'solve all conservation equations',
      remark = 'ihonly = 2',     remark = 'turn off material flow, heat transfer only',
      imphtc = 1,     remark = 'implicit eval of temp terms',
      remark = 'ihtc   = 0',     remark = 'turn off heat transfer',
      ihtc   = 2,     remark = 'turn on heat conduction through obstacles',
      ifrho  = 1,
      ifenrg = 2,     remark = 'fluid energy transport on',
      gz = -9.81,     remark = 'gravity',

      remark='trest   =  6.023',
      twfin   =  1000.0,  remark = 'simulation end, seconds',
      pltdt   =  1.0,   remark = 'plotting interval, seconds',
      hpltdt  =  1.0,    remark = 'history interval, seconds',
      delt    =  1.0e-5, remark = 'time step, seconds',
      remark = 'istdy   =  0',      remark = 'accelerate to steady state using non-phys
transient',
                        remark = 'minimum timestep',
      dtmax   =  0.01,    remark = 'maximum timestep',

      autot   =  2.0, remark = 'timestep by stability',
      omega   =  1.7, remark = 'default setting for over-relaxation factor',

      epsadj  =  1.0, remark = 'standard convergence criterion',

      igmres = 1,
```

```
    remark = 'iadix   =  1',   remark = 'pressure iteration options (x,y,z) ADI',
    remark = 'iadiy   =  1',
    remark = 'iadiz   =  1',
    ihelp = 2,
    ifrho  = 1,
    ifvelp = 0,
    ipdis  = 1, remark='hydrostatic pressure in z direction',

$END

$LIMITS

    itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
    itmax   =  10,    remark = 'allowable inner iteration count',
    itdtmx  =  100,
                        remark = 'adjust itmax early to quickly step through start-up',
    negtmx  =  100000,  remark = 'negative rhoe resets',
    ncflmx  =  1000,    remark = 'convection failures allowed',

$END

$PROPS

    remark  = 'set up properties on fluid 2 to allow for compressibility option',

    units   = 'si',
    rhof    = 1.225,
    mul     = 1.86e-5, remark = 'viscosity air',
    cvl     = 713.0,  remark = 'specific heat air',
    thcl    = 0.0264,  remark = 'thermal conductivity air',
    thexfl  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
    tstar   = 293.15,  remark = 'ref temp for air properties',
    remark  = 'rf2     = 287.',    remark = 'gas constant for air'

$END

$SCALAR
    remark = 'none needed for these simulations',
$END

$BCDATA

    remark = 'top wall is continuative (wt) or boundary 6',
    remark = 'set up as no ventilation',
    remark = 'made all bc continuative to start so cask is set in infinite air',

    wl     = 1,    remark = 'low x, symmetric',
    wr     = 2,    remark = 'high x, continuative',
    wf     = 1,    remark = 'low y, symmetric',
    wbk    = 2,    remark = 'high y, continuative',
    wb     = 2,    remark = 'low z, continuative',
    wt     = 5,    remark = 'high z, constant pressure',
    remark = 'eventually add cross-velocity at top of cask if necessary',

    tbcd = 300.0,
    pbc(6) = 101252.8965,
    remark = 'f boundaries are automatically 0 (mat 2)',

$END

   nxcelt = 100,
     px(1) = -2.4336375,  nxcell(1) = 100,
     px(2) =  2.4336375,

   nycelt = 100,
     py(1) = -2.4336375,  nycell(1) = 100,
     py(2) =  2.4336375,

   nzcelt = 100,
     pz(1) = -0.2159000,  nzcell(1) = 100,
     pz(2) =  6.0,
```

```
  $MESH

      remark = 'full Cartesian mesh',
      nxcelt    = 180,
        px(1)   = -2.4336375,  nxcell(1)   = 10, remark = '4ft air gap beyond cask',
        px(2)   = -1.2144375,  nxcell(2)   = 10, remark = 'overpack neutron shielding outside
diameter'
,
        px(3)   = -1.0890250,  nxcell(3)   = 3, remark = 'overpack multilayer shell outside
diameter',
        px(4)   = -1.0572750,  nxcell(4)   = 10, remark = 'overpack baseplate diameter',
        px(5)   = -0.9366250,  nxcell(5)   = 6, remark = 'overpack inner shell outside diameter',
        px(6)   = -0.8731250,  nxcell(6)   = 1, remark = 'overpack inner shell inside diameter',
        px(7)   = -0.8683650,  nxcell(7)   = 1, remark = 'MPC base plate outside diameter',
        px(8)   = -0.8540750,  nxcell(8)   = 1, remark = 'outside MPC shell diameter',
        px(9)   = -0.8477250,  nxcell(9)   = 2, remark = 'inside MPC shell diameter',
        px(10)  = -0.8216900,  nxcell(10)  = 2, remark = 'being fuel basket',
        px(11)  = -0.8137525,  nxcell(11)  = 10, remark = 'end basket, left edge in assemblies
7,13',
        px(12)  = -0.5842000,  nxcell(12)  = 2, remark = 'begin basket, right edge in assemblies
7,13',
        px(13)  = -0.5762625,  nxcell(13)  = 3, remark = 'end basket, left edge in assemblies
3,19',
        px(14)  = -0.5288280,  nxcell(14)  = 7, remark = 'left edge in assemblies 8,14',
        px(15)  = -0.3496945,  nxcell(15)  = 3, remark = 'right edge in assemblies 3,19',
        px(16)  = -0.3022600,  nxcell(16)  = 2, remark = 'begin basket, right edge in assemblies
8,14',
        px(17)  = -0.2943225,  nxcell(17)  = 3, remark = 'end basket, left edge in assemblies
4,20',
        px(18)  = -0.2517902,  nxcell(18)  = 7, remark = 'left edge in assemblies 1,9,15,23',
        px(19)  = -0.0677545,  nxcell(19)  = 3, remark = 'right edge in assemblies 4,20',
        px(20)  = -0.0252222,  nxcell(20)  = 2, remark = 'right edge in assemblies 1,9,15,23 -
begin ba
sket',
        px(21)  = -0.0172847,  nxcell(21)  = 2, remark = 'end basket,  start air',
        px(22)  =  0.0000000,  nxcell(22)  = 2, remark = 'air',
        px(23)  =  0.0172847,  nxcell(23)  = 2, remark = 'end air, begin basket',
        px(24)  =  0.0252222,  nxcell(24)  = 3, remark = 'end basket, left edge in assemblies
2,10,16,2
4',
        px(25)  =  0.0677545,  nxcell(25)  = 7, remark = 'left edge in assemblies 5,21',
        px(26)  =  0.2517902,  nxcell(26)  = 3, remark = 'right edge in assemblies 2,10,16,24',
        px(27)  =  0.2943225,  nxcell(27)  = 2, remark = 'right edge in assemblies 5,21, begin
basket',
        px(28)  =  0.3022600,  nxcell(28)  = 3, remark = 'end basket, left edge in assemblies
11,17',
        px(29)  =  0.3496945,  nxcell(29)  = 7, remark = 'left edge in assemblies 6,22',
        px(30)  =  0.5288280,  nxcell(30)  = 3, remark = 'right edge in assemblies 11,17',
        px(31)  =  0.5762625,  nxcell(31)  = 2, remark = 'right edge in assemblies 6,22, begin
basket',
        px(32)  =  0.5842000,  nxcell(32)  = 10, remark = 'end basket, left edge assemblies 12,18',
        px(33)  =  0.8137525,  nxcell(33)  = 2, remark = 'right edge assemblies 12,18, begin
basket',
        px(34)  =  0.8216900,  nxcell(34)  = 2, remark = 'end fuel basket',
        px(35)  =  0.8477250,  nxcell(35)  = 1, remark = 'inside MPC shell diameter',
        px(36)  =  0.8540750,  nxcell(36)  = 1, remark = 'outside MPC shell diameter',
        px(37)  =  0.8683650,  nxcell(37)  = 1, remark = 'MPC base plate outside diameter',
        px(38)  =  0.8731250,  nxcell(38)  = 6, remark = 'overpack inner shell inside diameter',
        px(39)  =  0.9366250,  nxcell(39)  = 10, remark = 'overpack inner shell outside diameter',
        px(40)  =  1.0572750,  nxcell(40)  = 3, remark = 'overpack baseplate diameter',
        px(41)  =  1.0890250,  nxcell(41)  = 10, remark = 'overpack multilayer shell outside
diameter',
        px(42)  =  1.2144375,  nxcell(42)  = 10, remark = 'overpack neutron shielding outside
diameter'
,
        px(43)  =  2.4336375,                  remark = '4ft air gap beyond cask',

    nycelt    = 180,
        py(1)   = -2.4336375,  nycell(1)   = 10, remark = '4ft air gap beyond cask',
```

```
        py(2)  = -1.2144375,  nycell(2)  = 10, remark = 'overpack neutron shielding outside
diameter'
,
        py(3)  = -1.0890250,  nycell(3)  = 3, remark = 'overpack multilayer shell outside
diameter',
        py(4)  = -1.0572750,  nycell(4)  = 10, remark = 'overpack baseplate diameter',
        py(5)  = -0.9366250,  nycell(5)  = 6, remark = 'overpack inner shell outside diameter',
        py(6)  = -0.8731250,  nycell(6)  = 1, remark = 'overpack inner shell inside diameter',
        py(7)  = -0.8683650,  nycell(7)  = 1, remark = 'MPC base plate outside diameter',
        py(8)  = -0.8540750,  nycell(8)  = 1, remark = 'outside MPC shell diameter',
        py(9)  = -0.8477250,  nycell(9)  = 2, remark = 'inside MPC shell diameter',
        py(10) = -0.8216900,  nycell(10) = 2, remark = 'end fuel basket',
        py(11) = -0.8137525,  nycell(11) = 10, remark = 'bottom edge assemblies 23, 24, begin
basket'
,
        py(12) = -0.5842000,  nycell(12) = 2, remark = 'end basket, top edge assemblies 23,24',
        py(13) = -0.5762625,  nycell(13) = 3, remark = 'bottom edge assemblies 19,22, begin
basket',
        py(14) = -0.5288280,  nycell(14) = 7, remark = 'bottom edge assemblies 20,21',
        py(15) = -0.3496945,  nycell(15) = 3, remark = 'top edge assemblies 19,22',
        py(16) = -0.3022600,  nycell(16) = 2, remark = 'end basket, top edge assemblies 20,21',
        py(17) = -0.2943225,  nycell(17) = 3, remark = 'bottom edge assemblies 14,17, begin
basket',
        py(18) = -0.2517902,  nycell(18) = 7, remark = 'bottom edge assemblies 13,15,16,18',
        py(19) = -0.0677545,  nycell(19) = 3, remark = 'top edge assemblies 14,17',
        py(20) = -0.0252222,  nycell(20) = 2, remark = 'begin basket, top edge assemblies
13,15,16,18
',
        py(21) = -0.0172847,  nycell(21) = 2, remark = 'begin air, end basket',
        py(22) =  0.0000000,  nycell(22) = 2, remark = 'air',
        py(23) =  0.0172847,  nycell(23) = 2, remark = 'end air, begin basket',
        py(24) =  0.0252222,  nycell(24) = 3, remark = 'end basket, bottom edge assemblies
7,9,10,12'
,
        py(25) =  0.0677545,  nycell(25) = 7, remark = 'bottom edge assemblies 8,11',
        py(26) =  0.2517902,  nycell(26) = 3, remark = 'top edge assemblies 7,9,10,12',
        py(27) =  0.2943225,  nycell(27) = 2, remark = 'top edge assemblies 8, 11, begin basket',
        py(28) =  0.3022600,  nycell(28) = 3, remark = 'end basket, bottom edge assemblies 4,5',
        py(29) =  0.3496945,  nycell(29) = 7, remark = 'bottom edge assemblies 3,6',
        py(30) =  0.5288280,  nycell(30) = 3, remark = 'top edge assemblies 4,5',
        py(31) =  0.5762625,  nycell(31) = 2, remark = 'top edge assemblies 3,6, begin basket',
        py(32) =  0.5842000,  nycell(32) = 10, remark = 'end basket, bottom edge assemblies 1,2',
        py(33) =  0.8137525,  nycell(33) = 2, remark = 'top edge assemblies 1,2',
        py(34) =  0.8216900,  nycell(34) = 2, remark = 'end fuel basket',
        py(35) =  0.847725,   nycell(35) = 1, remark = 'inside MPC shell diameter',
        py(36) =  0.854075,   nycell(36) = 1, remark = 'outside MPC shell diameter',
        py(37) =  0.868365,   nycell(37) = 1, remark = 'MPC base plate outside diameter',
        py(38) =  0.873125,   nycell(38) = 6, remark = 'overpack inner shell inside diameter',
        py(39) =  0.936625,   nycell(39) = 10, remark = 'overpack inner shell outside diameter',
        py(40) =  1.057275,   nycell(40) = 3, remark = 'overpack base plate outside diameter',
        py(41) =  1.089025,   nycell(41) = 10, remark = 'overpack multilayer shell outside
diameter',
        py(42) =  1.2144375,  nycell(42) = 10, remark = 'overpack neutron shielding outside
diameter'
,
        py(43) =  2.4336375,                  remark = '4ft air gap beyond cask',


     nzcelt     = 99,
        pz(1)  = -0.2159000,  nzcell(1)  = 5, remark = 'bottom overpack base plate',
        pz(2)  = -0.0635000,  nzcell(2)  = 2, remark = 'top overpack base plate',
        pz(3)  =  0.0000000,  nzcell(3)  = 2, remark = 'bottom of fuel basket/bottom of MPC
shell',
        pz(4)  =  0.0635000,  nzcell(4)  = 5, remark = 'bottom overpack neutron shielding',
        pz(5)  =  0.3052800,  nzcell(5)  = 47, remark = 'begin fuel',
        pz(6)  =  4.1651200,  nzcell(6)  = 5, remark = 'top fuel',
        pz(7)  =  4.4037250,  nzcell(7)  = 2, remark = 'top overpack neutron shielding',
        pz(8)  =  4.4704000,  nzcell(8)  = 2, remark = 'top of fuel basket',
        pz(9)  =  4.5212000,  nzcell(9)  = 9, remark = 'top of MPC shell',
        pz(10) =  4.7910750,  nzcell(10) = 5, remark = 'top overpack layering system',
```

```
        pz(11) =  4.9434750,  nzcell(11) = 15, remark = 'top overpack idealized lid edge',
        pz(12) =  6.0,                         remark = '3+ feet higher than cask',
  $END
      nxcelt    = 90,
        px(1) =  0.0000000,  nxcell(1) = 2, remark = 'air',
        px(2) =  0.0172847,  nxcell(2) = 2, remark = 'end air, begin basket',
        px(3) =  0.0252222,  nxcell(3) = 3, remark = 'end basket, left edge in assemblies
2,10,16,24'
,
        px(4) =  0.0677545,  nxcell(4) = 7, remark = 'left edge in assemblies 5,21',
        px(5) =  0.2517902,  nxcell(5) = 3, remark = 'right edge in assemblies 2,10,16,24',
        px(6) =  0.2943225,  nxcell(6) = 2, remark = 'right edge in assemblies 5,21, begin
basket',
        px(7) =  0.3022600,  nxcell(7) = 3, remark = 'end basket, left edge in assemblies 11,17',
        px(8) =  0.3496945,  nxcell(8) = 7, remark = 'left edge in assemblies 6,22',
        px(9) =  0.5288280,  nxcell(9) = 3, remark = 'right edge in assemblies 11,17',
        px(10) =  0.5762625, nxcell(10) = 2, remark = 'right edge in assemblies 6,22, begin
basket',
        px(11) =  0.5842000, nxcell(11) = 10, remark = 'end basket, left edge assemblies 12,18',
        px(12) =  0.8137525, nxcell(12) = 2, remark = 'right edge assemblies 12,18, begin
basket',
        px(13) =  0.8216900,  nxcell(13) = 2, remark = 'end fuel basket',
        px(14) =  0.8477250,  nxcell(14) = 1, remark = 'inside MPC shell diameter',
        px(15) =  0.8540750,  nxcell(15) = 1, remark = 'outside MPC shell diameter',
        px(16) =  0.8683650,  nxcell(16) = 1, remark = 'MPC base plate outside diameter',
        px(17) =  0.8731250,  nxcell(17) = 6, remark = 'overpack inner shell inside diameter',
        px(18) =  0.9366250,  nxcell(18) = 10, remark = 'overpack inner shell outside diameter',
        px(19) =  1.0572750,  nxcell(19) = 3, remark = 'overpack baseplate diameter',
        px(20) =  1.0890250,  nxcell(20) = 10, remark = 'overpack multilayer shell outside
diameter',
        px(21) =  1.2144375,  nxcell(21) = 10, remark = 'overpack neutron shielding outside
diameter'
,
        px(22) =  2.4336375,                   remark = '4ft air gap beyond cask',
      remark = 'full Cartesian mesh',
      nxcelt    = 90,
        px(1) =  0.0000000,  nxcell(1) = 2, remark = 'air',
        px(2) =  0.0172847,  nxcell(2) = 2, remark = 'end air, begin basket',
        px(3) =  0.0252222,  nxcell(3) = 3, remark = 'end basket, left edge in assemblies
2,10,16,24'
,
        px(4) =  0.0677545,  nxcell(4) = 7, remark = 'left edge in assemblies 5,21',
        px(5) =  0.2517902,  nxcell(5) = 3, remark = 'right edge in assemblies 2,10,16,24',
        px(6) =  0.2943225,  nxcell(6) = 2, remark = 'right edge in assemblies 5,21, begin
basket',
        px(7) =  0.3022600,  nxcell(7) = 3, remark = 'end basket, left edge in assemblies 11,17',
        px(8) =  0.3496945,  nxcell(8) = 7, remark = 'left edge in assemblies 6,22',
        px(9) =  0.5288280,  nxcell(9) = 3, remark = 'right edge in assemblies 11,17',
        px(10) =  0.5762625, nxcell(10) = 2, remark = 'right edge in assemblies 6,22, begin
basket',
        px(11) =  0.5842000, nxcell(11) = 10, remark = 'end basket, left edge assemblies 12,18',
        px(12) =  0.8137525, nxcell(12) = 2, remark = 'right edge assemblies 12,18, begin
basket',
        px(13) =  0.8216900,  nxcell(13) = 2, remark = 'end fuel basket',
        px(14) =  0.8477250,  nxcell(14) = 1, remark = 'inside MPC shell diameter',
        px(15) =  0.8540750,  nxcell(15) = 1, remark = 'outside MPC shell diameter',
        px(16) =  0.8683650,  nxcell(16) = 1, remark = 'MPC base plate outside diameter',
        px(17) =  0.8731250,  nxcell(17) = 6, remark = 'overpack inner shell inside diameter',
        px(18) =  0.9366250,  nxcell(18) = 10, remark = 'overpack inner shell outside diameter',
        px(19) =  1.0572750,  nxcell(19) = 3, remark = 'overpack baseplate diameter',
        px(20) =  1.0890250,  nxcell(20) = 10, remark = 'overpack multilayer shell outside
diameter',
        px(21) =  1.2144375,  nxcell(21) = 10, remark = 'overpack neutron shielding outside
diameter'
,
        px(22) =  2.4336375,                   remark = '4ft air gap beyond cask',

      nycelt    = 90,
        py(1) =  0.0000000,  nycell(1) = 2, remark = 'air',
        py(2) =  0.0172847,  nycell(2) = 2, remark = 'end air, begin basket',
```

```
        py(3) =  0.0252222,  nycell(3) = 3, remark = 'end basket, bottom edge assemblies
7,9,10,12',
        py(4) =  0.0677545,  nycell(4) = 7, remark = 'bottom edge assemblies 8,11',
        py(5) =  0.2517902,  nycell(5) = 3, remark = 'top edge assemblies 7,9,10,12',
        py(6) =  0.2943225,  nycell(6) = 2, remark = 'top edge assemblies 8, 11, begin basket',
        py(7) =  0.3022600,  nycell(7) = 3, remark = 'end basket, bottom edge assemblies 4,5',
        py(8) =  0.3496945,  nycell(8) = 7, remark = 'bottom edge assemblies 3,6',
        py(9) =  0.5288280,  nycell(9) = 3, remark = 'top edge assemblies 4,5',
        py(10) =  0.5762625,  nycell(10) = 2, remark = 'top edge assemblies 3,6, begin basket',
        py(11) =  0.5842000,  nycell(11) = 10, remark = 'end basket, bottom edge assemblies 1,2',
        py(12) =  0.8137525,  nycell(12) = 2, remark = 'top edge assemblies 1,2',
        py(13) =  0.8216900,  nycell(13) = 2, remark = 'end fuel basket',
        py(14) =  0.847725,   nycell(14) = 1, remark = 'inside MPC shell diameter',
        py(15) =  0.854075,   nycell(15) = 1, remark = 'outside MPC shell diameter',
        py(16) =  0.868365,   nycell(16) = 1, remark = 'MPC base plate outside diameter',
        py(17) =  0.873125,   nycell(17) = 6, remark = 'overpack inner shell inside diameter',
        py(18) =  0.936625,   nycell(18) = 10, remark = 'overpack inner shell outside diameter',
        py(19) =  1.057275,   nycell(19) = 3, remark = 'overpack base plate outside diameter',
        py(20) =  1.089025,   nycell(20) = 10, remark = 'overpack multilayer shell outside
diameter',
        py(21) =  1.2144375,  nycell(21) = 10, remark = 'overpack neutron shielding outside
diameter'
,
        py(22) =  2.4336375,                  remark = '4ft air gap beyond cask'

    nycelt   = 90,
        py(1) =  0.0000000,  nycell(1) = 2, remark = 'air',
        py(2) =  0.0172847,  nycell(2) = 2, remark = 'end air, begin basket',
        py(3) =  0.0252222,  nycell(3) = 3, remark = 'end basket, bottom edge assemblies
7,9,10,12',
        py(4) =  0.0677545,  nycell(4) = 7, remark = 'bottom edge assemblies 8,11',
        py(5) =  0.2517902,  nycell(5) = 3, remark = 'top edge assemblies 7,9,10,12',
        py(6) =  0.2943225,  nycell(6) = 2, remark = 'top edge assemblies 8, 11, begin basket',
        py(7) =  0.3022600,  nycell(7) = 3, remark = 'end basket, bottom edge assemblies 4,5',
        py(8) =  0.3496945,  nycell(8) = 7, remark = 'bottom edge assemblies 3,6',
        py(9) =  0.5288280,  nycell(9) = 3, remark = 'top edge assemblies 4,5',
        py(10) =  0.5762625,  nycell(10) = 2, remark = 'top edge assemblies 3,6, begin basket',
        py(11) =  0.5842000,  nycell(11) = 10, remark = 'end basket, bottom edge assemblies 1,2',
        py(12) =  0.8137525,  nycell(12) = 2, remark = 'top edge assemblies 1,2',
        py(13) =  0.8216900,  nycell(13) = 2, remark = 'end fuel basket',
        py(14) =  0.847725,   nycell(14) = 1, remark = 'inside MPC shell diameter',
        py(15) =  0.854075,   nycell(15) = 1, remark = 'outside MPC shell diameter',
        py(16) =  0.868365,   nycell(16) = 1, remark = 'MPC base plate outside diameter',
        py(17) =  0.873125,   nycell(17) = 6, remark = 'overpack inner shell inside diameter',
        py(18) =  0.936625,   nycell(18) = 10, remark = 'overpack inner shell outside diameter',
        py(19) =  1.057275,   nycell(19) = 3, remark = 'overpack base plate outside diameter',
        py(20) =  1.089025,   nycell(20) = 10, remark = 'overpack multilayer shell outside
diameter',
        py(21) =  1.2144375,  nycell(21) = 10, remark = 'overpack neutron shielding outside
diameter'
,
        py(22) =  2.4336375,                  remark = '4ft air gap beyond cask'
    nycelt   = 180,
        py(1)  = -2.4336375,  nycell(1)  = 10, remark = '4ft air gap beyond cask',
        py(2)  = -1.2144375,  nycell(2)  = 10, remark = 'overpack neutron shielding outside
diameter'
,
        py(3)  = -1.0890250,  nycell(3)  = 3, remark = 'overpack multilayer shell outside
diameter',
        py(4)  = -1.0572750,  nycell(4)  = 10, remark = 'overpack baseplate diameter',
        py(5)  = -0.9366250,  nycell(5)  = 6, remark = 'overpack inner shell outside diameter',
        py(6)  = -0.8731250,  nycell(6)  = 1, remark = 'overpack inner shell inside diameter',
        py(7)  = -0.8683650,  nycell(7)  = 1, remark = 'MPC base plate outside diameter',
        py(8)  = -0.8540750,  nycell(8)  = 1, remark = 'outside MPC shell diameter',
        py(9)  = -0.8477250,  nycell(9)  = 2, remark = 'inside MPC shell diameter',
        py(10) = -0.8216900,  nycell(10) = 2, remark = 'end fuel basket',
        py(11) = -0.8137525,  nycell(11) = 10, remark = 'bottom edge assemblies 23, 24, begin
basket'
,
        py(12) = -0.5842000,  nycell(12) = 2, remark = 'end basket, top edge assemblies 23,24',
```

```
        py(13) = -0.5762625,  nycell(13) = 3, remark = 'bottom edge assemblies 19,22, begin
basket',
        py(14) = -0.5288280,  nycell(14) = 7, remark = 'bottom edge assemblies 20,21',
        py(15) = -0.3496945,  nycell(15) = 3, remark = 'top edge assemblies 19,22',
        py(16) = -0.3022600,  nycell(16) = 2, remark = 'end basket, top edge assemblies 20,21',
        py(17) = -0.2943225,  nycell(17) = 3, remark = 'bottom edge assemblies 14,17, begin
basket',
        py(18) = -0.2517902,  nycell(18) = 7, remark = 'bottom edge assemblies 13,15,16,18',
        py(19) = -0.0677545,  nycell(19) = 3, remark = 'top edge assemblies 14,17',
        py(20) = -0.0252222,  nycell(20) = 2, remark = 'begin basket, top edge assemblies
13,15,16,18
',
        py(21) = -0.0172847,  nycell(21) = 2, remark = 'begin air, end basket',
        py(22) =  0.0000000,  nycell(22) = 2, remark = 'air',
        py(23) =  0.0172847,  nycell(23) = 2, remark = 'end air, begin basket',
        py(24) =  0.0252222,  nycell(24) = 3, remark = 'end basket, bottom edge assemblies
7,9,10,12'
,
        py(25) =  0.0677545,  nycell(25) = 7, remark = 'bottom edge assemblies 8,11',
        py(26) =  0.2517902,  nycell(26) = 3, remark = 'top edge assemblies 7,9,10,12',
        py(27) =  0.2943225,  nycell(27) = 2, remark = 'top edge assemblies 8, 11, begin basket',
        py(28) =  0.3022600,  nycell(28) = 3, remark = 'end basket, bottom edge assemblies 4,5',
        py(29) =  0.3496945,  nycell(29) = 7, remark = 'bottom edge assemblies 3,6',
        py(30) =  0.5288280,  nycell(30) = 3, remark = 'top edge assemblies 4,5',
        py(31) =  0.5762625,  nycell(31) = 2, remark = 'top edge assemblies 3,6, begin basket',
        py(32) =  0.5842000,  nycell(32) = 10, remark = 'end basket, bottom edge assemblies 1,2',
        py(33) =  0.8137525,  nycell(33) = 2, remark = 'top edge assemblies 1,2',
        py(34) =  0.8216900,  nycell(34) = 2, remark = 'end fuel basket',
        py(35) =  0.847725,   nycell(35) = 1, remark = 'inside MPC shell diameter',
        py(36) =  0.854075,   nycell(36) = 1, remark = 'outside MPC shell diameter',
        py(37) =  0.868365,   nycell(37) = 1, remark = 'MPC base plate outside diameter',
        py(38) =  0.873125,   nycell(38) = 6, remark = 'overpack inner shell inside diameter',
        py(39) =  0.936625,   nycell(39) = 10, remark = 'overpack inner shell outside diameter',
        py(40) =  1.057275,   nycell(40) = 3, remark = 'overpack base plate outside diameter',
        py(41) =  1.089025,   nycell(41) = 10, remark = 'overpack multilayer shell outside
diameter',
        py(42) =  1.2144375,  nycell(42) = 10, remark = 'overpack neutron shielding outside
diameter'
,
        py(43) =  2.4336375,                 remark = '4ft air gap beyond cask'


     nzcelt    = 53,
        pz(1)  = -0.2159000,  nzcell(1)  = 5, remark = 'bottom overpack base plate',
        pz(2)  = -0.0635000,  nzcell(2)  = 2, remark = 'top overpack base plate',
        pz(3)  =  0.0000000,  nzcell(3)  = 2, remark = 'bottom of fuel basket/bottom of MPC
shell',
        pz(4)  =  0.0635000,  nzcell(4)  = 5, remark = 'bottom overpack neutron shielding',
        pz(5)  =  0.3052800,  nzcell(5)  = 1, remark = 'begin fuel',
        pz(6)  =  4.1651200,  nzcell(6)  = 5, remark = 'top fuel',
        pz(7)  =  4.4037250,  nzcell(7)  = 2, remark = 'top overpack neutron shielding',
        pz(8)  =  4.4704000,  nzcell(8)  = 2, remark = 'top of fuel basket',
        pz(9)  =  4.5212000,  nzcell(9)  = 9, remark = 'top of MPC shell',
        pz(10) =  4.7910750,  nzcell(10) = 5, remark = 'top overpack layering system',
        pz(11) =  4.9434750,  nzcell(11) = 15, remark = 'top overpack idealized lid edge',
        pz(12) =  6.0,                       remark = '3+ feet higher than cask',

