SOFTWARE VALIDATION TEST PLAN FOR FLOW-3D® VERSION 9.0

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INTRODUCTION

FLOW-3D® (Flow Science, Inc., 2005) is a general purpose computational fluid dynamics simulation software package founded on the algorithms for simulating fluid flow that were developed at Los Alamos National Laboratory in the 1960s and 1970s. The basis of the computer program is a finite volume formulation (in an Eulerian framework) of the equations describing the conservation of mass, momentum, and energy in a fluid. The code is capable of simulating two-fluid problems: (i) incompressible and compressible flow and (ii) laminar and turbulent flows. FLOW-3D has many auxiliary models for simulating phase change, non-Newtonian fluids, non-inertial reference frames, porous media flows, surface tension effects, and thermo-elastic behavior.

The code will be employed to simulate the flow and heat transfer processes in potential high-level waste repository drifts at Yucca Mountain and in support of other experimental and analytical work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA).

FLOW-3D uses an ordered grid scheme that is oriented along a Cartesian or a polar-cylindrical coordinate system. Fluid flow and heat transfer boundary conditions are applied at the six orthogonal mesh limit surfaces. The code uses the so-called "Volume of Fluid" formulation pioneered by Flow Science, Inc., to incorporate solid surfaces into the mesh structure and the computing equations. Three-dimensional solid objects are modeled as collections of blocked volumes and surfaces. In this way, the advantages of solving the difference equations on an orthogonal, structured grid are retained.

The code implements a Boussinesq approach to modeling buoyant fluids in an otherwise incompressible flow regime. The Boussinesq approximation neglects the effect of fluid (air) density dependence on the pressure of the air phase, but includes the density dependence on temperature. This approach will be heavily used in the simulation of in-drift air flow and heat transfer processes at Yucca Mountain. Fluid turbulence is included in the simulation equations via a choice of turbulence models incorporated into the software. It is up to the user to choose whether fluid turbulence is significant and, if so, which turbulence model is appropriate for a particular simulation.

1 SCOPE OF THE VALIDATION

FLOW-3D is capable of simulating a wide range of mass transfer, fluid flow, and heat transfer processes. This validation exercise considers the following four sets of test cases:

1. Natural and forced convection
2. Moisture transport with phase change
3. Radiation heat transfer between surfaces
4. Combined convection, radiation, and moisture transport with phase change

The validation test cases are summarized in the following subsections.

1.1 Natural and Forced Convection

The capabilities of the standard version of FLOW-3D Version 9.0 in the area of natural and forced convection are considered in this set of tests. Forced convection is another term for active ventilation. Without active (or forced) ventilation, natural ventilation may occur.

Five test cases are described in Section 6. The first three test cases progress from a theoretical consideration of a hypothetical laminar natural convection flow scenario to experimental treatments of heat transfer in laminar and turbulent flows. The fourth and fifth test cases address forced convection (or ventilation) in thermally perturbed enclosures. These test cases cover a range of processes and geometries relevant to preclosure and postclosure issues in facilities and drifts at Yucca Mountain and are summarized below.

1. Laminar flow of a fluid via natural convection from a vertical flat smooth surface. For this geometric configuration, the conservation equations for mass, momentum, and thermal energy are well known (e.g., Ostrach, 1953; Schlichting, 1968; Incropera and Dewitt, 1996). The FLOW-3D results of a hypothetical case are compared to the semi-analytical solution of the boundary-layer type conservation equations derived specifically for this case.

2. Natural convection in a closed square cavity. This type of flow field was the subject of an experimental study reported by Ampofo and Karayiannis (2003). Fine resolution measurements of the fluid velocity and temperature and wall heat flux are compared to the FLOW-3D simulation results.

3. Natural convection between two concentric cylinders. The experiment results reported in Kuehn and Goldstein (1978) are used to validate the FLOW-3D results.

4. Natural ventilation for a room with one inlet, one outlet, and a heat source in the room. This test case is modeled after the experiment described by Dubovsky, et al. (2001). In addition to a comparison against the measured data, FLOW-3D results will be compared to the results of another widely used computational fluid dynamics code, FLUENT® Version 4.52 (Fluent Inc., 1994).

5. Forced convection in a room when the fluid (air) is assumed to be compressible. A comparison of velocity and mass flow rates at the inlet and outlet of the system at steady state confirms boundary condition and overall mass balance implementation in the code.

1.2 Moisture Transport Test Cases

Two test cases are described in Section 7. They are simple hypothetical cases that will be solved by mathematical analyses and simulations of experiments.

1. Conduction heat transfer and vapor diffusion. In this case, the combined modes of thermal energy and mass transport by conduction and diffusion from a high-temperature surface to a low temperature surface are studied. If the relative humidity is not limited to a maximum of 100 (i.e., a supersaturated condition is allowed), then the governing differential equations describing these processes can be solved for a one-dimensional case exactly as described by Bird, et al. (1960). Conversely, if the relative humidity is

limited to a maximum of 100 percent, the governing equations are highly nonlinear and must be solved numerically. The moisture transport module is capable of solving both these scenarios. Predictions will be compared to the theoretical model of each scenario.