  $OBS
     nobs = 32,

     remark = 'create the obstacle field',
     remark = 'begin with fuel basket:  MPC-24, Holtec drawing 3926, sheet 2, rev 2',

     remark = 'thermal conductivity given in J/m-s-K at 400C',
     remark = 'data from Hi-Star FSAR Report HI-201260, chapter4',
     remark = 'see table 4.4.5 for PWR thermal conductivity',

     remark = 'general characteristics',
     remark = '24 locations for spent fuel of similar geometric config',
```

```
remark = 'lay in x-cut plates first, left to right',

remark = 'thermal conductivity = kobs unit:   Watt/m/K = kg-m/s3/K',
remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',

remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
remark = 'Report HI-2012610',
remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
remark = 'thermal conductivity values from Table 4.4.7: generalized',
remark = 'thermal conductivity vs. temperature',
remark = 'choosing values at 400C',
remark = 'rcobs = specific heat',

remark = '24 Basket',
remark = 'A',
iob(1) = 1, ioh(1) = 1, xl(1) = -0.3022600, xh(1) =  0.3022600,
                        yl(1) =  0.8137525, yh(1) =  0.8216900,
                        zl(1) =  0.0000000, zh(1) =  4.4831000,
                        kobs(1) = 2.286,
                        rcobs(1) = 544.28,

remark = 'B',
iob(2) = 1, ioh(2) = 1, xl(2) = -0.5842000, xh(2) =  0.5842000,
                        yl(2) =  0.5762625, yh(2) =  0.5842000,
                        zl(2) =  0.0000000, zh(2) =  4.4831000,

remark = 'C',
iob(3) = 1, ioh(3) = 1, xl(3) = -0.8216900, xh(3) =  0.8216900,
                        yl(3) =  0.2943225, yh(3) =  0.3022600,
                        zl(3) =  0.0000000, zh(3) =  4.4831000,

remark = 'D',
iob(4) = 1, ioh(4) = 1, xl(4) = -0.8216900, xh(4) =  0.8216900,
                        yl(4) =  0.0172847, yh(4) =  0.0252222,
                        zl(4) =  0.0000000, zh(4) =  4.4831000,

remark = 'A2',
iob(5) = 1, ioh(5) = 1, xl(5) = -0.3022600, xh(5) =  0.3022600,
                        yl(5) = -0.8216900, yh(5) = -0.8137525,
                        zl(5) =  0.0000000, zh(5) =  4.4831000,

remark = 'B2',
iob(6) = 1, ioh(6) = 1, xl(6) = -0.5842000, xh(6) =  0.5842000,
                        yl(6) = -0.5842000, yh(6) = -0.5762625,
                        zl(6) =  0.0000000, zh(6) =  4.4831000,

remark = 'C2',
iob(7) = 1, ioh(7) = 1, xl(7) = -0.8216900, xh(7) =  0.8216900,
                        yl(7) = -0.3022600, yh(7) = -0.2943225,
                        zl(7) =  0.0000000, zh(7) =  4.4831000,

remark = 'D2',
iob(8) = 1, ioh(8) = 1, xl(8) = -0.8216900, xh(8) =  0.8216900,
                        yl(8) = -0.0252222, yh(8) = -0.0172847,
                        zl(8) =  0.0000000, zh(8) =  4.4831000,

remark = 'A3',
iob(9) = 1, ioh(9) = 1, xl(9) =  0.8137525, xh(9) =  0.8216900,
                        yl(9) = -0.3022600, yh(9) =  0.3022600,
                        zl(9) =  0.0000000, zh(9) =  4.4831000,

remark = 'B3',
iob(10) = 1, ioh(10) = 1, xl(10) =  0.5762625, xh(10) = 0.5842000,
                          yl(10) = -0.5842000, yh(10) = 0.5842000,
                          zl(10) =  0.0000000, zh(10) = 4.4831000,

remark = 'C3',
iob(11) = 1, ioh(11) = 1, xl(11) =  0.2943225, xh(11) = 0.3026600,
                          yl(11) = -0.8216900, yh(11) = 0.8216900,
                          zl(11) =  0.0000000, zh(11) = 4.4831000,
```

```
remark = 'D3',
iob(12) = 1, ioh(12) = 1, xl(12) =  0.0172847, xh(12) = 0.0252222,
                          yl(12) = -0.8216900, yh(12) = 0.8216900,
                          zl(12) =  0.0000000, zh(12) = 4.4831000,

remark = 'A4',
iob(13) = 1, ioh(13) = 1, xl(13) = -0.8216900, xh(13) = -0.8137525,
                          yl(13) = -0.3022600, yh(13) =  0.3022600,
                          zl(13) =  0.0000000, zh(13) =  4.4831000,

remark = 'B4',
iob(14) = 1, ioh(14) = 1, xl(14) = -0.5842000, xh(14) = -0.5762625,
                          yl(14) = -0.5842000, yh(14) =  0.5842000,
                          zl(14) =  0.0000000, zh(14) =  4.4831000,

remark = 'C4',
iob(15) = 1, ioh(15) = 1, xl(15) = -0.3022600, xh(15) = -0.2943225,
                          yl(15) = -0.8216900, yh(15) =  0.8216900,
                          zl(15) =  0.0000000, zh(15) =  4.4831000,

remark = 'D4',
iob(16) = 1, ioh(16) = 1, xl(16) = -0.0252222, xh(16) = -0.0172847,
                          yl(16) = -0.8216900, yh(16) =  0.8216900,
                          zl(16) =  0.0000000, zh(16) =  4.4831000,


remark = 'lay in 1/2in thick MPC shell at phi67.25in',
remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
remark = 'pages 3 and 4',
iob(23) = 2, ioh(23) = 1, ral(23) =  0.8477250, rah(23) = 0.8731250,
remark = 'actual spacing - eliminated b/c of grid resolution rah(23) =  0.854075,',
                          zl(23)  =  0.0000000, zh(23)  =  4.5212000,
                          kobs(2) = 0.0478,
                          rcobs(2) = 502.41,

remark = 'lay in MPC base plate 2.5in thick',
remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
remark = 'page 2(thickness), page 3(diameter)',
iob(24) = 3, ioh(24) = 1, ral(24) =  0.0000000, rah(24) = 0.8731250, remark = '0.8683625',
                          zl(24)  = -0.0635000, zh(24)  = 0.0000000,
                          kobs(3) = 0.0478,
                          rcobs(3) = 502.41,

remark = 'not including MPC lid - am assuming system is open',
remark = 'not including drain sump or fuel basket support rails',

remark = 'lay in overpack components',
remark = 'Holtec print 3913:  Hi-Star 100 Overpack Elevation View',
remark = 'base plate, page 2',
remark = '6in thick, 83.5in outside diameter',
iob(25) = 4, ioh(25) = 1, ral(25) =  0.0000000, rah(25) =  1.0572750,
                          zl(25)  = -0.21590000, zh(25) = -0.0635000,
                          kobs(4) = 30.3456,
                          rcobs(4) = 418.67,

remark = 'overpack inner shell, page 2',
remark = 'simplified to incorporate the full cask wall',
remark = '68.75in inside diameter, 73.75in outside diameter',
remark = '191.125in height from cask base plate',
iob(26) = 5, ioh(26) = 1, ral(26) =  0.8731250, rah(26) =  0.9366250,
                          zl(26)  = -0.0635000, zh(26)  =  4.7910750,
                          kobs(5) = 2.8117,
                          rcobs(5) = 502.41,

remark = 'overpack multilayered shells',
remark = 'simplified to incorporate the full cask wall',
remark = '73.75in inside diameter, 6 in thick 4x1.25 gamma layers + 1in shell',
iob(27) = 6, ioh(27) = 1, ral(27) =  0.9366250, rah(27) =  1.0890250,
                          zl(27)  = -0.0635000, zh(27)  =  4.7910750,
                          kobs(6) = 2.8117,
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                          rcobs(6) = 502.41,

remark = 'overpack neutron shielding',
remark = 'simplified to incorporate neutron shield and radial channels that form the shell',
remark = 'details from page 6',
remark = 'thickness of neutron shield = 4-7/16in + thickness of channel 1/2in = 4-15/16in',
remark = 'idealized inside diameter = 85.75in, outside diameter = 95.625in',
remark = 'height runs from 8-3/4in off cask base to 173-1/8in',
iob(28) = 7, ioh(28) = 1, ral(28) =  1.0890250, rah(28) =  1.2144375,
                          zl(28)  =  0.0635000, zh(28)  =  4.4037250,
                          kobs(7) = 2.8117,
                          rcobs(7) = 1632.85,

remark = 'overpack - approximation of outside rim around lid',
remark = 'idealized inside diameter = 68.75in, outside diameter = 83.25in',
remark = '6in thick',
remark = 'approximating from page 2, print 3913',
iob(29) = 8, ioh(29) = 1, ral(29) =  0.8731250, rah(29) =  1.0572750,
                          zl(29)  =  4.7910750, zh(29)  =  4.9434750,
                          kobs(8) = 2.8117,
                          rcobs(8) = 1632.85,

remark = 'ready to lay in the PWRs and heat source information',
remark = 'supposition:  PWR completely fill open area in MPC basket formation',
remark = 'doing this until better geometry provided',
remark = 'shortening PWR units by 12in on each end (centered)'
remark = 'based on info from PA Cox - check with Amit/Bis - ok',

remark = 'thermal conductivity is based on design specifications of Table 4.4.5',
remark = 'trend line created from data shown then conservatively extrapolated',
remark = 'to 400C;  values implemented at 232.22C from table',

remark = 'power values based on worst case scenario; 19008 total Watts, from',
remark = 'Table 4.4.18:  MPC-24 Basket Peak Fuel Claddings Temp as Function...',
tobs(1) = 0.0,


remark = 'lay in new 24 assembly',
remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',
iob(30) = 9, ioh(30) = 1, xl(30) = -0.2517902, xh(30) = -0.0252222,
                          yl(30) =  0.5842000, yh(30) =  0.8137525,
                          zl(30) =  0.3052800, zh(30) =  4.1651200,
                          kobs(9) = 0.696,
                          rcobs(9) = 234.46,
                          pobs(1,9) = 792,
                          twobs(1,9)=600,
                          tobs(9)=0,

remark = 'Slot 2',
iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                           yl(31) =  0.5842000, yh(31) =  0.8137525,
                           zl(31) =  0.3052800, zh(31) =  4.1651200,
                           kobs(10) = 0.696,
                           rcobs(10) = 234.46,
                           pobs(1,10) = 792,
                           twobs(1,10)=600,
                           tobs(10)=0,

remark = 'Slot 3',
iob(32) = 11, ioh(32) = 1, xl(32) = -0.5762625, xh(32) = -0.3496945,
                           yl(32) =  0.3496945, yh(32) =  0.5762625,
                           zl(32) =  0.3052800, zh(32) =  4.1651200,
                           kobs(11) = 0.696,
                           rcobs(11) = 234.46,
                           pobs(1,11) = 792,
                           twobs(1,11)=600,
                           tobs(11)=0,

remark = 'Slot 4',
iob(33) = 12, ioh(33) = 1, xl(33) = -0.2943225, xh(33) = -0.0677545,
                           yl(33) =  0.3022600, yh(33) =  0.5288280,
```

```
                                zl(33) =  0.3052800, zh(33) =  4.1651200,
                                kobs(12) = 0.696,
                                rcobs(12) = 234.46,
                                pobs(1,12) = 792,
                                twobs(1,12)=600,
                                tobs(12)=0,

remark = 'Slot 5',
iob(34) = 13, ioh(34) = 1, xl(34) =  0.0677545, xh(34) = 0.2943225,
                                yl(34) =  0.3022600, yh(34) = 0.5288280,
                                zl(34) =  0.3052800, zh(34) = 4.1651200,
                                kobs(13) = 0.696,
                                rcobs(13) = 234.46,
                                pobs(1,13) = 792,
                                twobs(1,13)=600,
                                tobs(13)=0,

remark = 'Slot 6',
iob(35) = 14, ioh(35) = 1, xl(35) =  0.3496945, xh(35) = 0.5762625,
                                yl(35) =  0.3496945, yh(35) = 0.5762625,
                                zl(35) =  0.3052800, zh(35) = 4.1651200,
                                kobs(14) = 0.696,
                                rcobs(14) = 234.46,
                                pobs(1,14) = 792,
                                twobs(1,14)=600,
                                tobs(14)=0,

remark = 'Slot 7',
iob(36) = 15, ioh(36) = 1, xl(36) = -0.8137525, xh(36) = -0.5842000,
                                yl(36) =  0.0252222, yh(36) =  0.2517902,
                                zl(36) =  0.3052800, zh(36) =  4.1651200,
                                kobs(15) = 0.696,
                                rcobs(15) = 234.46,
                                pobs(1,15) = 792,
                                twobs(1,15)=600,
                                tobs(15)=0,

remark = 'Slot 8',
iob(37) = 16, ioh(37) = 1, xl(37) = -0.5288280,  xh(37) = -0.3022600,
                                yl(37) =  0.0677545,  yh(37) =  0.2942590,
                                zl(37) =  0.3052800,  zh(37) =  4.1651200,
                                kobs(16) = 0.696,
                                rcobs(16) = 234.46,
                                pobs(1,16) = 792,
                                twobs(1,16)=600,
                                tobs(16)=0,

remark = 'Slot 9',
iob(38) = 17, ioh(38) = 1, xl(38) = -0.2517902, xh(38) = -0.0252222,
                                yl(38) =  0.0252222, yh(38) =  0.2517902,
                                zl(38) =  0.3052800, zh(38) =  4.1651200,
                                kobs(17) = 0.696,
                                rcobs(17) = 234.46,
                                pobs(1,17) = 792,
                                twobs(1,17)=600,
                                tobs(17)=0,

remark = 'Slot 10',
iob(39) = 18, ioh(39) = 1, xl(39) =  0.0252222, xh(39) = 0.2517902,
                                yl(39) =  0.0252222, yh(39) = 0.2517902,
                                zl(39) =  0.3052800, zh(39) = 4.1651200,
                                kobs(18) = 0.696,
                                rcobs(18) = 234.46,
                                pobs(1,18) = 792,
                                twobs(1,18)=600,
                                tobs(18)=0,

remark = 'Slot 11',
iob(40) = 19, ioh(40) = 1, xl(40) =  0.3022600, xh(40) =  0.5288280,
                                yl(40) =  0.0677545, yh(40) =  0.2942590,
                                zl(40) =  0.3052800, zh(40) =  4.1651200,
```

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                                kobs(19) = 0.696,
                                rcobs(19) = 234.46,
                                pobs(1,19) = 792,
                                twobs(1,19)=600,
                                tobs(19)=0,

remark = 'Slot 12',
iob(41) = 20, ioh(41) = 1, xl(41) =  0.5842000, xh(41) = 0.8137525,
                           yl(41) =  0.0252222, yh(41) = 0.2517902,
                           zl(41) =  0.3052800, zh(41) = 4.1651200,
                           kobs(20) = 0.696,
                           rcobs(20) = 234.46,
                           pobs(1,20) = 792,
                           twobs(1,20)=600,
                           tobs(20)=0,

remark = 'Slot 13',
iob(42) = 21, ioh(42) = 1, xl(42) = -0.8137525, xh(42) = -0.5842000,
                           yl(42) = -0.2517902, yh(42) = -0.0252222,
                           zl(42) =  0.3052800, zh(42) =  4.1651200,
                           kobs(21) = 0.696,
                           rcobs(21) = 234.46,
                           pobs(1,21) = 792,
                           twobs(1,21)=600,
                           tobs(21)=0,

remark = 'Slot 14',
iob(43) = 22, ioh(43) = 1, xl(43) = -0.5288280,  xh(43) = -0.3022600,
                           yl(43) = -0.2942590,  yh(43) = -0.0677545,
                           zl(43) =  0.3052800,  zh(43) =  4.1651200,
                           kobs(22) = 0.696,
                           rcobs(22) = 234.46,
                           pobs(1,22) = 792,
                           twobs(1,22)=600,
                           tobs(22)=0,

remark = 'Slot 15',
iob(44) = 23, ioh(44) = 1, xl(44) = -0.2517902, xh(44) = -0.0252222,
                           yl(44) = -0.2517902, yh(44) = -0.0252222,
                           zl(44) =  0.3052800, zh(44) =  4.1651200,
                           kobs(23) = 0.696,
                           rcobs(23) = 234.46,
                           pobs(1,23) = 792,
                           twobs(1,23)=600,
                           tobs(23)=0,

remark = 'Slot 16',
iob(45) = 24, ioh(45) = 1, xl(45) =  0.0252222,  xh(45) =  0.2517902,
                           yl(45) = -0.2517902,  yh(45) = -0.0252222,
                           zl(45) =  0.3052800,  zh(45) =  4.1651200,
                           kobs(24)= 0.696,
                           rcobs(24) = 234.46,
                           pobs(1,24) = 792,
                           twobs(1,24)=600,
                           tobs(24)=0,

remark = 'Slot 17',
iob(46) = 25, ioh(46) = 1, xl(46) =  0.3022600,  xh(46) =  0.5288280,
                           yl(46) = -0.2942590,  yh(46) = -0.0677545,
                           zl(46) =  0.3052800,  zh(46) =  4.1651200,
                           kobs(25) = 0.696,
                           rcobs(25) = 234.46,
                           pobs(1,25) = 792,
                           twobs(1,25)=600,
                           tobs(25)=0,

remark = 'Slot 18',
iob(47) = 26, ioh(47) = 1, xl(47) =  0.5842000,  xh(47) =  0.8137525,
                           yl(47) = -0.2517902,  yh(47) = -0.0252222,
                           zl(47) =  0.3052800,  zh(47) =  4.1651200,
                           kobs(26) = 0.696,
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                                rcobs(26) = 234.46,
                                pobs(1,26) = 792,
                                twobs(1,26)=600,
                                tobs(26)=0,

   remark = 'Slot 19',
   iob(48) = 27, ioh(48) = 1, xl(48) = -0.5762625, xh(48) = -0.3496945,
                                yl(48) = -0.5762625, yh(48) = -0.3496945,
                                zl(48) =  0.3052800, zh(48) =  4.1651200,
                                kobs(27) = 0.696,
                                rcobs(27) = 234.46,
                                pobs(1,27) = 792,
                                twobs(1,27)=600,
                                tobs(27)=0,

   remark = 'Slot 20',
   iob(49) = 28, ioh(49) = 1, xl(49) = -0.2943225, xh(49) = -0.0677545,
                                yl(49) = -0.5288280, yh(49) = -0.3022600
                                zl(49) =  0.3052800, zh(49) =  4.1651200,
                                kobs(28) = 0.696,
                                rcobs(28) = 234.46,
                                pobs(1,28) = 792,
                                twobs(1,28)=600,
                                tobs(28)=0,

   remark = 'Slot 21',
   iob(50) = 29, ioh(50) = 1, xl(50) =  0.0677545,  xh(50) =  0.2943225,
                                yl(50) = -0.5288280,  yh(50) = -0.3022600,
                                zl(50) =  0.3052800,  zh(50) =  4.1651200,
                                kobs(29) = 0.696,
                                rcobs(29) = 234.46,
                                pobs(1,29) = 792,
                                twobs(1,29)=600,
                                tobs(29)=0,

   remark = 'Slot 22',
   iob(51) = 30, ioh(51) = 1, xl(51) =  0.3496945,  xh(51) =  0.5762625,
                                yl(51) = -0.5762625,  yh(51) = -0.3496945,
                                zl(51) =  0.3052800,  zh(51) =  4.1651200,
                                kobs(30) = 0.696,
                                rcobs(30) = 234.46,
                                pobs(1,30) = 792,
                                twobs(1,30)=600,
                                tobs(30)=0,

   remark = 'Slot 23',
   iob(52) = 31, ioh(52) = 1, xl(52) = -0.2517902, xh(52) = -0.0252222,
                                yl(52) = -0.8137525, yh(52) = -0.5842000,
                                zl(52) =  0.3052800, zh(52) =  4.1651200,
                                kobs(31) = 0.696,
                                rcobs(31) = 234.46,
                                pobs(1,31) = 792,
                                twobs(1,31)=600,
                                tobs(31)=0,

   remark = 'Slot 24',
   iob(53) = 32, ioh(53) = 1, xl(53) =  0.0252222, xh(53) =  0.2517902,
                                yl(53) = -0.8137525, yh(53) = -0.5842000,
                                zl(53) =  0.3052800, zh(53) =  4.1651200,
                                kobs(32) = 0.696,
                                rcobs(32) = 234.46,
                                pobs(1,32) = 792,
                                twobs(1,32)=600,
                                tobs(32)=0,

$END
  nobs = 15,

   remark = 'create the obstacle field',
   remark = 'begin with fuel basket:  MPC-24, Holtec drawing 3926, sheet 2, rev 2',
```

```
remark = 'thermal conductivity given in J/m-s-K at 400C',
remark = 'data from Hi-Star FSAR Report HI-201260, chapter4',
remark = 'see table 4.4.5 for PWR thermal conductivity',

remark = 'general characteristics',
remark = '24 locations for spent fuel of similar geometric config',

remark = 'lay in x-cut plates first, left to right',

remark = 'thermal conductivity = kobs unit:   Watt/m/K = kg-m/s3/K',
remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',

remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
remark = 'Report HI-2012610',
remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
remark = 'thermal conductivity values from Table 4.4.7: generalized',
remark = 'thermal conductivity vs. temperature',
remark = 'choosing values at 400C',
remark = 'rcobs = specific heat',

remark = '24 Basket',
remark = 'A',
iob(1) = 1, ioh(1) = 1, xl(1) =  0.0000000, xh(1) =  0.3022600,
                        yl(1) =  0.8137525, yh(1) =  0.8216900,
                        zl(1) =  0.0000000, zh(1) =  4.4831000,
                        kobs(1) = 2.286,
                        rcobs(1) = 544.28

remark = 'B',
iob(2) = 1, ioh(2) = 1, xl(2) =  0.0000000, xh(2) =  0.5842000,
                        yl(2) =  0.5762625, yh(2) =  0.5842000,
                        zl(2) =  0.0000000, zh(2) =  4.4831000,

remark = 'C',
iob(3) = 1, ioh(3) = 1, xl(3) =  0.0000000, xh(3) =  0.8216900,
                        yl(3) =  0.2943225, yh(3) =  0.3022600,
                        zl(3) =  0.0000000, zh(3) =  4.4831000,

remark = 'D',
iob(4) = 1, ioh(4) = 1, xl(4) =  0.0000000, xh(4) =  0.8216900,
                        yl(4) =  0.0172847, yh(4) =  0.0252222,
                        zl(4) =  0.0000000, zh(4) =  4.4831000,

remark = 'A3',
iob(5) = 1, ioh(5) = 1, xl(5) =  0.8137525, xh(5) =  0.8216900,
                        yl(5) =  0.0000000, yh(5) =  0.3022600,
                        zl(5) =  0.0000000, zh(5) =  4.4831000,

remark = 'B3',
iob(6) = 1, ioh(6) = 1, xl(6) =  0.5762625, xh(6) = 0.5842000,
                        yl(6) =  0.0000000, yh(6) = 0.5842000,
                        zl(6) =  0.0000000, zh(6) = 4.4831000,

remark = 'C3',
iob(7) = 1, ioh(7) = 1, xl(7) =  0.2943225, xh(7) = 0.3026600,
                        yl(7) =  0.0000000, yh(7) = 0.8216900,
                        zl(7) =  0.0000000, zh(7) = 4.4831000,

remark = 'D3',
iob(8) = 1, ioh(8) = 1, xl(8) =  0.0172847, xh(8) = 0.0252222,
                        yl(8) =  0.0000000, yh(8) = 0.8216900,
                        zl(8) =  0.0000000, zh(8) = 4.4831000,

remark = 'lay in 1/2in thick MPC shell at phi67.25in',
remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
remark = 'pages 3 and 4',
iob(10) = 3, ioh(10) = 1, ral(10) =  0.8477250, rah(10) = 0.8731250,
remark = 'actual spacing - eliminated b/c of grid resolution rah(23) =  0.854075,',
                          zl(10)  =  0.0000000, zh(10)  =  4.5212000,
                          kobs(3) = 0.0478,
```

```
                          rcobs(3) = 502.41,

remark = 'lay in MPC base plate 2.5in thick',
remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
remark = 'page 2(thickness), page 3(diameter)',
iob(11) = 4, ioh(11) = 1, ral(11) =  0.0000000, rah(11) = 0.8731250, remark = '0.8683625',
                          zl(11)  = -0.0635000, zh(11)  = 0.0000000,
                          kobs(4) = 0.0478,
                          rcobs(4) = 502.41,

remark = 'not including MPC lid - am assuming system is open',
remark = 'not including drain sump or fuel basket support rails',

remark = 'lay in overpack components',
remark = 'Holtec print 3913:  Hi-Star 100 Overpack Elevation View',
remark = 'base plate, page 2',
remark = '6in thick, 83.5in outside diameter',
iob(12) = 5, ioh(12) = 1, ral(12) =  0.0000000, rah(12) =  1.0572750,
                          zl(12)  = -0.21590000, zh(12) = -0.0635000,
                          kobs(5) = 30.3456,
                          rcobs(5) = 418.67,

remark = 'overpack inner shell, page 2',
remark = 'simplified to incorporate the full cask wall',
remark = '68.75in inside diameter, 73.75in outside diameter',
remark = '191.125in height from cask base plate',
iob(13) = 6, ioh(13) = 1, ral(13) =  0.8731250, rah(13) =  0.9366250,
                          zl(13)  = -0.0635000, zh(13)  =  4.7910750,
                          kobs(6) = 2.8117,
                          rcobs(6) = 502.41,

remark = 'overpack multilayered shells',
remark = 'simplified to incorporate the full cask wall',
remark = '73.75in inside diameter, 6 in thick 4x1.25 gamma layers + 1in shell',
iob(14) = 7, ioh(14) = 1, ral(14) =  0.9366250, rah(14) =  1.0890250,
                          zl(14)  = -0.0635000, zh(14)  =  4.7910750,
                          kobs(7) = 2.8117,
                          rcobs(7) = 502.41,

remark = 'overpack neutron shielding',
remark = 'simplified to incorporate neutron shield and radial channels that form the shell',
remark = 'details from page 6',
remark = 'thickness of neutron shield = 4-7/16in + thickness of channel 1/2in = 4-15/16in',
remark = 'idealized inside diameter = 85.75in, outside diameter = 95.625in',
remark = 'height runs from 8-3/4in off cask base to 173-1/8in',
iob(15) = 8, ioh(15) = 1, ral(15) =  1.0890250, rah(15) =  1.2144375,
                          zl(15)  =  0.0635000, zh(15)  =  4.4037250,
                          kobs(8) = 2.8117,
                          rcobs(8) = 1632.85,

remark = 'overpack - approximation of outside rim around lid',
remark = 'idealized inside diameter = 68.75in, outside diameter = 83.25in',
remark = '6in thick',
remark = 'approximating from page 2, print 3913',
iob(16) = 9, ioh(16) = 1, ral(16) =  0.8731250, rah(16) =  1.0572750,
                          zl(16)  =  4.7910750, zh(16)  =  4.9434750,
                          kobs(9) = 2.8117,
                          rcobs(9) = 1632.85,

remark = 'ready to lay in the PWRs and heat source information',
remark = 'supposition:  PWR completely fill open area in MPC basket formation',
remark = 'doing this until better geometry provided',
remark = 'shortening PWR units by 12in on each end (centered)'
remark = 'based on info from PA Cox - check with Amit/Bis - ok',

remark = 'thermal conductivity is based on design specifications of Table 4.4.5',
remark = 'trend line created from data shown then conservatively extrapolated',
remark = 'to 400C;  values implemented at 232.22C from table',

remark = 'power values based on worst case scenario; 19008 total Watts, from',
remark = 'Table 4.4.18:  MPC-24 Basket Peak Fuel Claddings Temp as Function...',
```

```
 tobs(1) = 0.0,


 remark = 'lay in new 24 assembly',
 remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',

 remark = 'Slot 2',
 iob(17) = 10, ioh(17) = 1, xl(17) =  0.0252222, xh(17) =  0.2517902,
                            yl(17) =  0.5842000, yh(17) =  0.8137525,
                            zl(17) =  0.3052800, zh(17) =  4.1651200,
                             kobs(10) = 0.696,
                             rcobs(10) = 234.46,
                             pobs(1,10) = 792,

 remark = 'Slot 5',
 iob(18) = 11, ioh(18) = 1, xl(18) =  0.0677545, xh(18) = 0.2943225,
                            yl(18) =  0.3022600, yh(18) = 0.5288280,
                            zl(18) =  0.3052800, zh(18) = 4.1651200,
                            kobs(11) = 0.696,
                            rcobs(11) = 234.46,
                            pobs(1,11) = 792,

 remark = 'Slot 6',
 iob(19) = 12, ioh(19) = 1, xl(19) =  0.3496945, xh(19) = 0.5762625,
                            yl(19) =  0.3496945, yh(19) = 0.5762625,
                            zl(19) =  0.3052800, zh(19) = 4.1651200,
                            kobs(12) = 0.696,
                            rcobs(12) = 234.46,
                            pobs(1,12) = 792,

 remark = 'Slot 10',
 iob(20) = 13, ioh(20) = 1, xl(20) =  0.0252222, xh(20) = 0.2517902,
                            yl(20) =  0.0252222, yh(20) = 0.2517902,
                            zl(20) =  0.3052800, zh(20) = 4.1651200,
                            kobs(13) = 0.696,
                            rcobs(13) = 234.46,
                            pobs(1,13) = 792,

 remark = 'Slot 11',
 iob(21) = 14, ioh(21) = 1, xl(21) =  0.3022600, xh(21) =  0.5288280,
                            yl(21) =  0.0677545, yh(21) =  0.2942590,
                            zl(21) =  0.3052800, zh(21) =  4.1651200,
                            kobs(14) = 0.696,
                            rcobs(14) = 234.46,
                            pobs(1,14) = 792,

 remark = 'Slot 12',
 iob(22) = 14, ioh(22) = 1, xl(22) =  0.5842000, xh(22) = 0.8137525,
                            yl(22) =  0.0252222, yh(22) = 0.2517902,
                            zl(22) =  0.3052800, zh(22) = 4.1651200,
                            kobs(15) = 0.696,
                            rcobs(15) = 234.46,
                            pobs(1,15) = 792,
$FL

   remark = 'setting 1atm in Pa',
   presi = 101325.0,

$END

$BF
$END

$TEMP

   remark = 'setting initial temps to 25C to get things started',
   tempi = 300.0,

$END

$GRAFIC
```

```
    icolor = 2,

    remark = 'jobsbk = 10,  jobsf = 14,',

    ncplts = 4,
    contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
    contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
    contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
    contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,
$END


$PARTS
$END
```

!**********!

Run id: CloseLid2DModel
CloseLid2DModel
23 August 2005 Chnaging the fluid properties to that of helium.
23 August 2005 Adding a lid on top of the cask.
22 August 2005 Updating the thermal conductivity of the obstacle from Table 4.4.7, 1.954*1.7307 in SI
units
22 August 2005 Modifying the properties of the power obstacle. Making it equal to one in FSAR
Also changing the boundary condition wr as wall instead of continuative.
09 August 2005 remoing top free portion of the air
03 August 2005 Modeling 24 MPC as one power source in cylindrical geometry. Cv air= 713.5 J/Kg 0K

22 July 2005 Modeling just one power source in 2 dimentional setting. removing all other obstacles
.
Cartesin geometry only.
05 July 2005 Default value of gas constant R was in wrong units. Corrected here.

20 June 2005
Updated informational fields

24 May 2005
Turning off air flow and allowing thermal progression only

11 May 2005 Chris Ryder asked that I look at the 24 Basket with different fuel.
Resetting obstacle field with this basket and fuel source. Basic parameters will be the same. Grid will need to be slightly reworked to accomodate new fuel spacing.

```
$XPUT

  icmprs  = 0,   remark = 'incompressible flow',
  iorder  = 3,   remark = 'setting iorder = 3 monotonically increasing',
  itb     = 0,   remark = 'no free surfaces',
```

```
nmat   = 1,   remark = '1 compressible mat',
iwsh   = 0,   remark = 'turn off wall shear',

remark = 'switch to remark out when flow on',
remark = 'ihonly = 0',    remark = 'solve all conservation equations',
remark = 'ihonly = 2',    remark = 'turn off material flow, heat transfer only',
imphtc = 1,    remark = 'implicit eval of temp terms',
remark = 'ihtc   = 0',    remark = 'turn off heat transfer',
ihtc   = 2,    remark = 'turn on heat conduction through obstacles',
ifrho  = 1,
ifenrg = 2,    remark = 'fluid energy transport on',
gz = -9.81,    remark = 'gravity',

remark='trest   = 6.023',
twfin   = 300.0,  remark = 'simulation end, seconds',
pltdt   = 5,   remark = 'plotting interval, seconds',
hpltdt  = 1.0,   remark = 'history interval, seconds',
delt    = 1.0e-5, remark = 'time step, seconds',
remark = 'istdy   = 0',    remark = 'accelerate to steady state using non-phys transient',
            remark = 'minimum timestep',
dtmax   = 0.01,   remark = 'maximum timestep',

autot   = 2.0, remark = 'timestep by stability',
omega   = 1.7, remark = 'default setting for over-relaxation factor',

epsadj  = 1.0, remark = 'standard convergence criterion',

igmres = 1,

remark = 'iadix   = 1',  remark = 'pressure iteration options (x,y,z) ADI',
remark = 'iadiy   = 1',
remark = 'iadiz   = 1',
ihelp = 2,
ifrho  = 1,
ifvelp = 0,
ipdis  = 1, remark='hydrostatic pressure in z direction',


$END

$LIMITS

itflmx  = 1000000, remark = 'maximum pressure iteration failures allowed',
itmax   = 10,   remark = 'allowable inner iteration count',
itdtmx  = 100,
            remark = 'adjust itmax early to quickly step through start-up',
```

```
   negtmx  =  100000,  remark = 'negative rhoe resets',
   ncflmx  =  1000,    remark = 'convection failures allowed',

 $END

 $PROPS

   remark  = 'set up properties on fluid 2 to allow for compressibility option',

   units   = 'si',
   rhof    = 0.178,  remark='1.2',
   mu1     = 1.9e-5, remark='1.86e-5', remark = 'viscosity air',
   cv1     = 2077.5, remark='713.5',   remark='oldvalue=1883.7',  remark = 'specific heat air',
   thc1    = 0.142,  remark='0.0264',  remark = 'thermal conductivity air',
   thexf1   = 1.0e-3, remark='3.48e-3', remark = 'thermal expansion: p594 (Batchelor, Fluid
Dynamic
s)',
   tstar   = 1000.0, remark = 'ref temp for air properties',
   remark  = 'rf2     = 287.',    remark = 'gas constant for air'

 $END

 $SCALAR
   remark = 'none needed for these simulations',
 $END

 $BCDATA

   remark = 'top wall is continuative (wt) or boundary 6',
   remark = 'set up as no ventilation',
   remark = 'made all bc continuative to start so cask is set in infinite air',

   wl    = 1,   remark = 'low x, symmetric',
   wr    = 2,   remark = 'high x',
   wf    = 1,   remark = 'low y, symmetric',
   wbk   = 1,   remark = 'high y',
   wb    = 2,   remark = 'low z',
   wt    = 5,   remark = 'high z, continuative',
   remark = 'eventually add cross-velocity at top of cask if necessary',
   tbcd=300.0,
   pbc(6) = 101266.8054123,
   remark = 'f boundaries are automatically 0 (mat 2)',


 $END
```

```
  nxcelt = 100,
   px(1) = -2.4336375,  nxcell(1) = 100,
   px(2) =  2.4336375,

  nycelt = 100,
   py(1) = -2.4336375,  nycell(1) = 100,
   py(2) =  2.4336375,

  nzcelt = 100,
   pz(1) = -0.2159000,  nzcell(1) = 100,
   pz(2) =  6.0,

$MESH

   remark = 'full Cartesian mesh',
   icyl    = 1,
   nxcelt   = 55,
    px(1) =  0.0000000,  nxcell(1) = 15, remark = 'power source',
    px(2) =  0.6302068,  nxcell(2) = 20, remark = 'airgap',
    px(3) =  0.8477250,  nxcell(3) = 10, remark = 'cylindrical walls',
    px(4) =  1.2144375,  nxcell(4) = 10, remark = 'gap between room and cask wall',
    px(5) =  2.4336375,

  nycelt   = 1,
    pya(1) =  0.0000000,  nycell(1) = 1, remark = 'air',
    pya(2) = 10.0000000,

  nzcelt    = 84,
    pz(1)  = -0.2159000,  nzcell(1)  = 5, remark = 'bottom overpack base plate',
    pz(2)  = -0.0635000,  nzcell(2)  = 2, remark = 'top overpack base plate',
    pz(3)  =  0.0000000,  nzcell(3)  = 2, remark = 'bottom of fuel basket/bottom of MPC shell',
    pz(4)  =  0.0635000,  nzcell(4)  = 5, remark = 'bottom overpack neutron shielding',
    pz(5)  =  0.3052800,  nzcell(5)  = 47, remark = 'begin fuel',
    pz(6)  =  4.1651200,  nzcell(6)  = 5, remark = 'top fuel',
    pz(7)  =  4.4037250,  nzcell(7)  = 2, remark = 'top overpack neutron shielding',
    pz(8)  =  4.4704000,  nzcell(8)  = 2, remark = 'top of fuel basket',
    pz(9)  =  4.5212000,  nzcell(9)  = 9, remark = 'top of MPC shell',
    pz(10) =  4.7910750,  nzcell(10) = 5, remark = 'top overpack layering system',
    pz(11) =  4.9434750,  remark='nzcell(11) = 15', remark = 'top overpack idealized lid edge',
    remark='pz(12) =  6.0',                remark = '3+ feet higher than cask',
$END


$OBS
  nobs = 9,
```

iob(1) = 1, ioh(1) = 1, ral(1) = 0.0000000, rah(1) = 0.8731250, remark = '0.8683625',
zl(1) = -0.0635000, zh(1) = 0.0000000,
kobs(1) = 19.038, remark='0.0478',
rcobs(1) = 502.41,

iob(2) = 2, ioh(2) = 1, ral(2) = 0.0000000, rah(2) = 1.0572750,
zl(2) = -0.21590000, zh(2) = -0.0635000,
kobs(2) = 30.3456,
rcobs(2) = 418.67,

iob(3) = 3, ioh(3) = 1, ral(3) = 0.8477250, rah(3) = 0.8731250,
zl(3) = 0.0000000, zh(3) = 4.5212000,
kobs(3) = 19.038, remark='0.0478',
rcobs(3) = 502.41,

iob(4) = 4, ioh(4) = 1, ral(4) = 0.8731250, rah(4) = 0.9366250,
zl(4) = -0.0635000, zh(4) = 4.7910750,
kobs(4) =19.038, remark=' 2.8117',
rcobs(4) = 502.41,

iob(5) = 5, ioh(5) = 1, ral(5) = 0.9366250, rah(5) = 1.0890250,
zl(5) = -0.0635000, zh(5) = 4.7910750,
kobs(5) = 19.038, remark='2.8117',
rcobs(5) = 502.41,

iob(6) = 6, ioh(6) = 1, ral(6) = 1.0890250, rah(6) = 1.2144375,
zl(6) = 0.0635000, zh(6) = 4.4037250,
kobs(6) = 2.8117,
rcobs(6) = 1632.85,

iob(7) = 7, ioh(7) = 1, ral(7) = 0.8731250, rah(7) = 1.0572750,
zl(7) = 4.7910750, zh(7) = 4.9434750,
kobs(7) = 2.8117,
rcobs(7) = 1632.85,

```
iob(8) = 8, ioh(8) = 1, ral(8) = 0.0000000, rah(8) = 0.6302068,
                zl(8) =  0.3052800, zh(8) =  4.1651200,
                kobs(8) = 3.3818,
                rcobs(8) = 234.46,
                pobs(1,8) = 528, remark='total power/4/9 or 19008/4/9',
                twobs(1,8) = 600,
                tobs(8)=0,

  remark= 'adding a lid at the top of the cask',

iob(9) = 9, ioh(9) = 1, ral(9) =  0.0000000, rah(9) = 0.8731250, remark = '0.8683625',
                zl(9)  = 4.7910750, zh(9)  = 4.9434750,
                kobs(9) = 19.038,
                rcobs(9) = 502.41,


$END
 nobs = 15,

  remark = 'create the obstacle field',
  remark = 'begin with fuel basket:  MPC-24, Holtec drawing 3926, sheet 2, rev 2',

  remark = 'thermal conductivity given in J/m-s-K at 400C',
  remark = 'data from Hi-Star FSAR Report HI-201260, chapter4',
  remark = 'see table 4.4.5 for PWR thermal conductivity',

  remark = 'general characteristics',
  remark = '24 locations for spent fuel of similar geometric config',

  remark = 'lay in x-cut plates first, left to right',

  remark = 'thermal conductivity = kobs unit:   Watt/m/K = kg-m/s3/K',
  remark = 'density * specific heat = rcobs unit:  J/m3/K = kg/m/s2/K',
  remark = 'lumped obstacle specific heat = mobs unit:   J/K = kg-m2/s2/K',

  remark = 'using Alloy X description of cask components from Hi Star 100 FSAR',
  remark = 'Report HI-2012610',
  remark = 'thermal conductivity values from Table 1.A.5:  Alloy X and constituent',
  remark = 'thermal conductivity values from Table 4.4.7: generalized',
  remark = 'thermal conductivity vs. temperature',
  remark = 'choosing values at 400C',
  remark = 'rcobs = specific heat',

  remark = '24 Basket',
  remark = 'A',
```

```
iob(1) = 1, ioh(1) = 1, xl(1) =  0.0000000, xh(1) =  0.3022600,
                yl(1) =  0.8137525, yh(1) =  0.8216900,
                zl(1) =  0.0000000, zh(1) =  4.4831000,
                kobs(1) = 2.286,
                rcobs(1) = 544.28,

remark = 'B',
iob(2) = 1, ioh(2) = 1, xl(2) =  0.0000000, xh(2) =  0.5842000,
                yl(2) =  0.5762625, yh(2) =  0.5842000,
                zl(2) =  0.0000000, zh(2) =  4.4831000,

remark = 'C',
iob(3) = 1, ioh(3) = 1, xl(3) =  0.0000000, xh(3) =  0.8216900,
                yl(3) =  0.2943225, yh(3) =  0.3022600,
                zl(3) =  0.0000000, zh(3) =  4.4831000,

remark = 'D',
iob(4) = 1, ioh(4) = 1, xl(4) =  0.0000000, xh(4) =  0.8216900,
                yl(4) =  0.0172847, yh(4) =  0.0252222,
                zl(4) =  0.0000000, zh(4) =  4.4831000,

remark = 'A3',
iob(5) = 1, ioh(5) = 1, xl(5) =  0.8137525, xh(5) =  0.8216900,
                yl(5) =  0.0000000, yh(5) =  0.3022600,
                zl(5) =  0.0000000, zh(5) =  4.4831000,

remark = 'B3',
iob(6) = 1, ioh(6) = 1, xl(6) =  0.5762625, xh(6) = 0.5842000,
                yl(6) =  0.0000000, yh(6) = 0.5842000,
                zl(6) =  0.0000000, zh(6) = 4.4831000,

remark = 'C3',
iob(7) = 1, ioh(7) = 1, xl(7) =  0.2943225, xh(7) = 0.3026600,
                yl(7) =  0.0000000, yh(7) = 0.8216900,
                zl(7) =  0.0000000, zh(7) = 4.4831000,

remark = 'D3',
iob(8) = 1, ioh(8) = 1, xl(8) =  0.0172847, xh(8) = 0.0252222,
                yl(8) =  0.0000000, yh(8) = 0.8216900,
                zl(8) =  0.0000000, zh(8) = 4.4831000,

remark = 'lay in 1/2in thick MPC shell at phi67.25in',
remark = 'see Holtec print 3923:  MPC Enclosure Vessel Lid Details',
remark = 'pages 3 and 4',
iob(10) = 3, ioh(10) = 1, ral(10) =  0.8477250, rah(10) = 0.8731250,
remark = 'actual spacing - eliminated b/c of grid resolution rah(23) =  0.854075,',
```

```
                zl(10)  =  0.0000000, zh(10)  =  4.5212000,
                kobs(3) = 0.0478,
                rcobs(3) = 502.41,

remark = 'lay in MPC base plate 2.5in thick',
remark = 'Holtec print 2923:  MPC Enclosure Vessel Elevation Details',
remark = 'page 2(thickness), page 3(diameter)',
iob(11) = 4, ioh(11) = 1, ral(11) =  0.0000000, rah(11) = 0.8731250, remark = '0.8683625',
                zl(11)  = -0.0635000, zh(11)  = 0.0000000,
                kobs(4) = 0.0478,
                rcobs(4) = 502.41,

remark = 'not including MPC lid - am assuming system is open',
remark = 'not including drain sump or fuel basket support rails',

remark = 'lay in overpack components',
remark = 'Holtec print 3913:  Hi-Star 100 Overpack Elevation View',
remark = 'base plate, page 2',
remark = '6in thick, 83.5in outside diameter',
iob(12) = 5, ioh(12) = 1, ral(12) =  0.0000000, rah(12) =  1.0572750,
                zl(12)  = -0.21590000, zh(12) = -0.0635000,
                kobs(5) = 30.3456,
                rcobs(5) = 418.67,

remark = 'overpack inner shell, page 2',
remark = 'simplified to incorporate the full cask wall',
remark = '68.75in inside diameter, 73.75in outside diameter',
remark = '191.125in height from cask base plate',
iob(13) = 6, ioh(13) = 1, ral(13) =  0.8731250, rah(13) =  0.9366250,
                zl(13)  = -0.0635000, zh(13)  =  4.7910750,
                kobs(6) = 2.8117,
                rcobs(6) = 502.41,

remark = 'overpack multilayered shells',
remark = 'simplified to incorporate the full cask wall',
remark = '73.75in inside diameter, 6 in thick 4x1.25 gamma layers + 1in shell',
iob(14) = 7, ioh(14) = 1, ral(14) =  0.9366250, rah(14) =  1.0890250,
                zl(14)  = -0.0635000, zh(14)  =  4.7910750,
                kobs(7) = 2.8117,
                rcobs(7) = 502.41,

remark = 'overpack neutron shielding',
remark = 'simplified to incorporate neutron shield and radial channels that form the shell',
remark = 'details from page 6',
remark = 'thickness of neutron shield = 4-7/16in + thickness of channel 1/2in = 4-15/16in',
remark = 'idealized inside diameter = 85.75in, outside diameter = 95.625in',
```

```
remark = 'height runs from 8-3/4in off cask base to 173-1/8in',
iob(15) = 8, ioh(15) = 1, ral(15) =  1.0890250, rah(15) =  1.2144375,
                zl(15)  =  0.0635000, zh(15)  =  4.4037250,
                kobs(8) = 2.8117,
                rcobs(8) = 1632.85,

remark = 'overpack - approximation of outside rim around lid',
remark = 'idealized inside diameter = 68.75in, outside diameter = 83.25in',
remark = '6in thick',
remark = 'approximating from page 2, print 3913',
iob(16) = 9, ioh(16) = 1, ral(16) =  0.8731250, rah(16) =  1.0572750,
                zl(16)  =  4.7910750, zh(16)  =  4.9434750,
                kobs(9) = 2.8117,
                rcobs(9) = 1632.85,

remark = 'ready to lay in the PWRs and heat source information',
remark = 'supposition:  PWR completely fill open area in MPC basket formation',
remark = 'doing this until better geometry provided',
remark = 'shortening PWR units by 12in on each end (centered)'
remark = 'based on info from PA Cox - check with Amit/Bis - ok',

remark = 'thermal conductivity is based on design specifications of Table 4.4.5',
remark = 'trend line created from data shown then conservatively extrapolated',
remark = 'to 400C;  values implemented at 232.22C from table',

remark = 'power values based on worst case scenario; 19008 total Watts, from',
remark = 'Table 4.4.18:  MPC-24 Basket Peak Fuel Claddings Temp as Function...',
tobs(1) = 0.0,


remark = 'lay in new 24 assembly',
remark = 'Slot 1:  MPC-24 Fuel Basket Arrangement, drawing # 3926, sheet 2',

remark = 'Slot 2',
iob(17) = 10, ioh(17) = 1, xl(17) =  0.0252222, xh(17) =  0.2517902,
                yl(17) =  0.5842000, yh(17) =  0.8137525,
                zl(17) =  0.3052800, zh(17) =  4.1651200,
                kobs(10) = 0.696,
                rcobs(10) = 234.46,
                pobs(1,10) = 792,

remark = 'Slot 5',
iob(18) = 11, ioh(18) = 1, xl(18) =  0.0677545, xh(18) = 0.2943225,
                yl(18) =  0.3022600, yh(18) = 0.5288280,
                zl(18) =  0.3052800, zh(18) = 4.1651200,
                kobs(11) = 0.696,
```

```
                    rcobs(11) = 234.46,
                    pobs(1,11) = 792,

  remark = 'Slot 6',
  iob(19) = 12, ioh(19) = 1, xl(19) =  0.3496945, xh(19) = 0.5762625,
                    yl(19) =  0.3496945, yh(19) = 0.5762625,
                    zl(19) =  0.3052800, zh(19) = 4.1651200,
                    kobs(12) = 0.696,
                    rcobs(12) = 234.46,
                    pobs(1,12) = 792,

  remark = 'Slot 10',
  iob(20) = 13, ioh(20) = 1, xl(20) =  0.0252222, xh(20) = 0.2517902,
                    yl(20) =  0.0252222, yh(20) = 0.2517902,
                    zl(20) =  0.3052800, zh(20) = 4.1651200,
                    kobs(13) = 0.696,
                    rcobs(13) = 234.46,
                    pobs(1,13) = 792,

  remark = 'Slot 11',
  iob(21) = 14, ioh(21) = 1, xl(21) =  0.3022600, xh(21) =  0.5288280,
                    yl(21) =  0.0677545, yh(21) =  0.2942590,
                    zl(21) =  0.3052800, zh(21) =  4.1651200,
                    kobs(14) = 0.696,
                    rcobs(14) = 234.46,
                    pobs(1,14) = 792,

  remark = 'Slot 12',
  iob(22) = 14, ioh(22) = 1, xl(22) =  0.5842000, xh(22) = 0.8137525,
                    yl(22) =  0.0252222, yh(22) = 0.2517902,
                    zl(22) =  0.3052800, zh(22) = 4.1651200,
                    kobs(15) = 0.696,
                    rcobs(15) = 234.46,
                    pobs(1,15) = 792,
$FL

  remark = 'setting 1atm in Pa',
  presi = 101325.0,

$END

$BF
$END

$TEMP
```

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   remark = 'setting initial temps to 25C to get things started',
   tempi = 300.0,

$END

$GRAFIC

   icolor = 2,

   remark = 'jobsbk = 10,  jobsf = 14,',

   ncplts = 4,
   contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
   contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
   contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
   contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,
$END


$PARTS
$END
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Initial Entry: Pavan Shukla and Sidney Chocron,
Date: 24 June 2005

Title: Thermal analysis of HI-STAR 100 cask system.

Personnel: Pavan Shukla, CNWRA, Division 20, and Sidney Chocron, Southwest Research Institute, Division 18,

Project: This portion of the notebook summarises the work done by Pavan Shukla, Sidney Chorcron, Wei Li, and Steve Green on thermal analysis of the HI-STAR 100 transportation cask. He objective of this project is to understand the thermal behaviour of the cask when it is closed and when it is open under ambient conditions. Axisymmetric two-dimentional models of the open and closed cask are developed using FLOW-3D and FLUENT.

Summary of entries in the Notebook

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Entry: Pavan Shukla, Febuary 27th, 2006

Single Fuel Assemble Model **Febuary 27th, 2006**

Run id: siglefuelassemblymodel (inputdeck is attached at the end)

Description:

The single-fuel assemble model is developed to model one fuel assembly in the open cask. This model can also be used to determine the thermal behavior of the fuel assemblies on the staging rack in the dry transfer facility. When the cask is open, the air will enter in the cask through the colder regions and exit from the hotter regions. The closed cask thermal analysis show that fuel basket with multiple fuel assemblies is hotter in the center and colder on the side. Therefore, when cask is open, the fluid will enter the cask through the space between fuel basket and multipurpose canister shell, and as air travel downwards, it will heat up. The fuel basket for twenty-four pressurized fuel assemblies has undercuts for the airflow, and they provide passage for the air flow. The hot air will presumably enter the fuel basket through these undercuts and flow upward in the channels between fuel assemblies. To model this airflow process, a simple single-fuel-assembly model is developed.

The single-feel-assembly two-dimensional model consists of a half of a fuel assembly and adjacent channel for the fluid flow. The model can be described in the Cartesian coordinate system where X and Y axis are in horizontal and vertical direction, and Z axis is in the direction perpendicular to the XY plane. A schematic diagram of the multipurpose furl canister cross section with twenty-four fuel basket is presented in the HI-STAR FSAR. All four sides of the 9th fuel assembly are simulated in the Flow-3D. A schematic diagram of the model is presented in Figure below. The fluid flow was modeled in the 1.538 cm wide channel which is half of distance between two adjacent fuel assemblies. The thermal effect of adjacent fuel assembly is accounted for by imposing the symmetry boundary condition at right boundary. The symmetry boundary condition is also applied at the left boundary. To simulate the effect of other half of the fuel assembly, the symmetry boundary condition is applied on the middle plane which is marked by dash line in the Figure . The fuel assembly is 3.5 meters high and 0.1135 meters wide. The thickness of the fuel assembly along Z direction is 90.64 cm. [4×8.92 inch], and a single mesh cell is assigned along the Z direction.

In this model, only conduction and convection heat transfer processes take place to remove heat form the fuel assembly. The top and bottom walls are open, and air enters through the bottom wall and leave at the top. The bottom wall is at a constant temperature, and air entering through the boundary is at a uniform constant temperature. The top wall is at a constant pressure and at a constant temperature. The top wall boundary condition ensures that if air enters through the

boundary, it will be at the ambient temperature. The left and right boundaries in the model are defined as symmetric walls, and the boundaries at Z=0 and Z=90.64 cm are defined as periodic.

The maximum power generated by a pressurized water reactor fuel assembly is 792 watts. In this model, the thickness of the fuel assembly in Z direction is equal to four times its width. Since heat is disspipated from the sidewalls, the decay heat load of the fuel assembly in this model is also 792 watts. Furthermore, in this model, the Alloy-X and boral panels are assumed to be part of the fuel assembly and their effective thermal conductivities same as that of the fuel assembly. The thermal conductivity of the fuel assemble is 0.16 watts/meter-°K. The input file is attached in the Appendix.

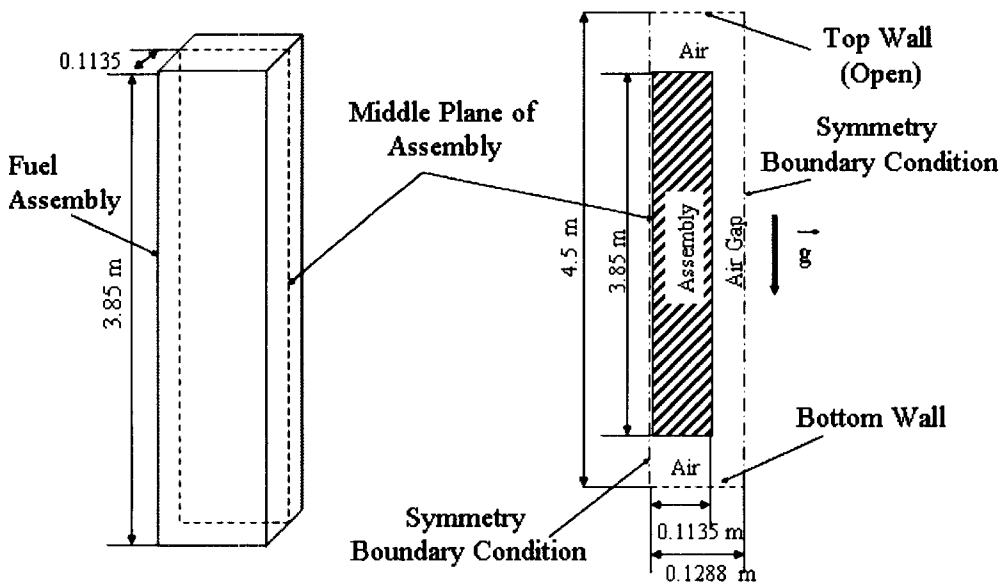

Figure: Schematic diagram of the single fuel assemble model.

Model Parameters:
The maximum power generated by a pressurized water reactor fuel assembly is 792 watts. In this model, the thickness of the fuel assembly in Z direction is equal to four times its width. Since heat is disspipated from the sidewalls, the decay heat load of the fuel assembly in this model is also 792 watts. Furthermore, in this model, the Alloy-X and boral panels are assumed to be part of the fuel assembly and their effective thermal conductivities same as that of the fuel assembly. The thermal conductivity of the fuel assemble is 0.16 watts/meter-°K.

Results: The model is simulated for two initial temperatures of fluid entering through the bottom wall in the model. The steady-state temperature profile of the fuel assembly with fluid entering at 350 °K is presented in Figure below. In this case, the fuel assembly attains a

maximum temperature of 530 °K . For fluid entering at 400 °K, the maximum temperature of the fuel assembly is 560 °K. The input file is attached in the Appendix.

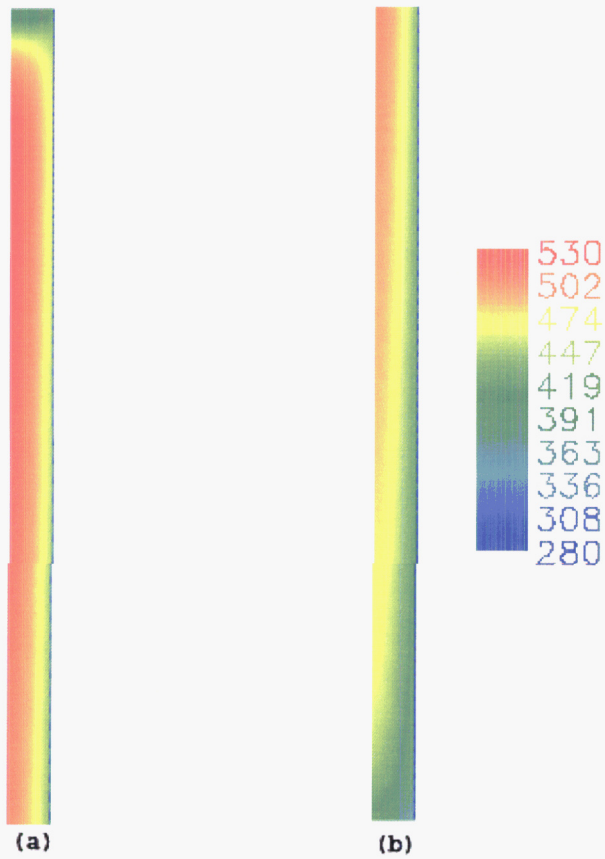

Figure: Steady State temperature distribution of the fuel assemble in the sigle fuel assemble model. This figure represents the fuel assemble into two parts: a) Upper part of the fuel assemble, b) Lower part of the fuel assembly.

Entry: Pavan Shukla, March 2nd, 2006

Testrun for FLUENT Version 6.2.16 **March 2nd, 2006**

Objective:

The comupational fluid dynamics software fluent was installed on computer # 3029. A test case was executed to validate the software, and to check its installation.

Problem Description

The initial test problem is taken from FLUENT manual, and it is titles as "Tutorial 1: Introduction to Using FLUENT: Fluid Flow and Heat Transfer in a mixing Elbow" in the FLUENT manual. The problem to be considered is shown schematically in Figure below. A cold fluid at 26 °C enters through the large pipe and mixes with a warmer uid at 40 °C in the elbow. The pipe dimensions are in inches, and the fluid properties and boundary conditions are given

in SI units.

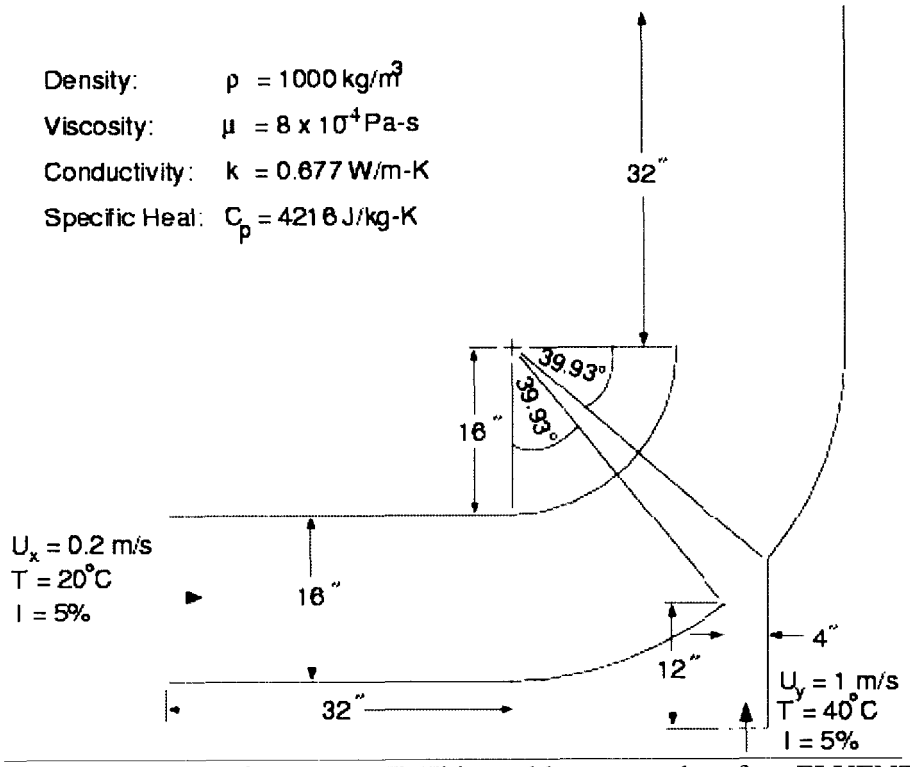

Figure: The initial test problem for FLUENT. This problem was taken fron FLUENT manual: Tutorial 1. Introduction to Using FLUENT: Fluid Flow and Heat Transfer in Mixing Elbow.

Results:
The problem is simulated using Fluent. The results are summarized below. The calculated velocity, and temperature distribution and in agreement with ones reported in the tutorial.

The predicted velocity distribution is presented in the following Figure. The calculated values are in agreement with one reported in FLUENT Tutorial#1 (Figure 1.5).

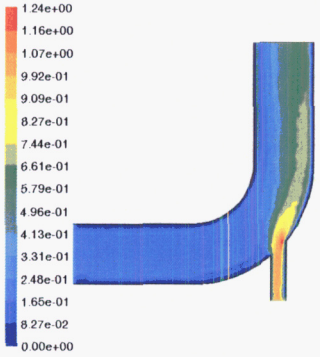

Figure: Calculated velocity distribution inside the elbow. The results are in agreement with one present in Figure 1.5 of the tutorial.

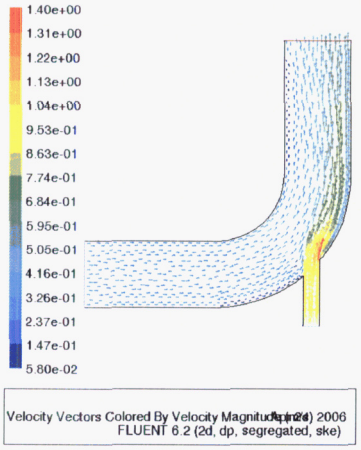

Figure: Velocity vectors inside the elbow. The results are in agreement with one present in Figure 1.7 of the tutorial.

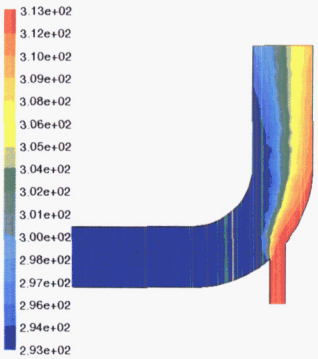

Figure: Calculated temperature distribution of the fluid inside the elbow. The results are in agreement with one presented in Figure 1.6 of the tutorial.

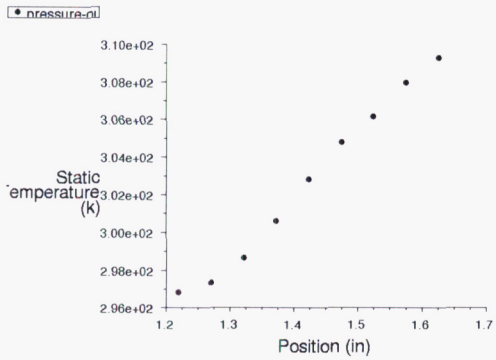

Figure: Temperature distribution at the outlet. Values are in agreement with ones reported in Figure 1.9.

The input and output files files are stored in the disk attched with this scientific note book. The files for this test run can be found in the subdirector called testcase. The input and output files are elbow-testrun.cas and elbow-testrun.dat.

Entry: Pavan Shukla, 15 March 2006

Objective: FLUENT is capable of modeling buoyancy-driven turbulent natural convection of a fluid phase, conduction of heat in solid objects, and radiation heat transfer between solid surfaces. Its ability to model natural convection and radiation heat transfer in a closed system is tested in this report. Two test cases are solved using FLUENT.

In the first test case, a heated cylinder is concentrically placed inside another cylinder. The annular cavity between cylinders is filled with nitrogen. The experimental results reported by Kuehn and Goldstein (1976, 1978) are used here to validate FLUENT Version 6.2.16.

In the second test case, the side walls of a square box are maintained at constant temperatures, and the top and bottom plates are thermally insulated. The buoyancy-driven natural convection and radiation heat transfer is modeled using FLUENT Version 6.2.16. In this report, the calculation results are compared to the results reported by Yücel, et al (1989) to validate the software.

Reference:

FLUENT, Inc. *FLUENT.* Version 6.2.16. FLUENT Incorporated: Lebanon, New Hampshire. 2005.

FLUENT, Inc. "FLUENT User's Manual." Version 6.2.16." FLUENT Incorporated: Lebanon, New Hampshire. 2006.

Final Safety Analysis Report for the HI-STAR 100 Dry Spent Fuel Storage System, HOLTEC International. December 2002.

Green, S., M. Clarke, D. Walter. "Software Validation Test Results for FLOW-3D, Version 9.0." San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2005.

Kuehn, T.H. and R.J. Goldstein. "An Experimental Study of Natural Convection Heat Transfer in Concentric and Eccentric Cylinder Annuli." *ASME Journal of FLUID Transfer.* Vol. 100. pp. 635–640. 1978.

Kuehn, T.H. and R.J. Goldstein. "An Experimental Study of Natural Convection Heat Transfer in the Annulus Between Horizontal Concentric Cylinders." *Journal of Fluid Mechanics.* Vol. 74, Part 4. pp. 635–640, pp. 695–719. 1976.

Patankar, S.V. *Numerical Heat Transfer and Fluid Flow.* Washington, DC: Hemisphere Pub. Corp. 1980.

Yücel A., S. Acharya, M.L. Williams. "Natural Convection and Radiation in a Square Enclosure." *Numerical Heat Transfer.* Part A. Vol. 15. pp. 261–278. 1989.

TEST CASE 1: Natural Convection in an Annulus Between Horizontal Concentric Cylinders

The first test case considerd natural convection between two isothermal concentric horizontal cylinders. The diameters of the inner and outer cylinders are 3.56 cm and 9.25 cm, respectively. The annulus space

between the two cylinders is filled with nitrogen. The inner cylinder is heated and maintained at a higher temperature with respect to the outer cylinder. As a result, the natural convection will ensue if temperature difference between the outer and inner cylinders is greater than a critical value. A schematic diagram of the problem is presented in Figure 6-1. Kuehn and Goldstein (1976, 1978) conducted an experimental study to measure the temperature distribution of the gas and wall heat flux. They considered concentric and eccentric configurations of the cylinders; however, only concentric configuration is considered for this validation study.

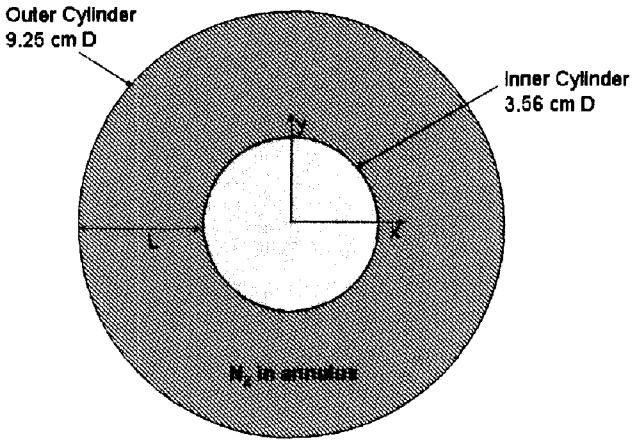

Figure: Schematic of Concentric Cylinders for Natural Convection Study. The Gravational Acceleration Is Along $-y$ Direction With Magnitude Equal to 9.81 m/s^2.

In the experimental setup, the length of both cylinders was 20.8 cm, and the annular space was filled with nitrogen at subatmospheric, atmospheric, and high pressures. The temperature difference between the inner and outer cylinders was maintained at different values to give pure conduction, laminar, and turbulent fluid flow conditions. The fluid flow regime can be characterized by the value of Rayleigh number, *Ra*, defined as

$$Ra = \frac{\rho^2 g\, \beta}{\mu^2} \Delta T\, L^3\, Pr \qquad (1)$$

where

ρ	—	gas density
g	—	acceleration due to gravity
β	—	thermal expansion coefficient of gas
μ	—	dynamic viscosity

L — $0.5(D_o - D_i)$ = gap width defined by the diameters of the cylinders
D_o — inner diameter of the outer cylinder
D_i — outer diameter of the inner cylinder
Pr — gas Prandtl Number

The experimental results are reported in terms of equivalent thermal conductivity k_{eq}, defined as

$$k_{eff} = \frac{Q \ln(D_o/D_i)}{2 \pi \Delta T k} \tag{2}$$

where
Q — heat transfer rate at inner cylinder per unit length (watts/meter)
ΔT — temperature difference between cylinders
k — conductivity of the gas

The reported results include the effects of end losses and radiation on total heat transfer. The simulation results are summarized by estimating the equivalent thermal conductivity, keq, using Eq. (2), and calculated values are compared to the experimental values.

Test Case 1 Input:

The input files for different flow conditions are developed and filed in FLUENT Version 6.2.16. These flow conditions correspond to Rayleigh numbers equal to 1.31×10^3, 6.19×10^4, 6.81×10^5, 2.51×10^6, 1.9×10^6, and 6.6×10^7 (Kuehn and Goldstein, 1978). The first two values of Rayleigh numbers represent the laminar flow; the second two values of Rayleigh numbers correspond to the transitional flow; and, for the last two values of Rayleigh numbers, the fluid flow is expected to be turbulent.

Test Case 1 Results:

The details of the validation test for this case are described in Scientific Notebook 704E. The test results are summarized in this report.

Six experimental conditions are selected for simulation with FLUENT Version 6.2.16. These six cases are listed in Table 1. The properties of nitrogen (Green, et al., 2005) at the selected conditions are listed in Table 2.

A two-dimensional model is developed to estimate the heat flux from the inner cylinder for different test conditions. In this model, the lengths of both the inner and outer cylinders are unity. The constant temperature boundary conditions is applied at the walls of the inner and outer cylinders. The computation domain between the two cylinders is divided in 3,600 cells, with 90 divisions on the circumference of each cylinder and 40 divisions along the radial direction. The mesh is finer in the boundary layer region located close to the cylinder.

The nitrogen pressure is varied between 0.11 and 35 atm, and the temperature difference between the two cylinders is varied between 0.91 and 53.5 °K [1.64 °F and 96.84 °F]. In the experimental study, the temperatures in the annulus were measured via Mach-Zender interferometry, and surface temperatures were measured with thermocouples.

The mesh resolution is chosen to adequately capture the expected temperature and velocity distributions for laminar, transitional, and turbulent flow domains. Keuhn and Goldstein (1978) reported that turbulent eddies are observed at the top of the inner cylinder for Ra $\approx 2 \times 10^5$. At increasing Rayleigh numbers, more of the flow is turbulent until at Ra $\approx 10^8$, where the upper half of the annulus is clearly in turbulent flow, but the lower half is in laminar flow. The standard k-ε turbulence model in FLUENT Version 6.2.16 is used for simulations of the higher Rayleigh number flows where transitional and turbulent flow field is expected.

A sample of the fluid flow field with temperature distribution predicted by FLUENT Version 6.2.16 is shown in the Figure below. These results are for the case of $Ra = 6.6 \times 10^7$. As seen in the figure, a symmetric circulation pattern is observed between the cylinders. The flow field in Figure 6-2 is mean flow velocity distribution. Time-dependent flow oscillations are not shown.

Table 1. Selected Experiments for FLUENT® Version 6.2.16 Simulations

Ra	P atm	ΔT °C	½(Ti + To) °C
1.31×10^3	0.110	53.5	51.1
6.19×10^4	0.977	38.0	44.4
6.81×10^5	8.46	4.29	27.3
2.51×10^6	34.6	0.91	27.7
1.90×10^7	34.7	7.01	29.1
6.60×10^7	35.0	28.7	40.8

Table 2. Properties of Nitrogen for FLUENT® Version 6.2.16 Simulation Conditions

Ra	ρ kg/m3	β 1/K	μ Pa×sec	Cp J/(kg ×°K)	k W/(m × ×°K)	FLUENT®Input File Name
1.31×10^3	0.1158	3.08×10^{-3}	1.903×10^{-5}	1,033.37	0.0274	K-G_Ra1-3e03.cas
6.19×10^4	1.051	3.15×10^{-3}	1.875×10^{-5}	1,033.37	0.0270	K-G_Ra6-2e04.cas
6.81×10^5	9.627	3.32×10^{-3}	1.810×10^{-5}	1,034.97	0.02627	K-G_Ra6-8e05.cas
2.51×10^6	39.40	3.323×10^{-3}	1.859×10^{-5}	1,041.07	0.02793	K-G_Ra2-5e06.cas
1.90×10^7	39.32	3.309×10^{-3}	1.865×10^{-5}	1,041.07	0.02802	K-G_Ra1-9e07.cas
$6.60 \times 10_7$	38.07	3.185×10^{-3}	1.916×10^{-5}	1,040.67	0.02874	K-G_Ra6-6e07.cas

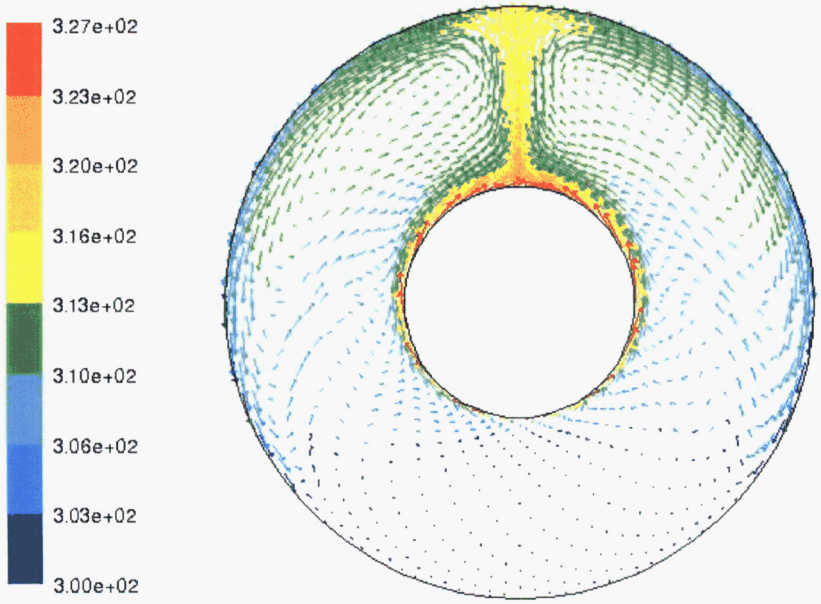

Figure: Predicted Fluid Temperature and Velocity Vectors for Natural Convection Between Cylinders. The Rayleigh Number Is 6.6 × 107.

Table 3. Equivalent Thermal Conductivity k_{eq} From Experiments and Simulations				
Ra	Q from simulations (watts/meter)	k_{eq} experiment	k_{eq} FLEUNT® Version 6.2.16	Deviation Percent
1.31 × 103	10.48	1.14	1.09	4.6
6.19 × 104	20.88	3.32	3.1	6.8
6.81 × 105	4.31	5.6	5.81	3.8
2.51 × 106	1.34	7.88	8.03	1.9
1.90 × 107	18.77	13.27	14.53	9.5
6.60 × 107	115.81	18.65	21.35	14.48

Note: The input and output files for this test are attached with the disk attached with this scientific notebook. The table below provides the list of input and output files.

Table 4. Input output files for validation test case 1.

Ra	FLUENT®Input File Name	FLUENT® Output File Name
1.31 × 103	K-G_Ra1-3e03.cas	K-G_Ra1-3e03.dat
6.19 × 104	K-G_Ra6-2e04.cas	K-G_Ra6-2e04.dat
6.81 × 105	K-G_Ra6-8e05.cas	K-G_Ra6-8e05.dat
2.51 × 106	K-G_Ra2-5e06.cas	K-G_Ra2-5e06.dat
1.90 × 107	K-G_Ra1-9e07.cas	K-G_Ra1-9e07.dat
6.60 × 107	K-G_Ra6-6e07.cas	K-G_Ra6-6e07.dat

TEST CASE 2: Natural Convection and Radiation in a Square Enclosure

The second test case considers the natural convection of fluid in a square enclosure. The side walls of the enclosure are maintained at constant temperature, whereas the bottom and top plates are adiabatic. This test case illustrates FLUENT's capability to model natural convection and radiation heat transfer.

A schematic diagram of the problem is presented in Figure 6-3, where the right side wall is maintained at temperature Th equal to 2,000 °K and the left side wall is maintained at temperature Tc equal to 1000 °K. In this system, the heat is transferred from the hotter wall to the colder wall by way of natural convection and radiation. This problem was first studied by Yücel, et al., (1989). They solved the governing equation for momentum, energy using SIMPLER (semi-implicit method for pressure linked equation revised). This method is described in detail by Patankar (1980). The governing equation for radiation was solved by a discrete ordinate method as described in the Fluent User's Manual (2006).

The fluid inside the enclosure is Newtonian, incompressible, gray, absorbing, emitting, and isotopically scattering. All the physical properties of the fluid are assumed to be constant except density. The properties of the fluid used in the test case are listed in Table 4. The flow is assumed to be laminar and two-dimensional, and the fluid density dependence on temperature is represented by the Boussinesq approximation (Patankar, 1980). The gravitational acceleration is assumed to be 6.94×10^{-4}. For this test problem, the Rayleigh number, Ra, between the hot and cold plates is 5×10^{6}, which indicate that the fluid flow is laminar.

This test case is simulated for four conditions. The first condition corresponds to modeling natural convection without radiation heat transfer. In the remaining calculations, the radiation heat transfer and natural convection is simultaneously modeled for optical thickness, τ, of the fluid equal to 1.0, 5.0, and 0.2. The optical thickness, τ, of the fluid is defined as

$$\tau = (K + \sigma) L \tag{3}$$

where

K — Absorption coefficient

σ — Scattering coefficient

L — Length of the fluid zone

The test results are summarized by calculating the overall Nusselt number, Nu, for total heat transfer from the hot wall to the cold wall and the Nusselt number for radiation heat transfer, NuR. The overall Nu is defined as

$$Nu = \frac{\bar{q}L}{k(T_h - T_c)} \tag{4}$$

where

$\bar{q}$ = average heat flux at the hotter wall

k = conductivity of the gas

The Nusselt number for radiation heat transfer, NuR, is obtained by replacing average heat flux $\bar{q}$ with heat flux $\bar{q}_r$ due to radiation heat transfer. The obtained values of Nu and NuR are compared to those reported by Yücel, et al. (1989) using S8 linear quadrature for discrete ordinates method

Test Case 2 Input

Four input files are created. The first input file corresponds to the case of natural convection without radiation. The input file name for this condition is natconrad.cas. The remaining three input files, natconrad_tau_1.cas, natconrad_tau_5.cas, natconrad_tau_p2.cas, correspond to optical thicknesses equal to 1, 5, and 0.2, respectively.

Test Case 2 Procedure

FLUENT Version 6.2.16 will be run using a uniform grid resolution for the four test conditions. The simulation results will be used to compute average wall heat flux and the overall Nusselt number, Nu, and the radiation Nusselt number, NuR. The computed values of Nu and NuR will be compared to the values reported by Yücel, et al. (1989).

Expected Results for Test Case 2

The acceptance criterion for the simulated equivalent thermal conductivity will be a deviation of no more than 5 percent of the reported value by Yücel, et al. (1989).

Table 4. Physical and Thermal Properties of Fluid Used in the Square Enclosure Test Case # 2.

Property	Value
Density ρ	1000 kg/m3

Heat capacity Cp	1103 J/(kg ×°K)
Viscosity μ	0.001 Pa×sec
Thermal expansion coefficient β	0.0001 1/°K
Absorption coefficient K	1.0, 5.0, and 0.2 m1
Scattering coefficient σ	0.0 m1
Optical thickness $\tau = (K+\sigma)L$	1.0, 5.0, and 0.2

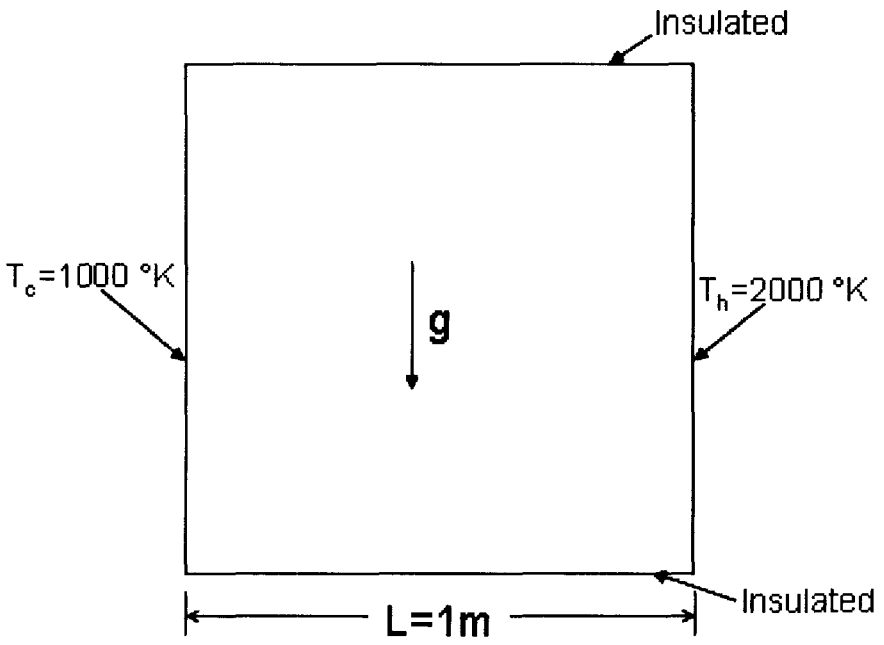

Figure: Schematic Representation of the Square Enclosure for the test case 2. The Gravitational Acceleration is 6.94×10^{-4} m/s^2

Results for Test Case # 2:

The details of this validation test are described in Scientific Notebook 704E. The test results are summarized in this report.

A two-dimensional model is developed to estimate the heat flux from the hot wall. A uniform mesh with 50 grid points in horizontal and vertical direction is created. This mesh was also selected by Yücel, et al. (1989) for calculations. The top and bottom walls of the enclosure are adiabatic, (i.e., heat flux is zero across these surfaces). The top and bottom walls do not participate in radiation. The governing equations are solved using FLUENT Version 6.2.16.

The average heat flux at the hot plate is calculated using FLUENT's menu driven postprocessor. The postprocessor separately calculates the overall average heat flux and radiation heat flux. These values are then used to calculate the overall Nusselt number, Nu, and radiation Nusselt number, NuR, using Eq. (4). The calculated overall Nusselt number, Nu, is given in Table 6-5. The deviation in Nu is within five percent of reported values by Yücel, et al. (1989). Similarly,

the Nusselt number due to radiation heat transfer, NuR, is listed in Table 6-6. The values of NuR are also with five percent of reported results by Yücel, et al. (1989).

A sample of the fluid flow field with temperature distribution calculated by FLUENT Version 6.2.16 is shown in Figure 6-4. These results are for the case of $\tau = 1$. As seen in the figure, the fluid circulation pattern is observed in the enclosure.

Table 5. Overall Nusselt Numbers, Nu, on the Hot Wall as Reported by Yücel, et al. (1989), and by FLUENT Version 6.2.16 Simulation Results

Test Condition	$\bar{q}$ (watts/meter^2)	Nu (Yücel, et al., 1989)	Nu (FLUENT® Version 6.2.16)	Deviation Percent
Nonradiating	218890.5	13.76	14.30	3.90
$\tau = 1$	579907.2	38.93	37.88	2.71
$\tau = 5$	485001.46	31.76	31.68	0.26
$\tau = 0.2$	684101.9	46.11	44.68	3.09

Table 6 Radiation Nusselt Numbers, Nu_R, on the Hot Wall as Reported by Yücel, et al. (1989), and by FLUENT Version 6.2.16 Simulation Results

Test Condition	$\bar{q}_r$ (watts/meter^2)	Nu_R (Yücel, et al., 1989)	Nu_R (FLUENT® Version 6.2.16)	Deviation Percent
$\tau = 1$	465723.05	31.28	30.42	2.75
$\tau = 5$	368232.06	23.64	24.05	1.74
$\tau = 0.2$	550083.97	37.40	35.93	3.93

Table 7. Input output files for the Test Case 2 (Validation Study)

Test Condition	Input File	Output File
Nonradiating	`natconrad.cas`	`natconrad.dat`
$\tau = 1$	`natconrad_tau_1.cas`	`natconrad_tau_1.dat`
$\tau = 5$	`natconrad_tau_5.cas`	`natconrad_tau_5.dat`
$\tau = 0.2$	`natconrad_tau_p2.cas`	`natconrad_tau_p2.dat`

The input and output files are stored in the disk attached with this scientific notebook. The files are located in the directory called natcondrad.

Entry: Pavan Shukla, 10 April 2006

Closed Cask model of the HI-STAR 100 system using FLOW-3D **April 10th, 2006**

Run id: closedcaskmodel01 (inputdeck is attached at the end)

Description: This model was implemented using FLOW-3D. The input deck is attached in the end. He model simulates the HI-STAR 100 system when it is closed. The fluid inside the cask is helium and fluid outside is air. The fuel baskets with fuel assemblies is modeled as a homogenized power sourse with a uniform effective thermal conductivity. The gap between MPC wall and overpack is also assumed to be filled with helium. The cask is assumed to be sitting on the concrete base which is 2.5 meter in radius, and 0.9144 meter in height. The thermal conductivity of concrete is 0.8 Watts/(meter-°K). The thermal conductivity of the fuel assembly is 3.382 Watts/(meter-°K). The boundary conditions and other important parameters such as thermal conductivity of the cask were obtained from HI-STAR 100 Final Safety Analysis report.

Description of the HI-STAR 100 Cask System: The Holtec international has been granted a licence to manufacture the HI STAR 100 cask system for the dry storage of the spent fuel nuclear assemblies. The fuel assemblies will also be transported to the fuel handling facility in these storage casks. The cylindrical shaped storage system consists of two discrete components: a) the multipurpose canister, and b) the storage and transport overpack. The multipurpose canister shell is placed inside the overpack. A description of different component of the storage system is given the following subsections.

Multi-Purpose Canisters: The inner component of the storage system is called the multi-purpose canister. This component consists of a honeycombed fuel basket, a baseplate, canister shell, a lid, and a closure ring. A schematic diagram HI-STAR 100 cask system showing he multipurpuse canister shell (MPC) is prepsented in Figure 1. The dimenstions of the different componenets of the cask system are provided in Table 1. The thicknesses of the shell wall and base plates are 0.5 inch and 2.5 inch, respectively. This shell is expected to me made of an alloy identified as Alloy X in Final Safety Analysis Report for HI STAR 100 transport systems. The thermal conductivity of Alloy X and other materials used in the cask are given in Table 2. The surface emmisivity of material used in the cask are given in Table 3. A honey combed basket is placed inside the canister shell where fuel assemblies are placed.

Fuel Basket: The fuel basket is a honey combed structure that is placed inside the multipurpose canister shell. The basket has square-shaped fuel compartments where fuel assemblies are inserted prior to closing of the multipurpose canister shell. Each fuel compartment panel has Boral thermal neutron absorber. The Boral is sandwiched between a sheathing plate and the box panel, and it covers the entire length of the active fuel region. The fuel basket has twenty-four fuel compartment and it is used for storing pressurized water reactor fuel assemblies. In Figure 1, The green square panels represent the Boral thermal neutron absorber. At the bottom and top of the fuel basket panels, there are circular shaped undercuts that provide a passage for the fluid to flow. These fuel baskets are also called MPC-24. A fuel baskets with sixty-eight fuel compartments is called as MPC-68, and it is are used to store the boiling water reactor fuel

assemblies. However, in this report, the thermal analysis has been carried out for the MPC-24 systems only.

When transportation cask is closed, the multipurpose canister shell is filled with pressurized helium, which acts as a non reacting gas medium for passive rejection of heat generated by fuel assemblies. The thermal conductivity of helium and air at different temperatures are given in Table 4. The viscosity, heat capacity, and molucular weight of helium and air are provided in Table 5. The fuel basket support brackets and drainage pipe were not included in the thermal analysis. These components were replaced by the open space.

Overpack: The HI-STAR 100 cask system's overpack is a multi-walled cylindrical vessel with a base plate and a closure lid. . The overpack is made of alloy steel. Lifting trunnions that are attached to the overpack walls and drainage ports are not shown in Figure 1. These sub-components were not modeled in the thermal analysis. The innermost wall of the overpack is 2.5 inch thick and it's made of nickel steel. The adjacent multi-layered shell region, which consist of a 1.25 inch thick gamma layers and four one-inch thick outer layers surrounding the gamma layer, were modeled as one 5.25 inch thick layer. In the fabrication process, the multilayered system will develop contact resistance due microscopic pockets of entrapped air. Since thermal conductivity of the air is lower than base metal, a higher resistance to thermal conduction will develop. The effective thermal conductivity of the multi-layered system can be estimated by the following expression

$$K_{eff} = r_0 \log\left(\frac{r_5}{r_0}\right)\left[\sum_{i=1}^{5}\frac{\delta}{K_{air}}\frac{r_0}{r_i} + \frac{r_0 \log\frac{r_5}{r_0}}{r_i K_{cst}}\right]^{-1}$$

where

K_{eff} – effective intermediate shell region conductivity

r_0 – inner radius of the inner intermediate shell

r_i – outer radius of ith intermediate shell

δ – interfacial air gap

K_{air} – thermal conductivity of the air

K_{cst} – carbon steel thermal conductivity

The r_0, r_i, and δ are provided in Table 6. The calculated values of K_{eff} are given in Table 7.

To minimize doses from gamma and neutron radiation emitted by fuel assemblies, overpack is surrounded by the neutron shielding material. This material is placed inside the radial channels which are vertically welded to the outer most surface of the overpack's circumference. These radial channels are also acts as thermal fins for improved heat transfer between overpack and

outer surrounding. The cavities of radial channel segments are filled together by the neutron shield material and silicone sponge The silicone sponge acts as thermal expansion foam to compress as neutron shield expands.

The neutron shielding material is made of neutron poison material boron carbide and aluminum. Holtec International has proposed Holtite-A as neutron absorbing material. Holtile-A meets the required criterion for neutron absorbing material as specified in 10CRF72.104, 10CRF72.106, and 10CRF72.126. The effective thermal conductivity of radial channel plus Holtite-A system are given in HI-STAR 100 Final Safety Analysis report (Table 4.4.8). These values are also reported again in Table 3.

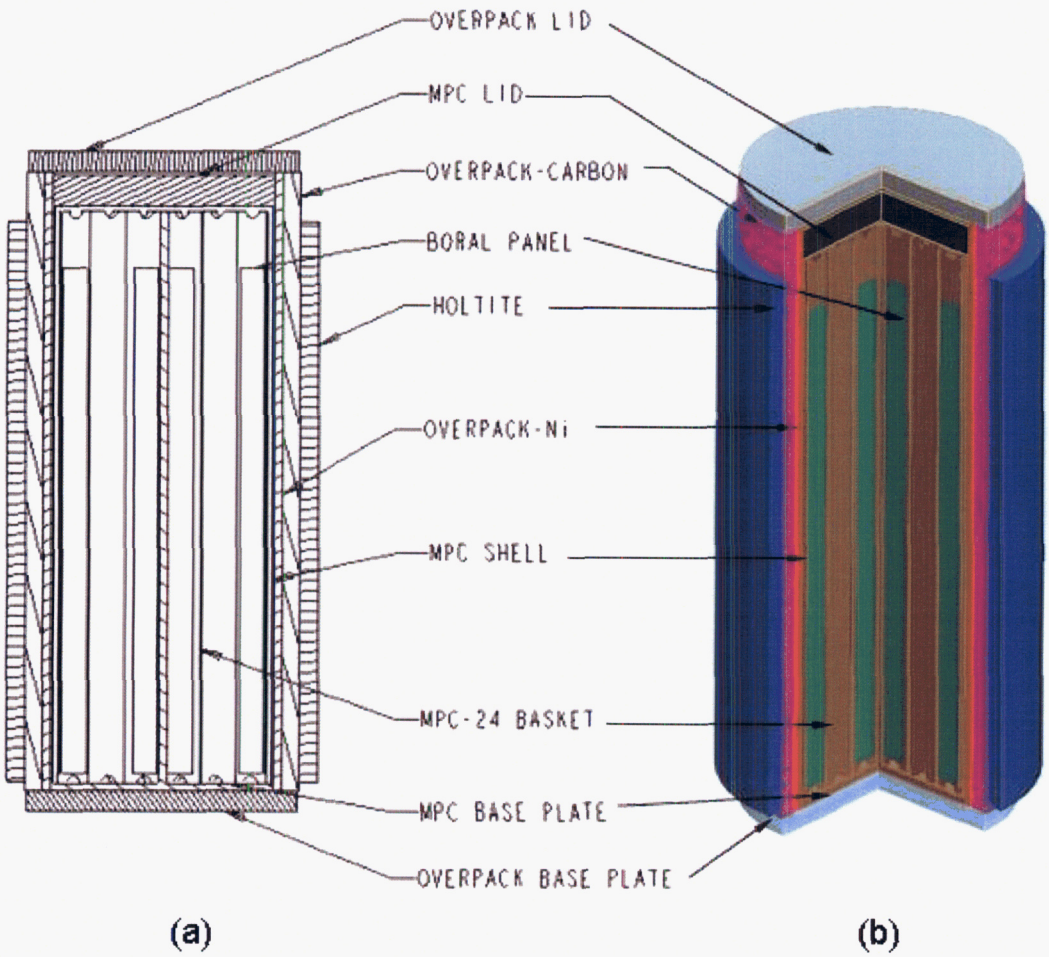

Figure 1: HI-STAR 100 cask system. (a) Two dimentional view, (b) Three dimentional view.

Table 1: Dimensions of different component of HI-STAR 100 Cask System			
Component of HI-STAR 100 System	Inner Radius (inch)	Outer Radius (inch)	Height (inch)
Multipurpose Canister Base Plate	0.0	34.1875	2.5
Multipurpose Canister Shell	33.6875	34.1875	178.0

Multipurpose Canister Lid	0.0	34.1875	9.5
Overpack Base Plate	0.0	41.625	6.0
Overpack-Ni layer	34.375	36.875	191.125
Overpack-Carbon Layer	36.875	42.125	191.125
Overpak Lid	0.0	42.125	6.0
Holtite	42.125	48.0	173.125

Table 2. Thermal conductivity of HI-STAR 100 Cask System Materials			
Components of the HI-STAR 100 System	Thermal conductivity (watts/meter-°K)		
	@ 93.33 °C [200 °F]	**@ 232.2 °C [450 °F]**	**@ 371.1 °C [700 °F]**
Multipurpose Canister Shell and Base Plate (Alloy X)	14.54	16.96	19.04
Overpack's Inner Shell and Base plate	42.23	41.36	38.77
Holtite-A and Carbon Steel Radial Connector System (Holtite)	3.38	3.14	2.85

Table 3: Surface Emmisivity of components used in HI-STAR 100 Cask System.	
Component	Emmisivity
Fuel Basket	0.36
Multipurpose Canister Shell, Base Plate, and Lid	0.36
Overpack Base Plate, Inner Shell, and Lid	0.66
Painted Surfaces	0.85

Table 4. Thermal Conductivity of Air and Helium		
Temperature	**Air K_{air} (Watts/meter-°K)**	**Helium K_{helium} (Watts/meter-°K)**
93.33 °C [200 °F]	2.994×10^{-2}	1.689×10^{-1}
232.2 °C [450 °F]	3.894×10^{-2}	2.231×10^{-1}
371.1 °C [700 °F]	4.707×10^{-2}	2.762×10^{-1}

Table 5. Properties of Helium and Air.			
Material	Heat Capacity Cp (Jouls/kg-°K)	Viscosity μ (kg/meter-sec)	Molecular Weight

Helium	5193	1.8×10^{-5}	4.0026
Air	1006.43	1.9×10^{-5}	28.996

Table 6. Parameter values used to calculated effective intermediate shell thermal conductivity.

Parameter	Value
r_0	36.785 inch
r_1	38.375 inch
r_2	39.375 inch
r_3	40.375 inch
r_4	41.375 inch
r_5	42.375 inch
δ	2000 μm

Table 7. Calculated values (using Equation 2-1) of effective intermediate shells (Overapck-carbon) thermal conductivity at 200 °F, 450 °F, and 700 °F

Temperature	K_{eff} (watts/meter-°K)
93.33 °C [200 °F]	11.58
232.2 °C [450 °F]	13.82
371.1 °C [700 °F]	15.24

Table 8: Thermal conductivity of components used in closed cask model of HI-STAR 100 Cask System using FLOW-3D

Component	K_{air} (Watt/meter-°K)
Multipurpose canister shell, base plate and lid	16.96
Overpack base plate, innershell, and lid	41.2
Overpack five adjacent carbon layers	11.58
Holtite	3.38
Concrete base	0.8

Heat Transfer From Overpack Surface:
In addition, another closed cask model is simulated where thermal conductivity of different component is defined as piecewise linear function of temperature. The thermal conductivity of different materials at three temperatures (200 °F , 450 °F, and 700 °F) are input in the FLUENT. This model is a validation study of the thermal model of HI-STAR 100 system reported by HOLTEC International. In this model, only radiation and conduction heat transfer is modeled

inside the cask, whereas, the heat dissipation from overpack's outer surface to the ambient air take place via natural convection and radiation heat transfer. The governing equation for radiative and convective heat transfer from the cask surface to the enviornment can be expressd as

$$q = h(T_S - T_A) + \sigma\varepsilon(T_S^4 - T_A^4) \quad (1)$$

where

q	-	heat flux (Watts/m^2)
h	-	heat transfer coefficient (Watts/ m^2-°K)
T_S, T_A	-	surface, ambient temperatures (°K)
σ	-	Stefan-Boltzmann constant(=5.67*10^{-8} Watts/m^2-°K^4)
ε	-	surface emmisivity

The following correlations were suggested by Jacob and Hawkins [Jacob, M. and Hawkins, G.A.,"Elements of Heat Transfer", John Wiley & Sons, New York, 1957] for natural convection heat transfer from the heated horizontal and vertical surfaces in the turbulent fluid flow regime:

$$h = 1.25(T_S - T_A)^{1/3}(Horizontal) \quad (2)$$

and

$$h = 1.08(T_S - T_A)^{1/3}(Vertical) \quad (3)$$

In the thermal models for the closed cask, the more conservative heat transfer for the vertical surfaces is applied to all exposed overpack surfaces.

In FLOW-3D Version 9.0, only a constant value of heat transfer coefficient can be assigned to an exposed surface. Therefore, initial calculations are performed with an assumed value of heat transfer coefficient, and surface temperatures of exposed surfaces of the overpack are obtained. Then, the heat transfer coefficient h is calculated by using the average value of surface temperature for horizontal and vertical surface using the heat transfer equations, which is again inputted to obtain new temperature profile of the overpack surfaces. This process is repeated till average value of surface temperature in successive steps are same.

Fluid Density

In both FLOW-3D and FLUENT, fluid density is modeled as an incompressible ideal gas. The density of gas ρ can be represented by

$$\rho = \frac{PM}{RT} \quad (4)$$

P	-	specified pressure of the gas (pascal)
M	-	molecular weight of the gas (mol/kg)
R	-	universal gas constant, 8.3144 J/mol-°K
T	-	temperature of the gas (°K)

The incompressible ideal gas approximation represent the gas density only as a function of temperature.

Heat Load of the Cask: The MPC-24 fuel basket can host twenty-four pressurised water reactor fuel assemblies. The furl assembly has design basis decay heat generation rate of 792 Watts.

Therefore, the heat load of a MPC -24 fuel basket is 19008 Watts. The heat generation is supposed to be non-uniformly distributed over the entire length of the fuel, however, it is assumed to be uniform.

Ambient Conditions: The ambient air temperature is 80 °F for the thermal analysis of HI-STAR 100 system.

Concrete Pad: The cask system is placed on a Independent Spent Fuel Storage Installation pad. In the thermal models, the pad is conservatively modeled as thirty six inch thick concrete cylinder with its radius to that of overpack base plate. The upper surface of the concrete surface is in contact with the ovrepack base plate, and its bottom surface is at 60 °F. The thermal conductivity of the concrete is assumed to be 0.8 watts/m-°K(The thermal conductivity value is estimated from the reference cited below). The sidewalls of the concrete pad are assumed to be adiabatic.

Reference for thermal conductivity: Fundamentals of Heat and Mass Transfer by Frank. P. Incropea, David P. DeWitt, Fifth Edition, John Wiley and Sons, New York, 2002.

Model Parameters for Closed Cask Model Using FLOW-3D: The diameter and height of the power source is 30.92 inch [0.7854 meter] and 176.5 inch [4.483 meter], respectively. The diameter of the equivalent fuel source is obtained by equating the cross-sectional surface area of the fuel basket to that of cylindrical power source. The surface heat transfer coefficients are obtained as described in the previous section. The thermal conductivity of different component that are used in this model are listed in Table 8. A schematic diagram of the model is presented in the following Figure.

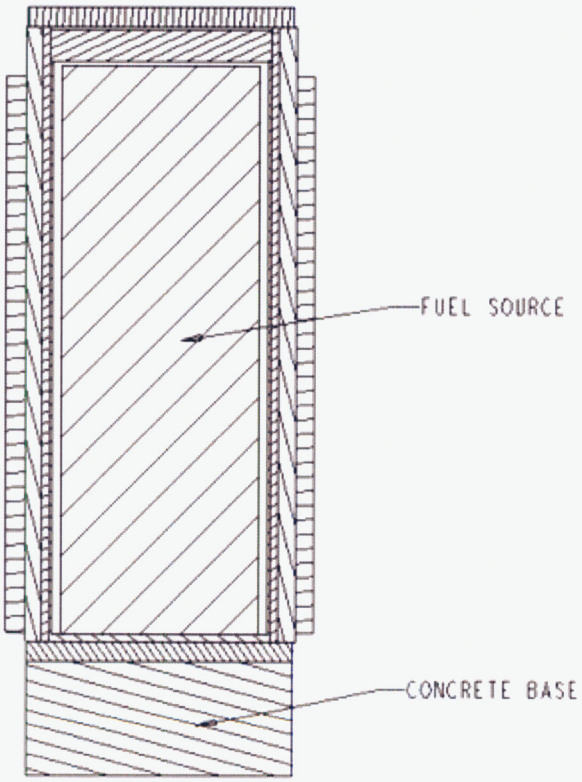

Figure: Closed cask model of HI-STAR 100 system.

Results: The model was simulated for 600 seconds. The maximum steady-state temperature of the fuel assemble is 752 °K for thermal conductivity of the fuel equal to 3.382 watts/m-°K.

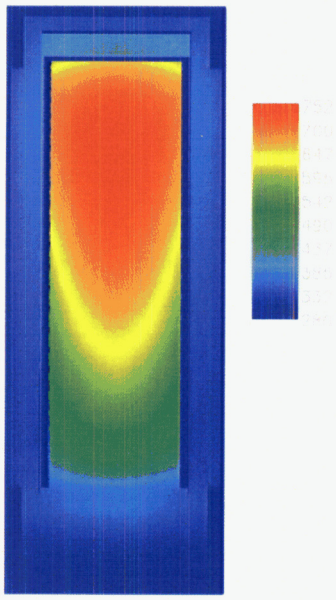

Figure 2 Simulation results of closedcaskmodel01 model. The maximum temperature of the fuel

assembly is 752 °K. The model is simulated using FLOW-3D. The input file is attached in the Appendix.

The model was again simulated for thermal conductivity of the fuel source equal to 2.59 and 1.92. The simulation results are presented below.

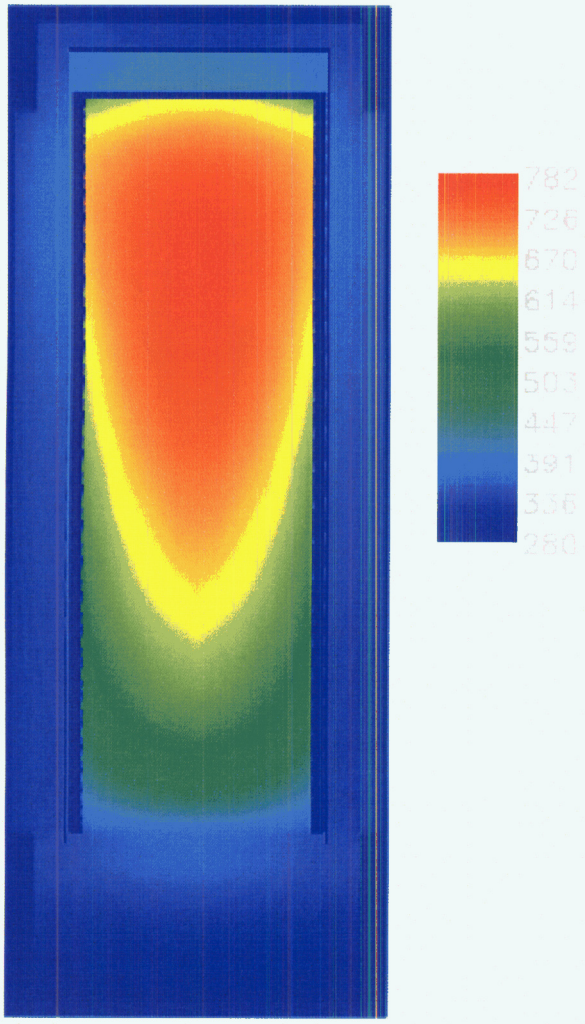

Figure 3: Thermal pattern inside the closed cask for fuel source thermal conductivity equal to 2.59. The maximum temperature of the fuel assemble is equal to 782 °K. The model is simulated using FLOW-3D.

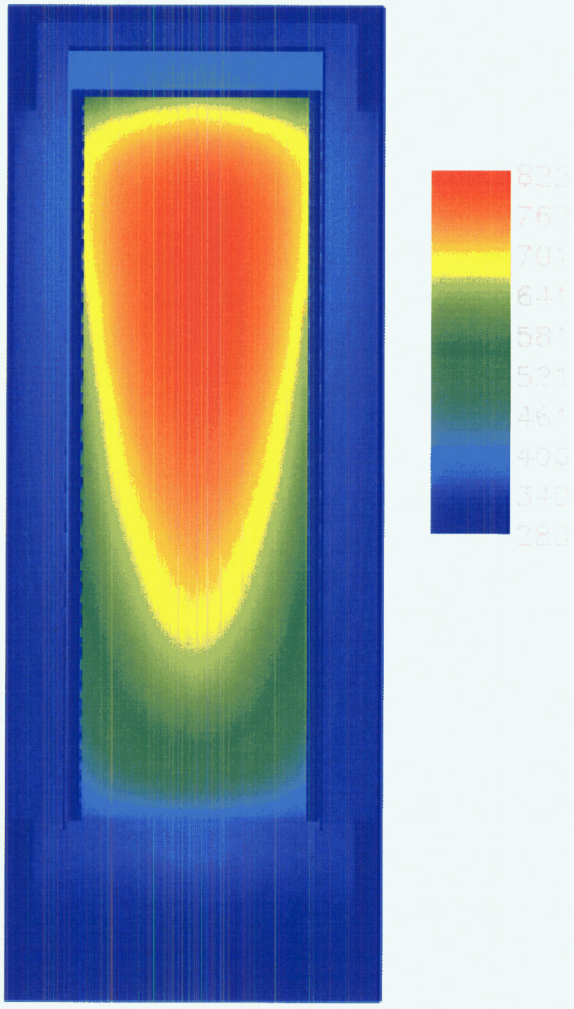

Figure 4: Thermal pattern inside the closed cask for fuel source thermal conductivity equal to 1.92. The maximum temperature of the fuel assemble is equal to 822 °K. The model is simulated using FLOW-3D.

The closed cask model is also simulated using FLUENT. The simulation resuts are presented below.

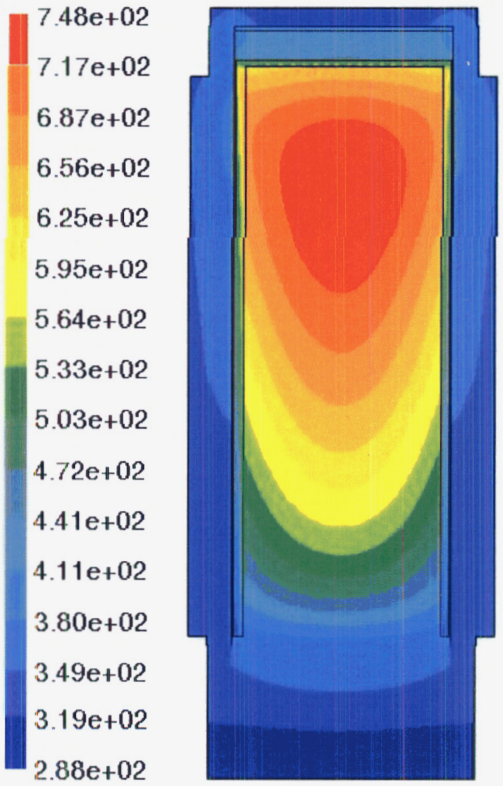

Figure 5: Simulation results of closed cask model using FLUENT. The maximum temperature of the fuel assembly is 748 °K for thermal conductivity of he Fuel equal to 3.382. The input and output files are in the disk attached with this scientific notebook.

The input and output files for the closed cask model using FLUENT are stored in HI-STAR100\ccmodel-FLOW3D.

Input Files: closedcask-half.dbs, closedcask-half.msh, closedcaskk382.cas
Outputfile: closedcaskk382.dat

Closed Cask model of the HI-STAR 100 system using FLUENT April 14th, 2006

Closed cask Model Using FLUENT:
The closed cask model of HI-STAR 100 system is developed using FLUENT Version 6.2.16. The objective of this work is to duplicate the results of the model developed by HOLTEC International in HI-STAR Final Safety Analysis report, and to demonstrate the capability to model HI-STAR 100 cask system. The schematic diagram of the model is presented above. In this model, the heat is transported from the fuel basket to multipurpose canister via radiation and conduction, and heat is rejected from overpack to ambient air via natural convection and radiation heat transfer. The closed cask model is simulated with and without solar radiation. In

this model, the thermal conductivity of the cask materials are defined as piecewise linear function of temperature.

Model Parameters: The dimension of different components in the model is same as one used for the closed cask model using FLOW-3D. The thermal conductivity of different materials is defined as a piecewise linear function of temperature, and thermal conductivity of different materials are given in Table 3, 4, and 5. The emissivity of the fuel basket and multipurpose canister shell is 0.36. The emmisivities of overpack material and overpack exposed surface are 0.66 and 0.85, respectively. The natural convection heat transfer coefficient, as defined in Equation 3, is valid between overpack exterior surface and ambient air.

The solar heat input to the exposed surface is determined based on 12-hours insolation levels recommended in 10 CFR 71.71. The solar insolation of 775 watts/m2 (800 Cal/cm2) is recommended for flat horizontal surface, and 388 watts/m2 (400 Cal/cm2) is for curved surfaces. The solar isolation on the overpack top surface is applied by defining the external thermal radiation temperature such that

The solar insolation on the exposed overpack surface is applied by adding a thin layer of transparent wall with its thickness equal to 0.25 inch. It is assumed that wall is completely transparent and solar insolation on the wall incidents from all directions. The wall has only one axisymmetric volume cell along its thickness. The thermal conductivity of the wall k is defined as

$$\kappa = ht_{wall} \tag{5}$$

where h is the heat transfer coefficient of the overpack exposed surface (defined in Equation 3) and t_{wall} is the thickness of the transparent wall. The solar absorptivity of the exposed overpack surface is conservatively assumed to be unity. Therefore, the incident solar insolation at horizontal and curved surface are divided by overpack surface emmisivity to account for loss due to reflection from the surface.

Results: The simulation results are presented in Figure 6 and 7.. The maximum predicted temperature of the fuel basket is 620 °Kwithout solar radiation, and maximum temperature of the fuel source is 635 °K with solar insolation. The HOLTEC International has reported the maximum temperature of the fuel basket to be 649.1 °K.

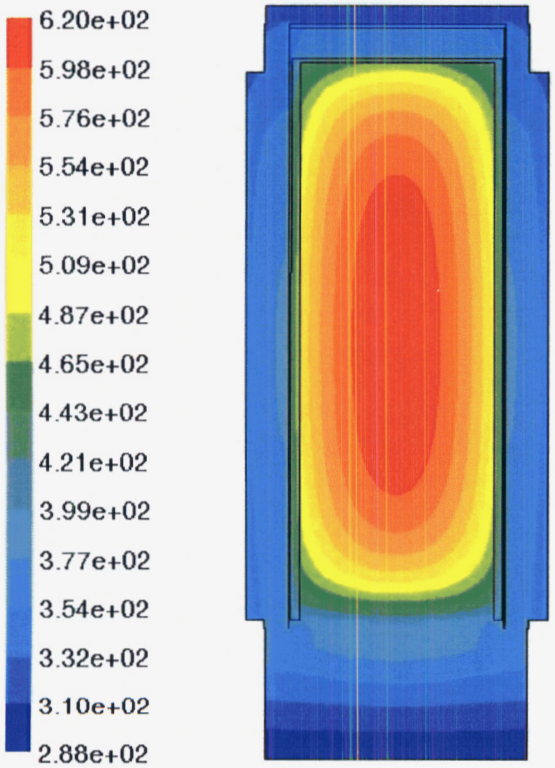

Figure 6: Closed cask model for HI-STAR 100 system. The model is simulated using FLUENT, and it accounts for radiation heat transfer within the cask. The solar heat load is taken to be zero.

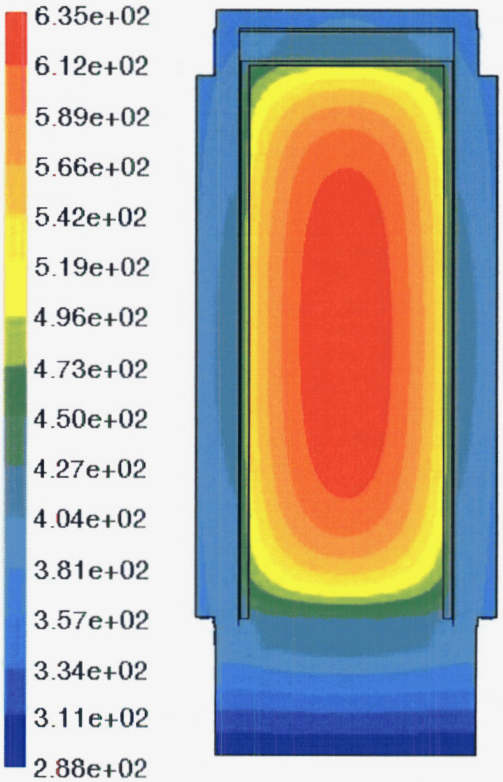

Figure 7: Closed cask model for HI-STAR 100 system. The model is simulated using FLUENT, and it accounts for radiation heat transfer within the cask. The solar insolation on horizontal surfaces is 775 watts/m^2 and 388 watts/m^2.

Open Cask model of the HI-STAR 100 system using FLUENT **April 23rd, 2006**

Open Cask Model Using FLUENT: CNWRA has developed a two-dimensional axisymmetric model of the HI-STAR 100 cask system when it is open and stored fuel assemblies are in direct contact with ambient air. When the cask is open, there is an active exchange of air between cask and surrounding. The model consists of an open cask and an hemispherical dome of air. The hemispherical dome represents the surrounding atmosphere near the open cask. The schematic diagram of the model is presented in Figure 9. At the boundary of the dome, the ambient air can enter or leave the computational domain at atmospheric pressure. The entering air temperature is fixed at 80 °F, while the temperature of the air existing the dome is determined by the model. The radius of the domain (200 inch) is approximately five time the height of the cask.

In this model, the twenty-four pressurized water reactor fuel assemblies and fuel basket is represented in two different ways:

1) A cylindrical homogenized fuel source with an effective thermal conductivity.
2) Three concentric cylindrical fuel source with annular gaps in between cylinders. The annular gap provide channels for fluid flow.

In the first representation, the effective thermal conductivity of the fuel medium is calculated by replacing the helium with air in the fuel basket. This approach gives a lower values of effective thermal conductivty of the fuel basket than for helium. The effective thermal conductivity of the fuel basket is calculated using geometric mean approximation and details are given in the Allendix.

In the second representation of the fuel basket with fuel assemblies are represented as three separate power source. These three fuel source represent the portions of fuel basket with four, eight, and twelve fuel assemblies. A schematic diagram of this representation if given in Figure 10, the fuel assemblies are bundeled in groups of four, eight and twelve and represented as three separate fuel source. The inner and outer radius of three fuel source are given in Table 9.
It is expected that air will enter in the cask system through colder regions and exit through hotter sections. The MPC-24 fuel basket has undercuts to provide passage for airflow. In the open cask model with three fuel sources, the fuel source are raised by 2.8 inch to provide passage of air underneath them, and a schematic diagram of the HI-STAR 100 open cask system is presented in Figure 11.

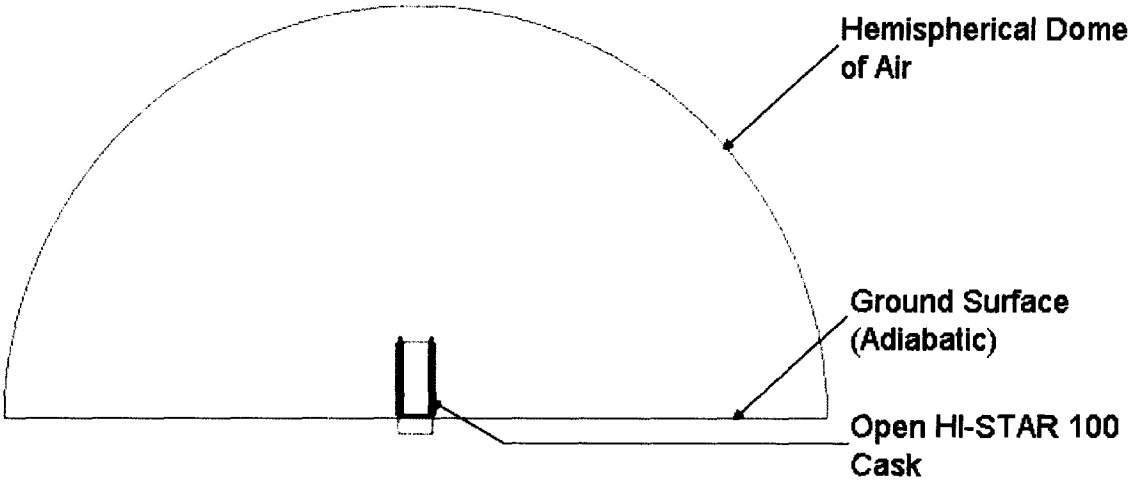

Figure 9: Open cask model for HI-STAR 100 system.

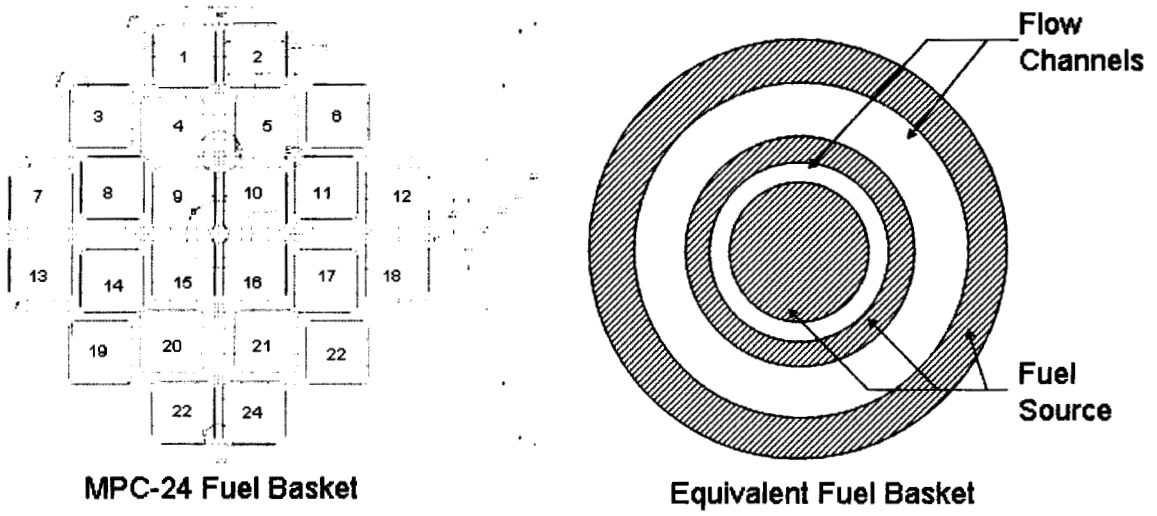

Figure 10: Representation of the MPC-24 Fuel basket as three equivalent fuel source

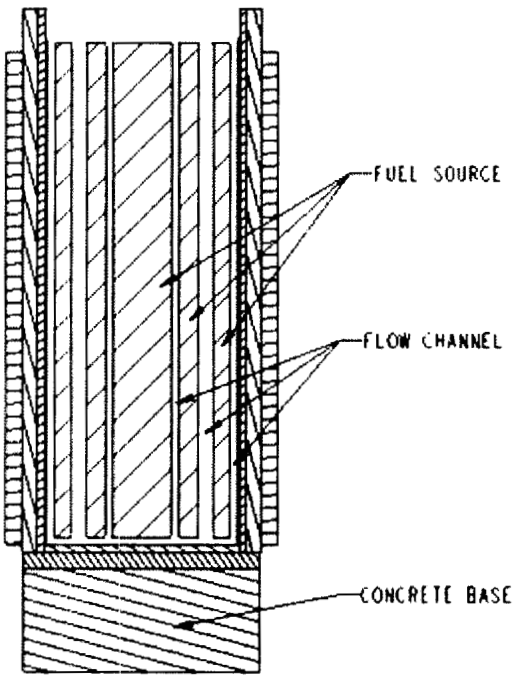

Figure 11: HI-STAR 100 cask system with modified representation of fuel basket with flow channels.

Table 9: Dimentions of equivalent fuel source in the open cask model with flow channels		
Component	Inner radius (inch)	Outer radius (inch)
Innermost fuel source	0	10.418
Second fuel source	13.075	19.698
Third fuel source	25.11	30.92

Model Parameters: In both representation of the fuel basket, the effective thermal conductivity of the equivalent fuel material is 1.692 watts/meter-°K (this value was obtained by geometric mean method. Calculations were performed by Steve Green (Div. 18)).. The model is simulated for no flow, laminar, and turbulent flow. The heat transfer from the overpack exterior surface to ambient is determined by the solution of convective and radiation heat transfer equations. For the turbulrnt flow, the model is simulated for k-ε (called as k epsilon) and k-Ω (k omega) turbulent flow models. The details of these turbulent models can be found in FLUENT User's manual.

Results: First, the results of the simulations for open cask model with the uniform cylindrical fuel sources are presented. The maximum temperature of the fuel source is 766 °K when only radiation and conduction heat transfer take place. The maximum temperature of the fuel source is 739 °K unde laminar flow conditions. The temperature distribution inside HI-STAR 100 system for these two conditions are presented in Figure 12 and 13. The thermal profile of HI-STAR 100 system under turbulent flow conditions are presented in Figure 14 and 15. The results show that maximum temperature of the fuel source is 731 °K for k-ε turbulence model, and 730 °K for k-Ω turbulence model. The results of the calculation are also summarized in Table 10. The radiation hear transfer is 92.44% and conduction heat transfer is 7.54% for under no flow condition. The percentage of conduction and convective heat transfer incenses to is 31.92% under laminar flow condition. As a result, the maximum tempearture of the fuel source is 739 °K. The conduction and convection heat transfer rate increase to 33.58 percent for k-ε turbulent flow model, 35.3 for k-Ω turbulence flow model.

Table 10. Summary of calculated results for the open HI-STAR 100 cask system with a homogeneous cylindrical fuel source.			
Model	Predicted Maximum Temperature	Percent Heat Dissipation by Radiation	Percent Heat Dissipation by Conduction and Convection
No Fluid Flow (Radiation and Conduction Only)	766 °K	92.44	7.56
Laminar Flow	738 °K	68.08	31.92
k-ε Turbulence Flow	731 °K	66.42	33.58
k-Ω Turbulence Flow	730 °K	64.7	35.3

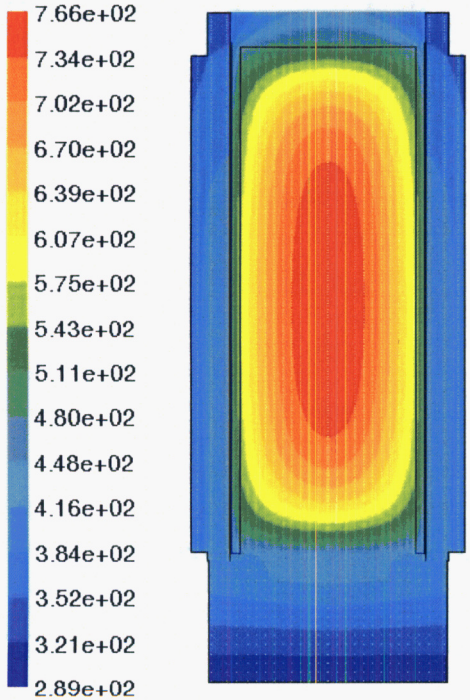

Figure 12: Open cask model of HI-STAR 100 System. Only radiation and cinduction model are employed.

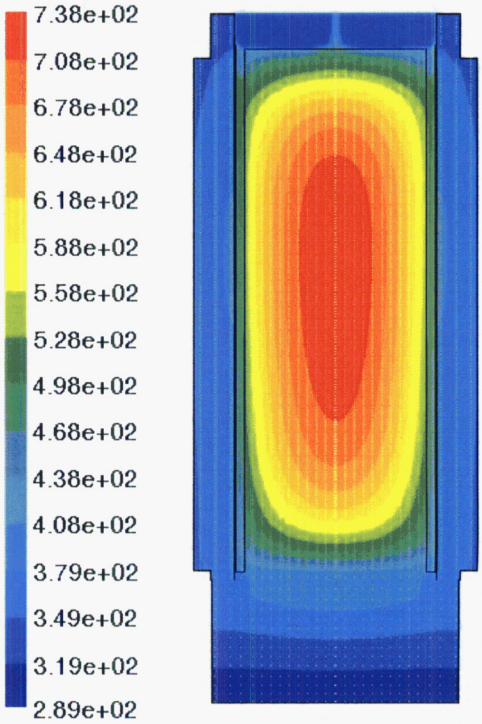

Figure 13: Open cask model of HI-STAR 100 System with Laminar FLOW model.

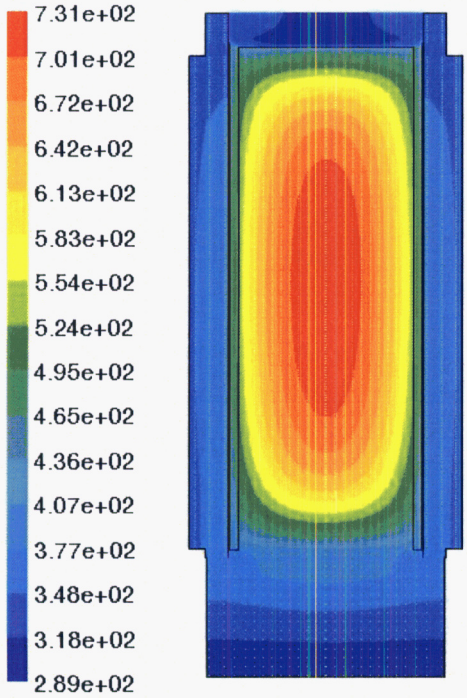

Figure 14: Open cask model of HI-STAR 100 System with k-ε turbulence flow model.

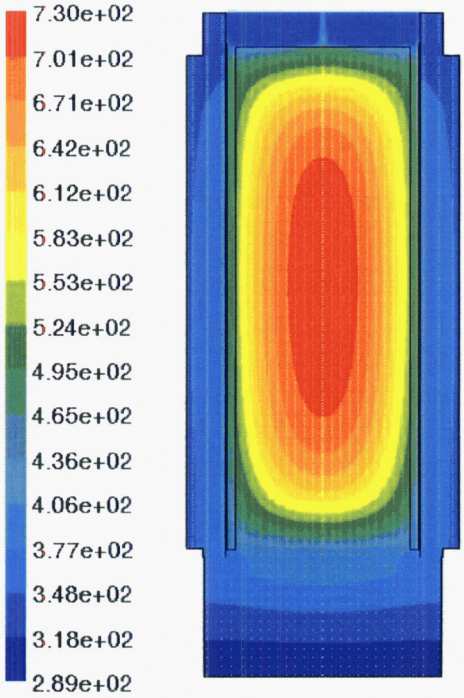

Figure 15 Open cask model of HI-STAR 100 System with k-Ω turbulence flow model.

When fuel basket and fuel assemblies are represented as three separate equivalent fuel source, the maximum predicted temperature is 755 °K in the presence of radiation and conduction heat transfer only. The calculation results are also summarized in Table 11, and the total percent of heat transfer by radiation under no flow condition is 92.3 percent The maximum temperature drops down to 501 °K when fluid is allowed to convect as laminar flow. In this case, the portion of heat transfer by conduction and convection increases to 74.4 percent. As a result, the most of heat is convected from the fuel source. The temperature distribution inside the open cask for these two conditions are presented in Figure 16 and 17. The maximum temperature of the fuel decreases to 427 °K when k-ε turbulence flow model is employed. The conduction and convection heat loss is 85.3 percent. However, the maximum temperature of the fuel increases back to 457 °K when k-omega turbulence model is used. The temperature distribution inside the cask for turbulence flow models is presented in Figure 18 and 19.

Table 11. Summary of calculated results for the open Hi-STAR cask system with thee fuel sources and flow channles in between.

Model	Predicted Maximum Temperature	Percent Heat Dissipation by Radiation	Percent Heat Dissipation by Conduction and Convection
No Fluid Flow (Radiation and Conduction Only)	755 °K	92.9	7.1
Laminar Flow	501 °K	25.6	74.4
k-ε Turbulence Flow	427 °K	14.7	85.3
k-Ω Turbulence Flow	457 °K	25.6	74.4

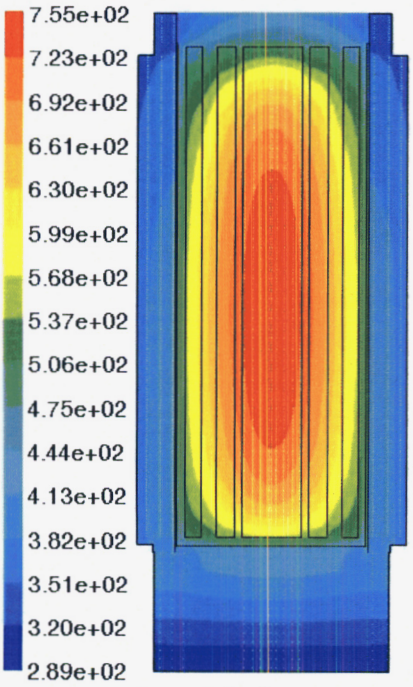

Figure 16: Open cask model of HI-STAR 100 System with fuel basket represented as three separate equivalent fuel source. Only radiation and cinduction model are employed.

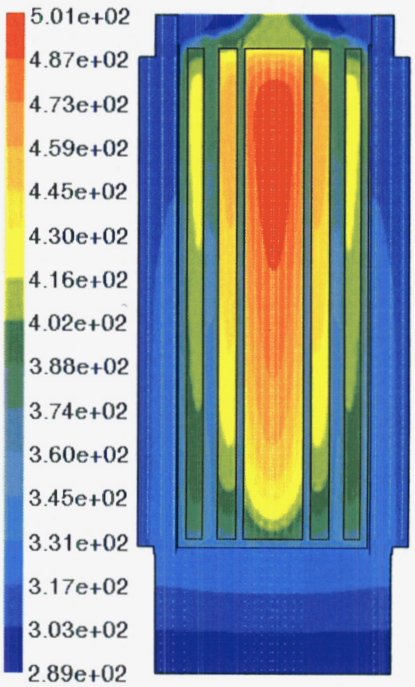

Figure 17: Open cask model of HI-STAR 100 System with fuel basket represented as three separate equivalent fuel source. Laminar fluid flow FLOW model is employed.

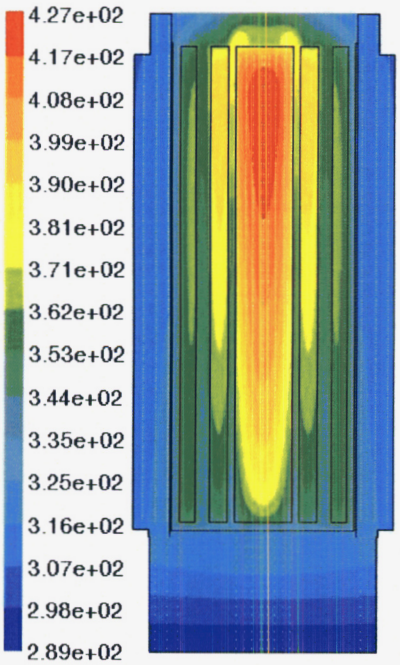

Figure 18: Open cask model of HI-STAR 100 System with fuel basket represented as three separate equivalent fuel source. k-ε turbulence flow model model is employed.

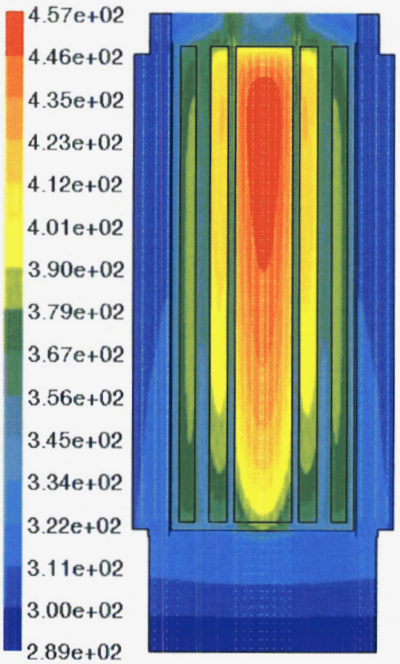

Figure 19: Open cask model of HI-STAR 100 System with fuel basket represented as three separate equivalent fuel source. k-Ω turbulence flow model model is employed.

Input and output files for open cask model:

With Single Equivalent Fuel Source:

Input Files:
Geometry was geterated in GAMBIT. File name: opencask-onefuel.dbs and opencask-onefuel.msh
The mesh file was imported in FLUENT and fluid area grid was adapted. The input and output files are listed in the table below. All files are stored in the attached disk in subdirectory called: HI-STAR100\ocmodel\onefuel\

Table: Input output files for open cask model with sigle equivalent fuel source.		
Flow Condition	FLUENT Input file	FLUENT output file
No Flow	opencask-onefuel-radcond.cas	opencask-onefuel-radcond.dat
Laminar Flow	opencask-onefuel-LAM.cas	opencask-onefuel-LAM.dat
k-ε turbulence flow model	opencask-onefuel-TurKE.cas	opencask-onefuel-TurKE.dat
k-Ω turbulence flow model	opencask-onefuel-TurKO.cas	opencask-onefuel-TurKO.dat

With Three Equivalent Fuel Source:

Input Files:
Geometry was geterated in GAMBIT. File name: opencask-channel.dbs and opencask-channel.msh
The mesh file was imported in FLUENT and fluid area grid was adapted. The input and output files are listed in the table below. All files are stored in the attached disk in subdirectory called: HI-STAR100\ocmodel\channel\

Table: Input output files for open cask model with three equivalent fuel source.		
Flow Condition	FLUENT Input file	FLUENT output file
No Flow	opencask-channel-radcond.cas	opencask-channel -radcond.dat
Laminar Flow	opencask-channel -LAM.cas	opencask-channel -LAM.dat
k-ε turbulence flow model	opencask-channel -TurKE.cas	opencask-channel -TurKE.dat
k-Ω turbulence flow model	opencask-channel -TurKO.cas	opencask-channel -TurKO.dat

APPENDIX

Entry: Pavan Shukla, Feb 20th, 2006

siglefuelassemblymodel

flatplate51: 2-D with open bottom, inflow at 350 K

27 Feb 2006 flatplate51 The air (ideal now) entering from the bottom is now at 350 K. Maximum temperature 530K in the assembly
06 Feb 2006 flatplate50 Some modifications requested by Pavan: gap geometry, full power, assembly conductivity, depth of the assembly.
Also the bottom is open and fresh air is entering the mesh from below.It looks like it is working fine with
a coarse mesh. Let's refine it. Ok, maximum temperature 527 K with finer mesh.
03 Aug 2005 flatplate19 Quick check changing Cv for air since Mary Ann's value seems to be wrong.
02 Aug 2005 flatplate17 Let's say that the initial obstacle temperature is 600K and see what happens ... It reaches steady state
faster than the cold guy, but the final temperature is the same, as hoped ...
01 Augu 2005 flatplate16 Steady state happens at around 200 secs, with the max temperature being 415 K. Let's run a coarse mesh
and see. The max temperature is now 404 K, so 11 K difference ...
28 July 2005 flatplate15r It is taking forever to Flow3D to see why reshyd does not work so I restart this guy from zero and
let it run up to 1000 s.
26 July 2005 flatplate15 I rerun it, did not realize that I chose symmetry on the lower boundary so power should be divided
by two. Added air gap at extremes
25 July 2005 flatplate15 Runs 08 thru 13 have been a success. Let's now solve conduction + convection problem. So we add the
nuclear reactor with it's power as an obstacle and see what happens. Temperature in this run rises
up to 500K and does not reach a steady state! Is there something wrong?
14 July 2005 flatplate07 Let's reduce the size of the problem so it runs faster. Then let's compare the following results:
1) discharge with differente bndry conditions 2) discharge to open space
14 July 2005 flatplate06 I think a pressure boundary condition in the upper part (x=0) is more realistic as far as the cask goes.
Will it be a big problem? It does not look like a problem, but let's do a more realistic condition.
14 July 2005 flatplate05 Let's see if with implicit heat transfer it goes faster.
14 July 2005 flatplate04 Ok, I think that even with the pressure iteration complaints this is working fine. Although it is slow.

12 July 2005 flatplate04 According to Flow3D manual press iteration problems arise if reversing flows and are not important if the
residue and the convergence criterior are close. The flow does reverse in this problem at the bottom.
And residues are not far from the convergence criterion.
Back to iadix=0 and large iterations (1000). 14 hours to complete the run. Very long!
12 July 2005 flatplate04 Hydrostatic distribution does not help with pressure iterations, but I think it is a nice idea.
Nevertheless the results looks very nice with the center of the gap with negative velocity and convection
happening on the wall. Let's restart it to see if we get rid of press iteration problems. Nope.
Now trying iadi.
11 July 2005 flatplate04 Natural convection was working great for a constant temperature wall. Let's use now a constant power
wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First
more realistic dimensions. So summarizing: 1) long field, 2) Constant Temp bound, 3) Symmetry in z.
The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never
getting the pressure iteration convergence problem). Let's limit it to 300 as Pavan's brother suggests.
Maybe the pressure iteration problems come from not having initial hydrostatic pressure distribution. Let's try.
10 July 2005 flatplate03 Now let's try natural convection with gravity along x-axis. The fluid is initially at rest. Steady state
is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.
It takes only around 1 s for steady.
10 July 2005 flatplate02 Incompressible, conduction only works fine, but time scale is enormous, 1e6 for 1 meter, let's reduce
the size of the field. For a 1 cm height mesh it works fine with heat transfer only. Timescale to steady
state around 400 s. I added slow velocity (high vel kills the time step) and I see the boundary layer
developing and heat transfer happening from the boundary. Steady state decreased to 2 s with the velocity!!
Also the characteristic distance where T drops from 350 to 329 is very small, around 1 cm or 1/10 of height.
10 July 2005 flatplate01 Trying to reproduce book analytical data
05 July 2005 pav04 Correcting rf2 to its real value.Run goes much faster!!
05 July 2005 pav03 Can this run coarser and faster? Ok, Pavan found that rf2 is wrong. I also think that we do not

need compresibility, but right now let's only care about the mesh. The result in the obstacle is the same,

but in the fluid that does not happen. Let's stay now with low resolution to play with it.

01 July 2005 pav02 Inherited from Pavan, steady state accelerator.

Goal is estimate the thermal contribution of one reactor.

24 June 2005

```
 $XPUT
  remark  = ' Advection Options',
    ifenrg  = 2,   remark = 'solve internal energy',
    ifrho   = 1,   remark = '=0 const dens, =1 density function of T, =2 solve transport, =3 second
order',
    iorder   = 1,      remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

  remark  = ' Convergence Criteria',
    epsadj  =  1.0, remark = 'multiplier for pressure iteration',
    epshtc  =  1.0, remark = 'multiplier for temp iteration',

  remark  = ' Heat Transfer Options',
    ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in obstacles
only',
    ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve obs
conduction',

  remark  = ' Explicit/Implicit Options',
    imphtc  = 1,   remark = '=0 explicit eval of temp, =1 fully implicit',
    imp     = 0,   remark = '=0 explicit press-vel incomp with incompress, =1 implicit coupling,
=2 ADI',
    impvis  = 0,   remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

  remark  = ' Flow mode options',
    icmprs  = 0,   remark = '0=incompr., 1=compressible flow',
    itb     = 0,   remark = 'no free surfaces',
    nmat    = 1,   remark = '1 compressible mat',

  remark  = ' Gravity',
    gx      = 9.81, remark = 'gravity -9,81',

  remark  = ' Initialization and Restart',
    ipdis   = 2,   remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x direct, =3 y
direct',
    trest   = 0.0  ,remark = ' restart time',

  remark  = ' Numerical options',
```

```
    ihelp  = 1,   remark = ' mentor help',
    istdy  = 0,   remark = ' =0 normal transients, =1 steady state accelerator for compress flow',
    omeght = 2.,  remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

  remark = ' Physical model options',
    iwsh   = 1,   remark = '=0 turn off wall shear',
    ifvis  = 0,   remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
    ivish  = 0,   remark = ' no viscous heating, =1 include visc heat',

  remark = ' Plot output',
    pltdt  = 10., remark = 'plotting interval, seconds',
    hpltdt = 100000.,remark = 'history interval, seconds',


  remark = ' Termination Control',
    twfin  = 1000.0, remark = 'simulation end, seconds',

  remark = ' Pressure interation options',
    iadix  = 0,   remark=' =0 SOR, =1 ADI',
    iadiy  = 0,   remark=' =0 SOR, =1 ADI',
    iadiz  = 1,   remark=' =0 SOR, =1 ADI',
    omega  = 1.7, remark = 'default setting for over-relaxation factor',

  remark = ' Time Step Control',
    delt   = 1.0e-5, remark = 'initial time step, seconds',
    dtmax  = 100.,   remark = 'maximum timestep',
    autot  = 2.0, remark = 'timestep by stability',

 $END

 $LIMITS

    itflmx = 1000000, remark = 'maximum pressure iteration failures allowed',
    itmax  = 1000,    remark = 'max press iter per time step',
    itdtmx = 100,     remark = ' max # of press iterations before time step reduced',
    idtht  = 20,      remark = ' max # of temp iter before dt reduced',
    ithtmx = 50,      remark = ' only when implicit heat transf., max # of temp iter per cycle',

    negtmx = 100000, remark = 'negative rhoe resets',
    ncflmx = 1000,   remark = 'convection failures allowed',

 $END

 $PROPS
```

```
   remark  = 'set up properties on fluid 2 to allow for compressibility option',

   units   = 'si',
   rhof    = 1.225,
   mu1     = 1.86e-5, remark = 'viscosity air',
   cv1     = 713. , remark = 'specific heat air',
   thc1    = 0.0264, remark = 'thermal conductivity air',
   thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
   tstar   = 293.15, remark = 'ref temp for air properties',
 $END


 $SCALAR
   remark = 'none needed for these simulations',
 $END

 $BCDATA

   wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
   wr    = 5, remark = 'high x',
   wf    = 1, remark = 'low y',
   wbk   = 1, remark = 'high y',
   wb    = 1, remark = 'low z',
   wt    = 1, remark = 'high z, continuative',

   pbc(1) = 101280.,
   tbc(1) = 300.,
   pbc(2) = 101325.,
   tbc(2) = 350.,

 $END
   tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
 $MESH
   nxcelt  = 150,
       px(1) = 0.0, nxcell(1) = 50,
       px(2) = 1.0, nxcell(2) = 25,
       px(3) = 2.0, nxcell(3) = 25,
       px(4) = 3.0, nxcell(4) = 50,
     px(5) = 4.50 ,

   nycelt  = 1,
     py(1)=0.0, nycell(1)=1,
     py(2)=.9064,  remark=' This includes the 4 faces of the assembly',
```

```
  nzcelt   = 23,
    pz(1)  = -0.1135,nzcell(1)  =  8,
    pz(2)  =  0.0,   nzcell(2)  = 15,
    pz(3)  = .01538,  remark='Pavan gave me the gap size',
$END

$OBS
  nobs=1,
  iob(1) = 1, ioh(1) = 1, xl(1) =   0.35, xh(1) =  4.20,
                  yl(1) =   0.  , yh(1) =  1.0,
                  zl(1) =  -.1135,zh(1)=  0.0,
                  kobs(1) = 0.169314,  remark=' Pavan gave me this number 6 Feb 2006',
                  rcobs(1) = 234.46,
                  pobs(1,1) =792., remark='Full power since the total surface corresponds to the
4 faces of the assembly',
                  twobs(1,1) = 600.,   remark=' this is the initial temperature of the obstacle',
                  tobs(1)  =0.,



$END

  iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                    yl(31) =  0.5842000, yh(31) =  0.8137525,
                    zl(31) =  0.3052800, zh(31) =  4.1651200,
                    kobs(10) = 0.696,
                    rcobs(10) = 234.46,
                    pobs(1,10) = 792,


$FL

   remark = 'setting 1atm in Pa',
   presi  = 101325.0,
   pvoid  = 101325.0,
   ui     = 0. ,
$END

$BF
$END

$TEMP

   remark = 'setting initial temps to 25C to get things started',
   tempi = 300.0,
```

```
 $END

 $GRAFIC

   icolor = 2,

   remark = 'jobsbk = 10,  jobsf = 14,',

   ncplts = 4,
   contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
   contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
   contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
   contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

 $END


 $PARTS
 $END
From schocron Fri Apr  7 10:24:53 2006
Date: Fri, 07 Apr 2006 10:24:53 -0500
To: schocron@swri.edu
Subject: c
Message-ID: <44368445.mailMLS11O02X@vader.div18.swri.edu>
User-Agent: nail 11.4 8/29/04
MIME-Version: 1.0
Content-Type: multipart/mixed;
 boundary="8AEVHTFGU0-=-IPH8MF4GX5-CUT-HERE-G62OMIX2SF-=-12IW7PL6OZ"

This is a multi-part message in MIME format.

--8AEVHTFGU0-=-IPH8MF4GX5-CUT-HERE-G62OMIX2SF-=-12IW7PL6OZ
Content-Type: text/plain; charset=us-ascii
Content-Transfer-Encoding: 7bit
Content-Disposition: inline

hola

--8AEVHTFGU0-=-IPH8MF4GX5-CUT-HERE-G62OMIX2SF-=-12IW7PL6OZ
Content-Type: application/octet-stream;
 charset=us-ascii
Content-Transfer-Encoding: 7bit
Content-Disposition: attachment;
 filename="prepin.inp"

flatplate50: 2-D with open bottom.
```

06 Feb 2006 flatplate50 Some modifications requested by Pavan: gap geometry, full power, assembly conductivity, depth of the assembly.

Also the bottom is open and fresh air is entering the mesh from below.It looks like it is working fine with

a coarse mesh. Let's refine it. Ok, maximum temperature 527 K with finer mesh.

03 Aug 2005 flatplate19 Quick check changing Cv for air since Mary Ann's value seems to be wrong.

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faster than the cold guy, but the final temperature is the same, as hoped ...

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and see. The max temperature is now 404 K, so 11 K difference ...

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wall with similar dimensions to the ones in the reactor. Afterwards let's incorporate the gap. First

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The run is going very slow,probably because of the pressure iteration stuff (I am using 100000, and never

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is very fast. I see again the boundary layer. I need a very high number of pressure iterations to converge.

It takes only around 1 s for steady.

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order',
    iorder  = 1,      remark = 'setting iorder = 3 monotonically increasing,0=linear,1=1st
order,2=2nd',

  remark  = ' Convergence Criteria',
    epsadj  =  1.0, remark = 'multiplier for pressure iteration',
    epshtc  =  1.0, remark = 'multiplier for temp iteration',

  remark  = ' Heat Transfer Options',
    ihonly  = 0,    remark = '=0 all, =1 energy only,=2 energy only zero vel,=3 heat in obstacles
only',
    ihtc    = 2,    remark = '=0 no heat trans, =1 evaluate heat, =2 evaluate heat and solve obs
conduction',

  remark  = ' Explicit/Implicit Options',
    imphtc  = 1,   remark = '=0 explicit eval of temp, =1 fully implicit',
    imp     = 0,   remark = '=0 explicit press-vel incomp with incompress, =1 implicit coupling,
=2 ADI',
    impvis  = 0,   remark = '=0 explicit viscous stress calc, =1 implicit, =2 ADI',

  remark  = ' Flow mode options',
    icmprs  = 0,   remark = '0=incompr., 1=compressible flow',
    itb     = 0,   remark = 'no free surfaces',
    nmat    = 1,   remark = '1 compressible mat',

  remark  = ' Gravity',
    gx      = 9.81, remark = 'gravity -9,81',

  remark  = ' Initialization and Restart',
    ipdis   = 2,   remark = '=0 uniform press, =1 hydrostatic press in z direction, =2 x direct, =3 y
direct',
    trest   = 0.0  ,remark = ' restart time',

  remark  = ' Numerical options',
    ihelp   = 1,   remark = ' mentor help',
    istdy   = 0,   remark = ' =0 normal transients, =1 steady state accelerator for compress flow',
    omeght  = 2.,  remark = ' overrelaxation factor for ADI implicit heat transf. Calcs',

  remark  = ' Physical model options',
    iwsh    = 1,   remark = '=0 turn off wall shear',
    ifvis   = 0,    remark = '=0 local viscos, =1 Prandtl, =2 turb energ, 3= k-eps, 4=RNG, =-1
large eddy',
    ivish   = 0,   remark = ' no viscous heating, =1 include visc heat',

  remark  = ' Plot output',
```

```
   pltdt  =  10., remark = 'plotting interval, seconds',
   hpltdt  =  100000.,remark = 'history interval, seconds',


 remark  = ' Termination Control',
   twfin  = 1000.0,  remark = 'simulation end, seconds',

 remark  = ' Pressure interation options',
   iadix  = 0,   remark=' =0 SOR, =1 ADI',
   iadiy  = 0,   remark=' =0 SOR, =1 ADI',
   iadiz  = 1,   remark=' =0 SOR, =1 ADI',
   omega  = 1.7,  remark = 'default setting for over-relaxation factor',

 remark  = ' Time Step Control',
   delt   =  1.0e-5, remark = 'initial time step, seconds',
   dtmax  =  100.,   remark = 'maximum timestep',
   autot  =  2.0, remark = 'timestep by stability',

 $END

 $LIMITS

   itflmx  =  1000000, remark = 'maximum pressure iteration failures allowed',
   itmax  =  1000,     remark = 'max press iter per time step',
   itdtmx  =  100,    remark = ' max # of press iterations before time step reduced',
   idtht  =  20,     remark = ' max # of temp iter before dt reduced',
   ithtmx  =  50,     remark = ' only when implicit heat transf., max # of temp iter per cycle',

   negtmx  =  100000,  remark = 'negative rhoe resets',
   ncflmx  =  1000,   remark = 'convection failures allowed',

 $END

 $PROPS

   remark  = 'set up properties on fluid 2 to allow for compressibility option',

   units  = 'si',
   rhof   = 1.225,
   mu1    = 1.86e-5, remark = 'viscosity air',
   cv1    = 713. ,  remark = 'specific heat air',
   thc1   = 0.0264,  remark = 'thermal conductivity air',
   thexf1  = 3.48e-3, remark = 'thermal expansion: p594 (Batchelor, Fluid Dynamics)',
   tstar  = 293.15,  remark = 'ref temp for air properties',
 $END
```

```
$SCALAR
   remark = 'none needed for these simulations',
$END

$BCDATA

   wl      = 5,  remark = 'low x, 1=symmetry,2=wall,3=continuative,4=periodic,5=specified
press,6=specified vel,7=GO,8=outflow,9=Grid Block',
   wr    = 5, remark = 'high x',
   wf    = 1, remark = 'low y',
   wbk   = 1, remark = 'high y',
   wb    = 1, remark = 'low z',
   wt    = 1, remark = 'high z, continuative',

   pbc(1) = 101280.,
   tbc(1) = 300.,
   pbc(2) = 101325.,
   tbc(2) = 300.,

$END
   tbcd   = 300., This guy seems to impose a temperature boundary condition that we do not
want.
$MESH
   nxcelt  = 150,
       px(1) = 0.0, nxcell(1) = 50,
       px(2) = 1.0, nxcell(2) = 25,
       px(3) = 2.0, nxcell(3) = 25,
       px(4) = 3.0, nxcell(4) = 50,
     px(5) = 4.50 ,

   nycelt  = 1,
     py(1)=0.0, nycell(1)=1,
     py(2)=.9064,  remark=' This includes the 4 faces of the assembly',

   nzcelt   = 23,
     pz(1) = -0.1135,nzcell(1) = 8,
     pz(2) = 0.0,  nzcell(2) = 15,
     pz(3) = .01538, remark='Pavan gave me the gap size',
$END

$OBS
  nobs=1,
  iob(1) = 1, ioh(1) = 1, xl(1) =  0.35, xh(1) = 4.20,
                  yl(1) =  0. , yh(1) = 1.0,
                  zl(1) = -.1135,zh(1)= 0.0,
```

```
                kobs(1) = 0.169314,  remark=' Pavan gave me this number 6 Feb 2006',
                rcobs(1) = 234.46,
                pobs(1,1) =792., remark='Full power since the total surface corresponds to the
4 faces of the assembly',
                twobs(1,1) = 600.,   remark=' this is the initial temperature of the obstacle',
                tobs(1)  =0.,


 $END

   iob(31) = 10, ioh(31) = 1, xl(31) =  0.0252222, xh(31) =  0.2517902,
                  yl(31) =  0.5842000, yh(31) =  0.8137525,
                  zl(31) =  0.3052800, zh(31) =  4.1651200,
                  kobs(10) = 0.696,
                  rcobs(10) = 234.46,
                  pobs(1,10) = 792,


 $FL

   remark = 'setting 1atm in Pa',
   presi  = 101325.0,
   pvoid  = 101325.0,
   ui     = 0. ,
 $END

 $BF
 $END

 $TEMP

   remark = 'setting initial temps to 25C to get things started',
   tempi = 300.0,

 $END

 $GRAFIC

   icolor = 2,

   remark = 'jobsbk = 10,  jobsf = 14,',

   ncplts = 4,
   contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
   contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
```

contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,

$END

$PARTS
$END

--8AEVHTFGU0-=-IPH8MF4GX5-CUT-HERE-G62OMIX2SF-=-12IW7PL6OZ--

****
Closedcaskmodel01
****

```
10 Apr    2006  ccask24  Same thing, k=3.382. Assmby: Tmax=752.1 K, Vertical
wall: Tmax= 347.0K, Tmin= 324.9 K,
                        Horizontal wall: Tmax=342.2 K, Tmin=339.3 K. The run
died after reaching steady state.
10 Apr    2006  ccask23  Pavan sent me another input deck with ridiculously
small changes in the temperature. Let's run it ...
03 Apr    2006  ccask21  Now max. temperature in assembly is 799 K. Vertical
wall: Tmax=350 K, Tmin=325.5K -> Tavg= 337.75K.
                        Horizontal wall: Tmax=344.3 K, Tmin=341.2 K ->
Tavg=342.75 K. We are still converged fortunately ...
                        Note: Flow3-D is still dying after reaching steady
state (so it claims). I guess we should report
                        this to Flow Science at some point.
31 Mar    2006  ccask19  In the ideal gas computation the R (gas constant)
was hardwired for air, I changed it for He.
23 Feb    2006  ccask17  k=2.59 W/m/K in obstacle 9. Assembly Tmax=723 K;
Vertical Wall: Tmax=350.4K Tmin=324.5 K
                        Horizontal wall: Tmax=343.2K Tmin=340.1K
23 Feb    2006  ccask16  Pavan wants to play a little with the thermal
conductivity of the assembly. k=1.92 W/m/K in obstacle 9
                        Assembly: Tmax=767K; Vertical wall: Tmax=350.7 K,
Tmin=324K; Horizontal wall: Tmax 343 K, Tmin=340 K
22 Feb    2006  ccask15  Iteration number 3 for DT=40 K, changed htcs. Max
Temp in assembly 692 K. Vertical wall: Tmax=350K
                        Tmin=325 K -> Tavg=337 K so DT=Tavge-300=37 K, very
close to the one assumed.
                        Horizontal wall: Tmax= 343.5 K Tmin = 340.5 ->
Tavge=342 -> DT=342-300= 42K, again very close. I guess
                        we can say we are converged!
22 Feb    2006  ccask14  We found in ccask13 vertical wall Tavge=328.6 K ,
and in horizontal: Tavge = 328.5 K. Let's adjust the heat
                        transfer coefficients for that DT=28K. Ok, max temp
694 K. Vertical wall: Tmax=351.8 K ,Tmin=326.5K -> Tav=339K
                        Horizontal wall: Tmax 345.4 Tmin 342.3 Tav=343.8K .
So, this time DT is around 40 K
21 Feb    2006  ccask13  Let's add now radiation to the void. Later change
heat transfer coef. to better reflect the real
```

temperature in horizontal and vertical walls. Max temperature in assembly 682 K. Steady-state reached in
57.1 secs, nice! Vertical wall: Tmax=339 K, Tmin=318.2 K; Horizontal wall: Tmax=330 K, Tmin=327 K.
21 Feb 2006 ccask12 Let's run now Helium as ideal gas. Remember, I do not need to change anything in the input deck, I
just need to run the user version of Flow-3D. Let's also watch if it still dies after reaching steady
state. Again it reaches steady state at around 130 secs. This time it does not dye! Good!!!
Steady state max temp. 702 K. In the vertical wall: Tmax=359.6 K, Tmin=330.5K; in the horizontal:
Tmax=348.9 K, Tmin=344.7 K
17 Feb 2006 ccask10 Input deck from Anurag. He changed void type to 1. It runs all right and reaches steady state at around
around 772 K. For some reason it dies afterwards, but I do not think it's important ...
15 Feb 2006 ccask09 Add a gap with He between MPC and overpack, added impvis=1 and max press iteration failures infinite.
Coarsen the mesh.
13 Feb 2006 ccask05: Pavan gave me new heat transfer coefficients based upon DT=360K with the old ones.
They do not seem to affect the results, maybe because of not reaching steady state?
13 Feb 2006 ccask05: Anurag did some mods to this.
10 Feb 2006 ccask04: Pavan and Anurag modified ccask03 input deck. This is the result ...
08 Feb 2006 ccask02: Coarse mesh
08 Feb 2006 ccask01: Code inherited from Pavan. Boussinesq approx. Two fluid run. Need to go to ideal gas for He and
switch on convection.
07 Febuary 2005 Modeling a Homegenised closed cask system. Results od this
calculations go in the report.
23 August 2005 Chnaging the fluid properties to that of helium.
23 August 2005 Adding a lid on top of the cask.
22 August 2005 Updating the thermal conductivity of the obstacle from Table 4.4.7, 1.954*1.7307 in SI units
22 August 2005 Modifying the properties of the power obstacle. Making it equal to one in FSAR
Also changing the boundary condition wr as wall instead of continuative.
09 August 2005 remoing top free portion of the air
03 August 2005 Modeling 24 MPC as one power source in cylindrical geometry. Cv air= 713.5 J/Kg 0K

22 July 2005 Modeling just one power source in 2 dimentional setting. removing all other obstacles.
Cartesin geometry only.
05 July 2005 Default value of gas constant R was in wrong units. Corrected here.

20 June 2005
Updated informational fields

24 May 2005
Turning off air flow and allowing thermal progression only

11 May 2005 Chris Ryder asked that I look at the 24 Basket with different fuel.
Resetting obstacle field with this basket and fuel source. Basic parameters will be
the same. Grid will need to be slightly reworked to accomodate new fuel spacing.

```
 $XPUT
      twfin   =  300.0,  remark = 'simulation end, seconds',
      gz = -9.81,     remark = 'gravity',
      ifenrg = 2,     remark = 'fluid energy transport on',
      ifrho  = 1,
      ihtc   = 2,     remark = 'turn  on heat conduction through obstacles',
      delt    =  1.0e-4, remark = 'time step, seconds',
      ipdis  = 1, remark='hydrostatic pressure in z direction',
      hpltdt  =  1.0,    remark = 'history interval, seconds',
      pltdt   =  5.,   remark = 'plotting interval, seconds',
      imphtc = 1,     remark = 'implicit eval of temp terms',
      icmprs  = 0,    remark = 'incompressible flow',
      iorder  = 3,    remark = 'setting iorder = 3 monotonically increasing',
      itb     = 1,    remark = 'no free surfaces Changed by Anurag',
      nmat    = 1,    remark = '1 compressible mat',
      iwsh    = 1,    remark = 'turn off wall shear',
      dtmax   =  0.01,    remark = 'maximum timestep',
      autot   =  2.0, remark = 'timestep by stability',
      omega   =  1.0, remark = 'default setting for over-relaxation factor',
      epsadj  =  1.0, remark = 'standard convergence criterion',
      remark='this was killing the run:igmres = 1,',
      ihelp = 2,
      ifrho  = 1,
      ifvelp = 0,
      impvis=1,
    iadix=1, iadiz=1,
  $END

  $LIMITS
       remark = 'maximum pressure iteration failures allowed',
  $END

  $PROPS
      remark  = 'set up properties on fluid 2 to allow for compressibility
option',
      units   = 'si',
      rhof    = 0.178, remark='1.2',
      mu1     = 1.9e-5, remark='1.86e-5', remark = 'viscosity air',
      cv1     = 2077.5, remark='713.5',   remark='oldvalue=1883.7',  remark =
'specific heat air',
      thc1    = 0.142, remark='0.0264',  remark = 'thermal conductivity air',
      thexf1  = 1.0e-3,  remark='3.48e-3', remark = 'thermal expansion: p594
(Batchelor, Fluid Dynamics)',
      tstar   = 1000.0,  remark = 'ref temp for air properties',
      remark  = 'rf2     = 287.',    remark = 'gas constant for air',
  $END

  $SCALAR
      remark = 'none needed for these simulations',
  $END
```

```
  $BCDATA
      remark = 'top wall is continuative (wt) or boundary 6',
      remark = 'set up as no ventilation',
      remark = 'made all bc continuative to start so cask is set in infinite
air',
      wl     = 1,    remark = 'low x, symmetric',
      wr     = 2,    remark = 'high x',
      wf     = 1,    remark = 'low y, symmetric',
      wbk    = 1,    remark = 'high y',
      wb     = 2,    remark = 'low z',
          remark = 'high z, continuative',
      remark = 'eventually add cross-velocity at top of cask if necessary',
      tbc(5) = 288.7,
      pbc(6) = 101266.805,
      remark = 'f boundaries are automatically 0 (mat 2)',
    fbc(6)=0.0,
    wt=5,
    tbc(2)=299.82,
    tbc(6)=299.82,
    ipbctp(6)=1,
    ipbctp(5)=1, ipbctp(2)=1,
  $END

  $MESH
      remark = 'cylindrical  mesh',
      icyl     = 1,
      nxcelt   = 51,
        px(1) =  0.0000000,  nxcell(1) = 10, remark = 'power source',
        px(2) =  0.7853680,  nxcell(2) = 10, remark = 'airgap',
        px(3) =  0.8556625,  nxcell(3) = 5, remark = 'MPC walls',
        px(4) =  0.8683625,  nxcell(4) = 10, remark = 'overpack and holtite-A
boundary',
        px(5) =  0.8731250,  nxcell(5) = 15, remark = 'overpack and holtite-A
boundary',
        px(6) =  1.2192000,  nxcell(6) =  1, remark = 'Adding two void spaces
after holtitle-A boundary',
        px(7) =  1.25,
    nycelt   = 1,
        pya(1) =  0.0000000,  nycell(1) = 1, remark = 'air',
        pya(2) = 10.0000000,
     nzcelt    = 76,
        pz(1)  = -1.1303000,  nzcell(1)  =10, remark= 'concrete base ',
        pz(2)  = -0.2159000,  nzcell(2)  = 5,  remark = 'bottom overpack base
plate',
        pz(3)  = -0.0635000,  nzcell(3)  = 5,  remark = 'MPC base plate',
        pz(4)  =  0.0000000,  nzcell(4)  =30, remark = 'bottom of fuel basket
and of MPC shell',
        pz(5)  =  4.4831000,  nzcell(5)  = 5,  remark = 'bottom overpack
neutron shielding',
        pz(6)  =  4.5212000,  nzcell(6)  = 5, remark = 'begin fuel',
        pz(7)  =  4.7625000,  nzcell(7)  = 10,  remark = 'top fuel',
        pz(8)  =  4.7910750,  nzcell(8)  = 5,  remark = 'top overpack neutron
shielding',
        pz(9)  =  4.9434750,  nzcell(9)  = 1,  remark = 'void spave on the
top of ',
        pz(10) =  4.9900000,
```

```
  $END

  $OBS
     nobs = 10,
     remark='MPC base Plate upuntil MPC shell interior wall',
     iob(1) = 1, ioh(1) = 1,     ral(1) =  0.0000, rah(1) = 0.8683625,
remark='0.8556625',
                                  zl(1) = -0.0635, zh(1)  = 0.0000000,
                                 kobs(1) = 16.960,
                                rcobs(1) = 502.41,
     remark='MPC Shell ',
     iob(2) = 2, ioh(2) = 1,     ral(2) =  0.8556625,  rah(2) = 0.8683625,
remark='0.8731250',
                                  zl(2)  =  0.0000000,  zh(2)  = 4.5212000,
                                 kobs(2) = 16.96, remark='0.8',
                                rcobs(2) = 502.41,
     remark='MPC Lid',
     iob(3) = 3, ioh(3) = 1,     ral(3) =  0.0000000,  rah(3) =0.8683625,
remark='0.8556625',
                                  zl(3)  =  4.5212,     zh(3)  =  4.7625,
                                 kobs(3) = 16.96,
                                 rcobs(3)= 502.41,
     remark='Overpack Base Plate',
     iob(4) = 4, ioh(4) = 1, ral(4) =  0.0000000, rah(4) =  1.0572750,
                               zl(4)  = -0.21590000, zh(4) = -0.0635000,
                               kobs(4) = 41.2,
                               rcobs(4) = 502.41,
                               hobv1(4)=5.19, remark='from Pavans excel
table',
                               hobe1(4)=4.8199e-8, remark='Pavan said
5.67051*10^(-8)*0.85',
     remark='overpack inner shell',
     iob(5) = 5, ioh(5) = 1, ral(5) =  0.8731250, rah(5) =  0.9366250,
                               zl(5)  = -0.0635000, zh(5)  =  4.7910750,
                               kobs(5) = 41.2,
                               rcobs(5) = 502.41,
     remark='overpack five adjacent layerrs',
     iob(6) = 6, ioh(6) = 1, ral(6) =  0.9366250, rah(6) =  1.0699750,
                              zl(6) = -0.0635000, zh(6)  =  4.7910750,
                               kobs(6) = 11.580,
                               rcobs(6) = 502.41,
                               hobe1(6)=4.8199e-8, remark='Pavan said
5.67051*10^(-8)*0.85',
                               hobv1(6)=5.19, remark='from Pavans excel
table',
     remark='overpack lid',
     iob(7) = 7, ioh(7) = 1, ral(7) =  0.0000000, rah(7) = 1.0699750,
                               zl(7) = 4.7910750, zh(7)  = 4.9434750,
                               kobs(7) = 41.2,
                               rcobs(7) = 502.41,
                               hobe1(7)=4.8199e-8, remark='Pavan said
5.67051*10^(-8)*0.85',
                               hobv1(7)=4.49, remark='from Pavans excel
table',
     remark='Holtite-A and carbon sttel connectors',
     iob(8) = 8, ioh(8) = 1, ral(8) =  1.0699750, rah(8) =  1.2192000,
                              zl(8) =  0.00635000, zh(8) =  4.4037250,
```

```
                                 kobs(8) = 3.3800,
                                rcobs(8) = 500.,
                                hobel(8)=4.8199e-8, remark='Pavan said
5.67051*10^(-8)*0.85',
                                hobvl(8)=5.19, remark='from Pavans excel
table',
     remark= 'power source',
     iob(9) = 9, ioh(9) = 1, ral(9) = 0.0000000, rah(9) = 0.785368,
                                zl(9) =  0.0000000, zh(9) =  4.4831,
                                kobs(9) = 3.382, remark='2.5874',
                                rcobs(9) = 234.46,
                                pobs(1,9) = 528., remark='total power/4/9 or
19008/4/9',
                                twobs(1,9) = 600.,
                                tobs(9)=0.,
     remark= 'concrete base',
     iob(10) = 10, ioh(10) = 1, ral(10) = 0.0000000, rah(10) = 1.057275,
                                zl(10) =  -1.1303, zh(10)  =-0.2159,
                                kobs(10) = 0.8,
                                rcobs(10) = 234.46,
                                hobvl(10)=0.,
    twobs(1,1)=300.0, twobs(1,2)=300.0, twobs(1,3)=300.0, twobs(1,4)=300.0,
    twobs(1,5)=300.0, twobs(1,6)=300.0, twobs(1,7)=300.0, twobs(1,8)=300.0,
    twobs(1,10)=300.0,
  $END

  $FL
      remark = 'setting 1atm in Pa',
    nfls=1, frah(1)=.88,  remark = 'Fluid region Changed by Anurag',
    fzh(1)=4.9434750,
    pvoid=101266.805,
    remark = 'setting pointer to indicate void type 1 for HT coefficients;
i.e. hobvl or hobel for radiation; changed by Anurag',
    xvr(1)=1.2, yvr(1)=0.001, zvr(1)=4.5, pvrd(1)=101266.805,
    tvrd(1)=299.82, ivht(1)=1, remark = 'ivht sets void type 1',
  $END

  $BF
  $END

  $TEMP
      remark = 'setting initial temps to 25C to get things started', remark =
'Fluid region Initial temp Changed by Anurag',
      tempi = 300.0,
    tvoid=299.82,
    ntmp=1, trah(1)=1.03, treg(1)=299.82,
  $END

  $GRAFIC
      icolor = 2,
      remark = 'jobsbk = 10,  jobsf = 14,',
      ncplts = 4,
      contyp(1) = 'f',  ictyp(1) = 1, iperc(1) = 3,
      contyp(2) = 'vel',ictyp(2) = 1, iperc(2) = 3,
      contyp(3) = 'tn', ictyp(3) = 1, iperc(3) = 3,
      contyp(4) = 'tw', ictyp(4) = 1, iperc(4) = 3,
  $END
```

```
 &renderspace
    ifrs=0,
    ifcomp=0,
 /
 $PARTS
  $END
```

```
FLUENT TEST CASE
Tutorial 1. Introduction to Using FLUENT: Fluid Flow and Heat Transfer in a
Mixing Elbow.
```

Effective thermal conductivity of fuel basket when it is in contact with air:

Effective Thermal Conductivity of a Composite Structure

Background and Objective

Nuclear waste storage canisters are sealed and pressurized with helium for normal operations. The helium provides an inert environment around the fuel rods and other materials. The helium also has a high thermal diffusivity with respect to other inert gases and can diffuse thermal energy more readily than many other gases. If a cask is opened in an air environment, however, the helium will be quickly replaced with the ambient air. This will lower the overall effective thermal conductivity in the spaces inside the canister and there is a possibility that the fuel rods could reach an unsafe temperature under these conditions.

The objective of the analysis presented here is to provide a methodology for estimating the thermal conductivity of a canister fuel basket in which the helium has been replaced with air. Such an estimate will be used in the overall thermal analysis of an open nuclear waste canister.

Assumptions

The following assumptions will be made for this analysis:

1. *The effective thermal conductivity of a helium-filled fuel basket is known from previous detailed analyses or laboratory measurements.*
2. *The gas in the canister is stationary. That is, convection heat transfer is neglected.*
3. *Thermal radiation between the canister internal components is neglected.*
4. *The fuel assembly unit cell is a geometrically square array of fuel rods*

References

*Beck, A. E., "Methods for Determining Thermal Conductivity and Thermal Diffusivity," **Handbook of Terrestrial Heat-Flow Density Determination**, Haenel, R., Rybach, L., Stegena, L. eds., Kluwer Academinc Publishers, Dordrect, 1988, pp. 87-124.*

*Holtec International, Chapter 4 - Thermal Evaluation, **Final Safety Analysis Report (FSAR), HI-STAR 100 Cask System**, Rev 1, December, 2002.*

Approach

The effective thermal conductivity of a helium-filled canister will be estimated with several different proposed mathematical models for computing effective thermal conductivity of composite materials. There are many such models described, for example, by Beck (1988). The estimates will be compared to the accepted value of the effective thermal conductivity of the helium-filled canister and the closest estimated value to the accepted value will dictate which model is the most accurate of those used. This model will then be used to estimate the effective thermal conductivity of an air-filled canister. This estimated value will be adjusted by the ratio of the estimated and accepted values for the helium-filled canister to arrive at the final estimate of the effective thermal conductivity of an air-filled canister.

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Composite Effective Thermal Conductivity

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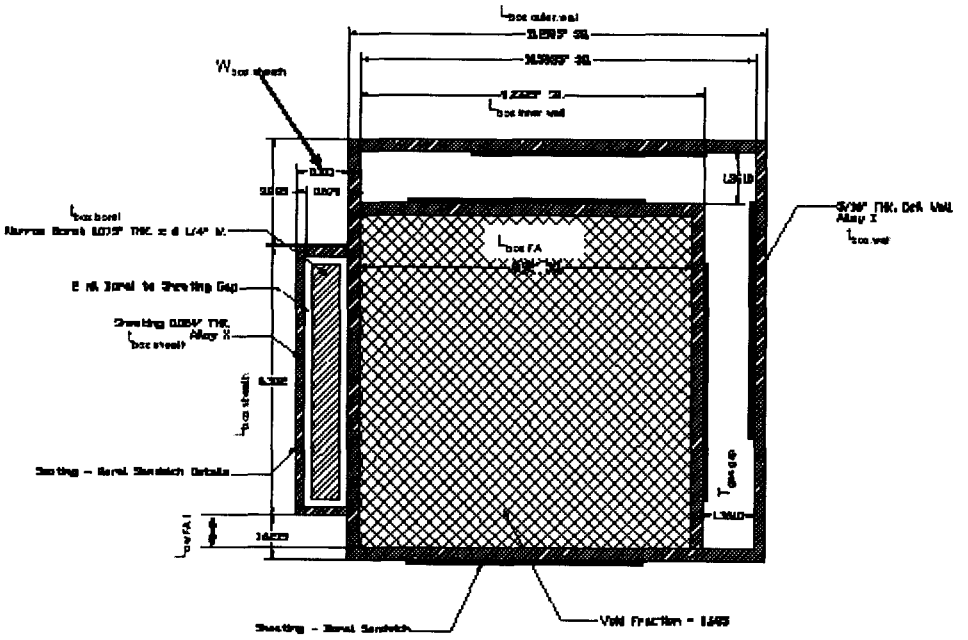

Figure 1. One Fuel Assembly "Box" in a Waste Canister, Typical

Effective Thermal Conductivity of Fuel Assembly and Fuel Assembly Box

Each of the fuel assembly matrices is contained within a box constructed or Alloy X (usually) that runs the entire length of the canister. Each face of the box has a layer of Boral shielding contained within an Allow X that holds the shield against the wall of the box. A highly simplified schematic of one fuel assembly box is shown in Figure 1. Approximate dimensions and the thermal conductivity of the materials in the walls of the box are as follows.

Fuel Assembly Box Geometry

$L_{box.outer.wall} := 11.2185 \cdot in$ *Length of fuel assembly box wall*

$L_{box.sheath} := 6.302 \cdot in$ *Length of fuel assembly sheath*

$t_{box.wall} := 0.3125 \cdot in$ *Thickness of fuel assembly box wall*

$t_{box.sheath} := 0.024 \cdot in$ *Thickness of fuel assembly sheath*

$t_{box.boral} := 0.075 \cdot in$ *Thickness of boral shield material*

$L_{ow.FA.t} := 1.6215 \cdot in - t_{box.wall}$ *Box wall not covered by sheath*

$t_{s.boral.gap} := 0.002 \cdot in$ *Gap between sheath and Boral*

$t_{gas.gap} := 1.361 \cdot in$ *Thickness of gas gap between the inner and outer walls*

$L_{box.inner.wall} := 9.2325 \cdot in$

$W_{box.sheath} := 0.103 \cdot in$ *Boral sheath height from box wall*

$L_{box.FA} := 8.92 \cdot in$ *Inside dimension of inner box holding the fuel rods*

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Property Values for the Fuel Assembly Box Materials

$k_{alloyX} := 9.8 \cdot \frac{BTU}{hr \cdot ft \cdot R}$ *Alloy X box wall and Boral sheath*

$k_{boral} := 47.84 \cdot \frac{BTU}{hr \cdot ft \cdot R}$ *Boral shielding inside sheath*

$h_{sheath_gap} := 100 \cdot \frac{watt}{m^2 \cdot K}$ *Effective heat transfer coefficient of sheath-boral interface*

The effective thermal conductivity of the fuel rod matrix will be approximated with various models for composite materials. The following is the setup for theses models

Definitions

$ORIGIN \equiv 1$ *Set the Mathcad definition for the array initial index to 1 (Default is 0). This will make identification of the terms in the property arrays more straightforward to most users.*

$N_{material} := 2$ *Number of materials in the matrix.*

$im := 1 .. N_{material}$ *Define indexes for constituent property vector(s)*

k_m (vector) *Thermal conductivities of constituent materials*

v_m (vector) *Volume fractions of constituent materials*

$n_{gas} := 2$ *Index of the gas in the material property vector*

Property Values for Materials inside the Fuel Assembly Box

Thermal conductivity	*Volume fraction*	*NOTE: Use R or K for the temperature in the thermal conductivity units. This is required by Mathcad*
$k_{m_1} := 3.50 \cdot \frac{BTU}{hr \cdot ft \cdot R}$	$v_{m_1} := .315$	*Fuel @ 450°F*
$k_{m_2} := 0.1289 \cdot \frac{BTU}{hr \cdot ft \cdot R}$	$v_{m_2} := .685$	*Helium at 450°F*
	$\sum_{i=1}^{N_{material}} v_{m_i} = 1$	*NOTE: The sum of the volume fractions **MUST** be one*
$k_{air} := 0.0225 \cdot \frac{BTU}{hr \cdot ft \cdot R}$		*Air at 450°F*

$k_{eff_He.known} := 0.284 \cdot \frac{BTU}{hr \cdot ft \cdot R}$ *Accepted value for the effective thermal conductivity of the W-14x14 Std Fuel Assembly*

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Radiation effects

The fuel rods can transfer heat between them via thermal radiation. This effect will be accounted for by an effecetive conductivity that is tempaeratrue dependent.

The 1-D radiaiton heat transfer between two one gray surfaces is given by

$Q_{rad} = \sigma \cdot F_{1,2} \cdot A_1 \cdot (T_1^4 - T_2^4)$ $\sigma := 5.67 \cdot 10^{-8} \cdot \frac{watt}{m^2 \cdot K^4}$ *Stefan-Boltzmann constant*

The factor F'1,2 incorporates the geometric view factor and the emissivities of the two surfaces.

$$F'_{1,2} = F_{1,2} \cdot \frac{1}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1}$$

We will assume that for most of the rods, all that each one can 'see' is other rods, so,

$F_{1,2} := 1$

The emssivity of the fuel rod cladding surfaces reommended in the Holtec HI-Star FSAR is

$\varepsilon_1 := 0.8$ $\varepsilon_2 := 0.8$ *CHECK THESE VALUES*

The radiative heat transfer equation can be rewritten as

$$Q_{rad} = \sigma \cdot F_{1,2} \cdot A_1 \cdot (T_1^2 - T_2^2) \cdot (T_1 + T_2) \cdot (T_1 - T_2)$$

If we assume that the temperature difference betweem two nearby fuels rods is much less than the average temperature, then this expression can be rewritten with the approximation

$$Q_{rad} = \sigma \cdot F_{1,2} \cdot A_1 \cdot 4 \cdot T_{avg}^3 \cdot (T_1 - T_2)$$

The heat transfer by conduction between these two surfaces through a medium with an effective thermal conductivity is

$$Q_{1,2} = \frac{k_{eff\,rad}}{d} \cdot A_1 \cdot (T_1 - T_2)$$

where d is the nominal distance between the surfaces. Comparing these two expression, one finds that

$$k_{eff\,rad} = \sigma \cdot F_{1,2} \cdot 4 \cdot T_{avg}^3 \cdot d$$

Substituting the numerical values:

$d := \frac{8.92 \cdot in}{14}$ *Nominal distance between two fuel rods*

$F'_{1,2} := \frac{1}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_2} - 1}$ $F'_{1,2} = 0.667$

$T_{avg} := (450 + 459.6) \cdot R$ *The assumed average temperature of the system*

$k_{eff\,FA,rad} := \sigma \cdot F'_{1,2} \cdot 4 \cdot T_{avg}^3 \cdot d$ $k_{eff\,FA,rad} = 0.182 \frac{BTU}{hr \cdot ft \cdot R}$

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Effective Thermal Conductivity Models for Composites

Arithemetic Mean

$$k_{eff\,c.He.am} := \sum_{i=1}^{N_{material}} \left(k_{m_i} \cdot v_{m_i}\right) \qquad k_{eff\,c.He.am} = 1.191 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff\,He.am} := k_{eff.c.He.am} + k_{eff.FA.rad} \qquad k_{eff\,He.am} = 1.373 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

$$\frac{k_{eff\,He.am} - k_{eff.He.known}}{k_{eff.He.known}} = 3.835$$

Variance from the accepted value as a fraction of the accepted value

$$k_{eff\,c.air\,am} := k_{eff\,c.He.am} - k_{m_{n_{gas}}} \cdot v_{m_{n_{gas}}} + k_{air} \cdot v_{m_{n_{gas}}} \qquad k_{eff\,c.air\,am} = 1.118 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff\,air.am} := k_{eff\,c.air.am} + k_{eff\,FA.rad} \qquad k_{eff\,air.am} = 1.3 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

Harmonic Mean

$$k_{eff\,c.He.hm} := \left[\sum_{i=1}^{N_{material}} \left(\frac{v_{m_i}}{k_{m_i}}\right)\right]^{-1} \qquad k_{eff\,c.He.hm} = 0.185 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff\,He.hm} := k_{eff\,c.He.hm} + k_{eff\,FA.rad} \qquad k_{eff\,He.hm} = 0.367 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

$$\frac{k_{eff\,He.hm} - k_{eff\,He.known}}{k_{eff\,He.known}} = 0.294$$

Variance from the accepted value as a fraction of the accepted value

$$k_{eff\,c.air\,hm} := \left[\frac{1}{k_{eff.c.He.hm}} - \frac{v_{m_{n_{gas}}}}{k_{m_{n_{gas}}}} + \frac{v_{m_{n_{gas}}}}{k_{air}}\right]^{-1} \qquad k_{eff\,c.air\,hm} = 0.033 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff\,air.hm} := k_{eff\,c.air\,hm} + k_{eff.FA.rad} \qquad k_{eff\,air.hm} = 0.215 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

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Geometric Mean

$$k_{eff.c.He.gm} := \prod_{i=1}^{N_{material}} \left(k_{m_i}\right)^{t_{m_i}}$$

$k_{eff.c.He.gm} = 0.365 \frac{BTU}{hr \cdot ft \cdot R}$ *Effective thermal conductivity with helium conduction only*

$$k_{eff.He.gm} := k_{eff.c.He.gm} - k_{eff.FA.rad}$$

$k_{eff.He.gm} = 0.547 \frac{BTU}{hr \cdot ft \cdot R}$ *Effective thermal conducibvity with combined conduction and radiation*

$$\frac{k_{eff.He.gm} - k_{eff.He.known}}{k_{eff.He.known}} = 0.926$$

Variance from the accepted value as a fraction of the accepted value

$$k_{eff.c.air.gm} := k_{eff.c.He.gm} \frac{\left(k_{air}\right)^{o_{m_{n_{gas}}}}}{\left(k_{m_{n_{gas}}}\right)^{t_{m_{n_{gas}}}}}$$

$k_{eff.c.air.gm} = 0.11 \frac{BTU}{hr \cdot ft \cdot R}$ *Effective thermal conductivity with helium conduction only*

$$k_{eff.air.gm} := k_{eff.c.air.gm} + k_{eff.FA.rad}$$

$k_{eff.air.gm} = 0.293 \frac{BTU}{hr \cdot ft \cdot R}$ *Effective thermal conducibvity with combined conduction and radiation*

Effective Thermal Conductivity of Fuel Assembly with Air

$$k_{eff.He.close} := k_{eff.He.hm}$$

$$k_{eff.air.close} := k_{eff.air.hm}$$

Pick the model that yields the estimate of the effective thermal conductivity that is closest to the accepted value for the effective thermal conductivity of the helium-filled canister.

$$k_{eff.air.final} := k_{eff.air.close} \frac{k_{eff.He.known}}{k_{eff.He.close}}$$

$k_{eff.air.final} = 0.166 \frac{BTU}{hr \cdot ft \cdot R}$ *This is the adjusted value for the estimate of the effective thermal conductivity of the fuel assembly unit cell*

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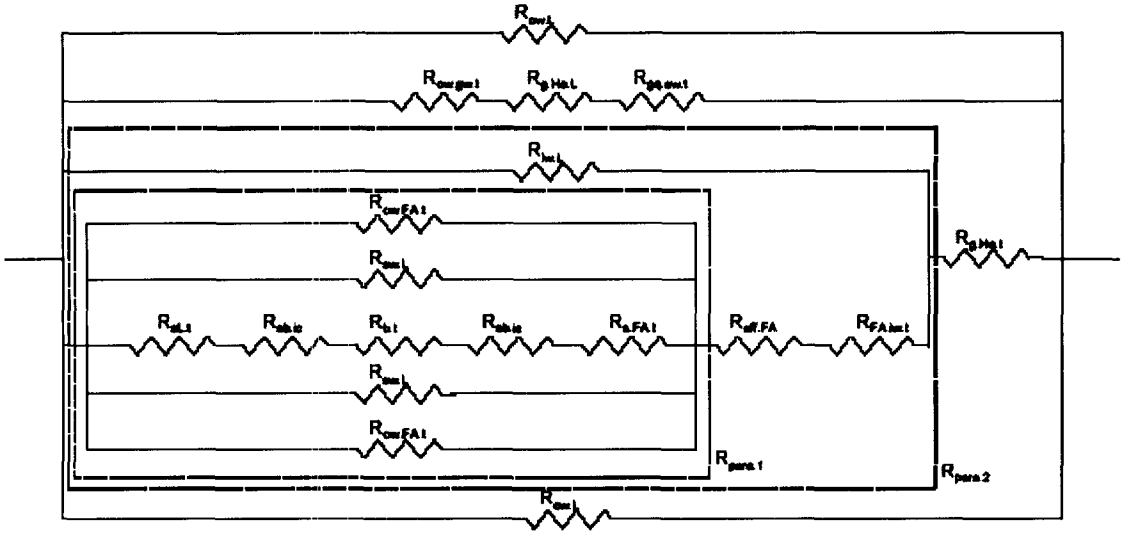
Thermal Model of Fuel Assembly Box Using Parallel-Series Resistor Network

The construction of the fuel assembly box leads to the following idealized thermal resistance network.



The definition of each of the thermal resistance in the network are

Path 1

$$R_{ow.L} := \left(\frac{k_{alloyX}}{L_{box.outer.wall}} \cdot t_{box.wall}\right)^{-1} \qquad R_{p1} := R_{ow.L}$$

Path 2

$$k_{g.L.rad} := \sigma \cdot F_{1,2} \cdot T_{avg}^{3} \cdot \frac{(L_{box.outer.wall} - 2 \cdot t_{box.wall})}{2}$$

$$R_{ow.gw.t} := \left(\frac{k_{alloyX}}{t_{box.wall}} \cdot t_{gas.gap}\right)^{-1} \qquad R_{g.He.L} := \left(\frac{k_{m_{n_{gas}}} + k_{g.L.rad}}{L_{box.outer.wall} - 2 \cdot t_{box.wall}} \cdot t_{gas.gap}\right)^{-1}$$

$$R_{g.air.L} := \left(\frac{k_{air} + k_{g.L.rad}}{L_{box.outer.wall} - 2 \cdot t_{box.wall}} \cdot t_{gas.gap}\right)^{-1} \qquad R_{gw.ow.t} := \left(\frac{k_{alloyX}}{t_{box.wall}} \cdot t_{gas.gap}\right)^{-1}$$

$$R_{p2.He} := R_{ow.gw.t} + R_{g.He.L} + R_{gw.ow.t}$$

$$R_{p2.air} := R_{ow.gw.t} + R_{g.air.L} + R_{gw.ow.t}$$

Path 3

$$R_{iw.L} := \left(\frac{k_{alloyX}}{L_{box.inner.wall} + t_{box.wall}} \cdot t_{box.wall}\right)^{-1} \qquad R_{p3} := R_{iw.L}$$

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Path 4

$$R_{ow.FA.t} := \left(\frac{k_{alloyX}}{t_{box.wall}} \cdot L_{ow.FA.t}\right)^{-1}$$

$$R_{p4} := R_{ow.FA.t}$$

Path 5

$$R_{sW.L} := \left(\frac{k_{alloyX}}{W_{box.sheath}} \cdot t_{box.sheath}\right)^{-1}$$

$$R_{p5} := R_{sW.L}$$

Path 6

$$R_{sL.t} := \left[\frac{k_{alloyX}}{t_{box.sheath}} \cdot \left(L_{box.sheath} - 2 \cdot t_{box.sheath}\right)\right]^{-1}$$

$$R_{b.t} := \left[\frac{k_{boral}}{t_{box.boral}} \cdot \left(L_{box.sheath} - 2 \cdot t_{box.sheath}\right)\right]^{-1}$$

$$R_{sb.ic.He} := \left[\frac{k_{m_{n_{gas}}}}{t_{s.boral.gap}} \cdot \left(L_{box.sheath} - 2 \cdot t_{box.sheath}\right)\right]^{-1}$$

$$R_{sb.ic.air} := \left[\frac{k_{air}}{t_{s.boral.gap}} \cdot \left(L_{box.sheath} - 2 \cdot t_{box.sheath}\right)\right]^{-1}$$

$$R_{s.FA.t} := \left[\frac{k_{alloyX}}{t_{box.wall}} \cdot \left(L_{box.sheath} - 2 \cdot t_{box.sheath}\right)\right]^{-1}$$

$$R_{sheath.t.He} := R_{sL.t} + R_{sb.ic.He} + R_{b.t} - R_{sb.ic.He}$$

$$R_{p6.He} := R_{sheath.t.He} + R_{s.FA.t}$$

$$R_{sheath.t.air} := R_{sL.t} + R_{sb.ic.air} - R_{b.t} + R_{sb.ic.air}$$

$$R_{p6.air} := R_{sheath.t.air} + R_{s.FA.t}$$

Path 7 is the same as Path 5

$$R_{p7} := R_{p5}$$

Path 8 is the same as Path 4

$$R_{p8} := R_{p4}$$

Path 9

$$R_{eff.air.FA} := \left(\frac{k_{eff.air.final}}{L_{box.FA}} \cdot L_{box.FA}\right)^{-1} \quad OR \quad R_{eff.He.FA} := \left(\frac{k_{eff.He.known}}{L_{box.FA}} \cdot L_{box.FA}\right)^{-1}$$

$$R_{FA.iw.t} := \left(\frac{k_{alloyX}}{t_{box.wall}} \cdot L_{box.FA}\right)^{-1}$$

$$R_{p9.He} := R_{eff.He.FA} - R_{FA.iw.t}$$

$$R_{p9.air} := R_{eff.air.FA} + R_{FA.iw.t}$$

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Path 10

$$k_{eff.gap.t.rad} := \sigma \cdot F_{1,2} \cdot 4 \cdot T_{avg}^{3} \cdot t_{gas.gap} \qquad k_{eff.gap.t.rad} = 0.39 \frac{BTU}{hr \cdot ft \cdot R}$$

$$R_{g.He.t} := \left[\frac{k_{m_{gas}} + k_{eff.gap.t.rad}}{t_{gas.gap}} \cdot (L_{box.FA} + t_{box.wall}) \right]^{-1}$$

$$R_{g.air.t} := \left[\frac{k_{air} + k_{eff.gap.t.rad}}{t_{gas.gap}} \cdot (L_{box.FA} + t_{box.wall}) \right]^{-1}$$

$$R_{p10.He} := R_{sheath.t.He} + R_{g.He.t} + R_{sheath.t.He}$$

$$R_{p10.air} := R_{sheath.t.air} + R_{g.air.t} + R_{sheath.t.air}$$

Path 11 is the same as Path 1

$$R_{p11} := R_{p1}$$

Following the rule of combining parallel and series resistors, the effective thermal resistance of a repeating box structure can be estimated as

$$R_{para1.He} := \left(R_{p4}^{-1} + R_{p5}^{-1} + R_{p6.He}^{-1} + R_{p7}^{-1} + R_{p8}^{-1} \right)^{-1}$$

$$R_{para1.air} := \left(R_{p4}^{-1} + R_{p5}^{-1} + R_{p6.air}^{-1} + R_{p7}^{-1} + R_{p8}^{-1} \right)^{-1}$$

$$R_{para2.He} := \left[R_{p3}^{-1} + \left(R_{para1.He} + R_{p9.He} \right)^{-1} \right]^{-1}$$

$$R_{para2.air} := \left[R_{p3}^{-1} + \left(R_{para1.air} + R_{p9.air} \right)^{-1} \right]^{-1}$$

$$R_{eff.box.He} := \left[R_{p1}^{-1} + R_{p2.He}^{-1} + \left(R_{para2.He} + R_{p10.He} \right)^{-1} + R_{p11}^{-1} \right]^{-1}$$

$$R_{eff.box.air} := \left[R_{p1}^{-1} + R_{p2.air}^{-1} + \left(R_{para2.air} + R_{p10.air} \right)^{-1} + R_{p11}^{-1} \right]^{-1}$$

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$R_{eff.box.He} = 0.789 \frac{R \cdot ft \cdot hr}{BTU}$ $R_{eff.box.He}^{-1} = 1.268 \frac{BTU}{hr \cdot ft \cdot R}$

Compare the effective thermal resistance/conductance of a fuel assembly box filled with air to that of box filled with helium.

$k_{eff.box.He} := R_{eff.box.He}^{-1}$ $k_{eff.box.He} = 1.268 \frac{BTU}{hr \cdot ft \cdot R}$

The 'known' value for the effective thermal conductivity of the entire fuel basket is tqaken from the Holtec HI-STAR 100 FSAR.

$k_{eff.box.He.known} := 1.495 \frac{BTU}{hr \cdot ft \cdot R}$

$\frac{k_{eff.box.He} - k_{eff.box.He.known}}{k_{eff.box.He.known}} = -0.152$

There is a 15% variance between the computed value of the effective thermal conductivity with He and the accepted value

$R_{eff.box.air} = 0.872 \frac{R \cdot ft \cdot hr}{BTU}$ $R_{eff.box.air}^{-1} = 1.147 \frac{BTU}{hr \cdot ft \cdot R}$

$k_{eff.box.air} := R_{eff.box.air}^{-1} \cdot \frac{L_{box.outer.wall}}{L_{box.outer.wall}}$

Effective thermal resistance, R, and conductance, R^{-1}, of the box structure. The thermal conductance is the conductance per unit depth and is used to compute the effective comparable to the thermal conductivity of a material

$k_{eff.box.air.final} := k_{eff.box.air} \frac{k_{eff.box.He.known}}{k_{eff.box.He}}$

Use the varaince for the He-related value to adjust the air-related value

$k_{eff.box.air.final} = 1.352 \frac{BTU}{hr \cdot ft \cdot R}$

*This shows that, by replacing the pressurized He with air at 1 atm in the fuel basket, the overall effective thermal conductivity will be raduced from 1.495 BTU/(hr*ft*R) to about 1.3 BTU/(hr*ft*R).*

This estimate is subject to many assumptions, idealizations, and approximations. There is likely a significant uncertainty in this estimate due to the nature of the technique used here.

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Thermal Model of Fuel Assembly Box Using Composite Material Model

$N_{material.mpc} := 4$

$impc := 1..N_{material.mpc}$ *Define indexes for constituent property vector(s)*

$k_{m.mpc}$ (vector) *Thermal conductivities of constituent materials*

$\phi_{m.mpc}$ (vector) *Volume fractions of constituent materials*

$n_{gas.mpc} := 2$ *Index of the gas in the material property vector*

Property Values for Materials inside the Fuel Assembly Box

$A_{tot.mpc} := L_{box.outer.wall}^2 + 2 \cdot L_{box.sheath} \cdot W_{box.sheath}$

$$A_{alloyX} := 4 \cdot (L_{box.outer.wall} - t_{box.wall}) \cdot t_{box.wall} \cdots - (L_{box.inner.wall} - t_{box.wall}) \cdot t_{box.wall} - L_{box.inner.wall} \cdot t_{box.wall} \cdots - 6 \cdot \left[L_{box.sheath} \cdot t_{box.sheath} - 2 \cdot (W_{box.sheath} - t_{box.sheath}) \cdot t_{box.sheath} \right]$$

$A_{boral} := 6 \cdot (L_{box.sheath} - 2 \cdot t_{box.sheath}) \cdot t_{box.boral}$

$A_{FA} := L_{box.FA}^2$ $\qquad L_{box.FA} + t_{box.wall} + t_{gas.gap} = 10.594\,in$

$$A_{He} := 0.685 \cdot A_{FA} \cdots - \left[L_{box.inner.wall} \cdot t_{gas.gap} + (L_{box.outer.wall} - 2 \cdot t_{box.wall}) \cdot t_{gas.gap} \right] \cdots - 4 \cdot (L_{box.sheath} \cdot W_{box.sheath})$$

$A_{fuel} := 0.315 \cdot A_{FA}$ $\qquad L_{box.sheath} - 2 \cdot t_{box.sheath} = 6.254\,in$

$L_{box.inner.wall} + t_{gas.gap} - 2 \cdot t_{box.wall} = 11.2185\,in$

Thermal conductivity *Volume fraction* *NOTE: Use R or K for the temperature in the thermal conductivity units. This is required by Mathcad*

$k_{m.mpc_1} := 3.50 \cdot \frac{BTU}{hr \cdot ft \cdot R}$ $\qquad \phi_{m.mpc_1} := \frac{A_{fuel}}{A_{tot.mpc}} + .001$ *Fuel @ 450°F*

$k_{m.mpc_2} := 0.1289 \cdot \frac{BTU}{hr \cdot ft \cdot R}$ $\qquad \phi_{m.mpc_2} := \frac{A_{He}}{A_{tot.mpc}}$ *Helium at 450°F*

$k_{m.mpc_3} := k_{boral}$ $\qquad \phi_{m.mpc_3} := \frac{A_{boral}}{A_{tot.mpc}}$ $\qquad k_{boral} = 47.84 \frac{BTU}{ft \cdot hr \cdot R}$

$k_{m.mpc_4} := k_{alloyX}$ $\qquad \phi_{m.mpc_4} := \frac{A_{alloyX}}{A_{tot.mpc}}$ $\qquad k_{alloyX} = 9.8 \frac{BTU}{ft \cdot hr \cdot R}$

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$$\sum_{i=1}^{N_{material.mpc}} \phi_{m.mpc_i} = 1$$ *NOTE: The sum of the volume fractions **MUST** be one*

Arithemetic Mean

$$k_{eff.c.mpc.He.am} := \sum_{i=1}^{N_{material.mpc}} \left(k_{m.mpc_i} \cdot \phi_{m.mpc_i}\right) \qquad k_{eff.c.mpc.He.am} = 3.392 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff.mpc.He.am} := k_{eff.c.mpc.He.am} + k_{eff.FA.rad} \qquad k_{eff.mpc.He.am} = 3.574 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

$$\frac{k_{eff.mpc.He.am} - k_{eff.box.He.known}}{k_{eff.box.He.known}} = 1.391$$ *Variance from the accepted value as a fraction of the accepted value*

$$k_{eff.c.mpc.air.am} := k_{eff.c.mpc.He.am} - k_{m_{t_{gas}}} \cdot \phi_{m_{n_{gas}}} + k_{air} \cdot \phi_{m_{n_{gas}}} \qquad k_{eff.c.mpc.air.am} = 3.319 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff.mpc.air.am} := k_{eff.c.mpc.air.am} + k_{eff.FA.rad} \qquad k_{eff.mpc.air.am} = 3.501 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

Harmonic Mean

$$k_{eff.c.mpc.He.hm} := \left[\sum_{i=1}^{N_{material.mpc}} \left(\frac{\phi_{m.mpc_i}}{k_{m.mpc_i}}\right)\right]^{-1} \qquad k_{eff.c.mpc.He.hm} = 0.205 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff.mpc.He.hm} := k_{eff.c.mpc.He.hm} + k_{eff.FA.rad} + k_{eff.gap.c.rad} \qquad k_{eff.mpc.He.hm} = 0.777 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducitivity with combined conduction and radiation

$$\frac{k_{eff.He.hm} - k_{eff.box.He.known}}{k_{eff.box.He.known}} = -0.754$$ *Variance from the accepted value as a fraction of the accepted value*

$$k_{eff.c.mpc.air.hm} := \left(\frac{1}{k_{eff.c.mpc.He.hm}} - \frac{\phi_{m_{t_{gas}}}}{k_{m_{n_{gas}}}} + \frac{\phi_{m_{n_{gas}}}}{k_{air}}\right)^{-1} \qquad k_{eff.c.mpc.air.hm} = 0.033 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff.mpc.air.hm} := k_{eff.c.air.hm} + k_{eff.FA.rad} + k_{eff.gap.c.rad} \qquad k_{eff.mpc.air.hm} = 0.605 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducibvity with combined conduction and radiation

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2/28/2006 8:03 AM

Composite Effective Thermal Conductivity

Replace He w/Air
Open Storage Cask

$$\phi_{m.mpc_1} := 1 - \sum_{i=2}^{N_{material.mpc}} \left(\phi_{m.mpc_i}\right)$$

Adjust the volume fraction of material 1 to yield exactly 1 for the sum. This is necessary to make the Product in the 'gm' come out with the proper units.

Geometric Mean

$$k_{eff.c.mpc.He.gm} := \prod_{i=1}^{N_{material.mpc}} \left(k_{m.mpc_i}\right)^{\phi_{m.mpc_i}} \qquad k_{eff.c.mpc.He.gm} = 0.563 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff.mpc.He.gm} := k_{eff.c.mpc.He.gm} + k_{eff.FA.rad} + k_{eff.gap.r.rad} \qquad k_{eff.mpc.He.gm} = 1.136 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducitivity with combined conduction and radiation

$$\frac{k_{eff.mpc.He.gm} - k_{eff.box.He.known}}{k_{eff.box.He.known}} = -0.24$$

Variance from the accepted value as a fraction of the accepted value

$$k_{eff.c.mpc.air.gm} := k_{eff.c.mpc.He.gm} \cdot \frac{\left(k_{air}\right)^{\phi_{m_{n_{gas}}}}}{\left(k_{m_{n_{gas}}}\right)^{\phi_{m_{n_{gas}}}}} \qquad k_{eff.c.mpc.air.gm} = 0.17 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conductivity with helium conduction only

$$k_{eff.mpc.air.gm} := k_{eff.c.mpc.air.gm} + k_{eff.FA.rad} + k_{eff.gap.r.rad} \qquad k_{eff.mpc.air.gm} = 0.743 \frac{BTU}{hr \cdot ft \cdot R}$$

Effective thermal conducitivity with combined conduction and radiation

The Geometric Mean is the closest to the acceptwd value of the overall thermal conductivity

$$k_{eff.mpc.air.final} := k_{eff.mpc.air.gm} \cdot \frac{k_{eff.box.He.known}}{k_{eff.mpc.He.gm}} \qquad k_{eff.mpc.air.final} = 0.978 \frac{BTU}{hr \cdot ft \cdot R}$$

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GEOSCIENCES AND ENGINEERING DIVISION

SCIENTIFIC NOTEBOOK REVIEW CHECKLIST RECORD

Scientific Notebook No. 704E Project Numbers: 20.06602.01.336

Accomplished

- [x] 1. Initial entries per QAP-001
- [x] 2. Dating of entries
- [x] 3. Corrections (crossed out, one line through w/initials/date)
- [x] 4. No White out used
- [x] 5. Page number visible on copy or original notebook
- [x] 6. In process entries per QAP-001
- [x] 7. Figure information present
- [x] 8. Text readable
- [x] 9. Copyrighted material is identified
- [x] 10. Permanent ink or type only
- [x] 11. Signing of entries (not required on each page)
- [x] 12. Electronic media in the scientific notebook properly labeled
- [x] 13. NRC Supplementary Scientific Notebook Questions are addressed.
- [x] 14. The independent, two person verification required by AP-019, Section 5.2.1.2(b) is complete

Any discrepancies must be resolved before notebook closeout.

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I have reviewed this scientific notebook and find it in agreement with QAP-001.

Manager's Signature 7-26-07 Date

Attach this completed form to the last page of the notebook.

Form QAP-01 (03/2007)