2. Moisture transport in a closed container. This test case is the simulation of the Condensation Cell Experiment as described by CNWRA Scientific Notebook #643. A closed container contains a heated pool of water at one end and a cooled wall at the other. A convection cell is established inside the container, and water evaporated from the pool is advected with and diffused through the air and is condensed on the cooled plate and parts of the other walls. The FLOW-3D simulation results are compared to the measured temperatures and steady condensation rates.

These cases are relevant to the postclosure issues of moisture transport in a repository drift in that the localized processes of evaporation and condensation are simulated and the thermodynamics of high-humidity air are included in the overall solution algorithm.

1.3 Thermal Radiation Test Cases

Two test cases are described in Section 8. Both are hypothetical cases that can be investigated using analytical solutions of thermal radiative heat transfer processes.

1. Thermal conduction and radiation between two surfaces. Simplifying assumptions leads to an exact solution for the overall heat transfer rate following the methods described by Siegel and Howell (1992). The FLOW-3D results will be compared to the analytical predictions.

2. Thermal radiation configuration factors. Radiation configuration factors are an important aspect of radiation modeling, and it is important that these computations be validated along with the radiation heat transfer analysis that employs the configuration factors. The first scenario to be tested is that of radiation between two partitioned cylinders in which the geometry can be considered two dimensional. The second scenario is a three-dimensional rectangular enclosure. The configuration factors computed by the radiation module will be compared to the results of the analytical solutions for these two cases.

These cases are relevant to the postclosure issues of thermal radiation exchange in a repository because it has been widely demonstrated that radiation heat transfer will play a significant—and sometimes dominant—role in the overall heat transfer processes in the drift. Radiation heat fluxes are dependent on geometry only through the configuration factors; therefore, physical size is not as important in this heat transfer mode as in convection and conduction. As long as the relative sizes of features are similar to the full scale, the geometric properties of the radiation exchange will be sufficiently tested.

1.4 Combined Heat Transfer Modes

A single test case with four different scenarios is described in Section 9. This test case is a hypothetical condition of heat transfer in a square two-dimensional enclosure and can be analyzed with accepted empirical correlations for the convection, radiation, and moisture transport aspects of the problem. The following scenarios were chosen to investigate the effects of moisture transport and radiation on convection.

- Only natural convection
- Natural convection with thermal radiation
- Natural convection with moisture transport with phase change
- Natural convection with radiation and moisture transport with phase change

This final case is relevant to the postclosure issues of thermal radiation exchange in a repository because it embodies all the modes of heat and mass transfer that are expected in the drift. This case tests the functionality of the two software modifications for radiation and moisture transport when they are applied together in the FLOW-3D computer code. The physical scale aspects of natural convection heat transfer are adequately addressed in the convection-only tests in Section 6. The radiation heat flux exchange is relatively insensitive to physical size, and phase change aspect of moisture transport is a local phenomenon. Consequently, this test case is considered adequate for validating the operation of the modified FLOW-3D in a mixed-mode heat transfer process.

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3 ENVIRONMENT

3.1 Software—Standard Installation

The FLOW-3D software package has been in use since the early 1980s. It was originally based on algorithms that were developed by the founders of Flow Science, Inc., when they were employed at Los Alamos National Laboratory. The original code was developed to be a general purpose computational fluid dynamics package that could simulate the effects of irregular solid objects; however, it was especially noted for its ability to simulate free surfaces and reduced gravity. The current version of the code is a much enhanced descendent of that early software package and is widely used in industry and government agencies. A description of the software may be found at the Flow Science, Inc., website (http:/www/flow3d.com).

This software validation uses Version 9.0 of FLOW-3D, which can operate in a WINDOWS or Linux/UNIX environment. The graphical user interface is started by clicking on the executable file. The user either creates a new simulation using the menus available in the graphical user interface, or a previously created setup file can be opened for continued work or modification. The setup file that is created by the user completely describes the simulation and is all that is required to recreate results for a particular scenario. Computational fluid dynamics simulations often take many hours or even days to complete; hence, users should retain files holding simulation results for future analyses and postprocessing.

3.2 Software Modifications

The FLOW-3D software as delivered by the vendor includes options for customizing the program for special flow and heat transfer processes not covered in the basic code capabilities. The base code was modified in accordance with the requirements described by Green (2006). The code modifications are understandable by an advanced user of the FLOW-3D software. A complete description of the modifications, the underlying theory, and the details of the modifications are described in Scientific Notebook #536E.

The basic FLOW-3D code is not capable of simulating the transport processes associated with the high humidity conditions that could be present in waste repository drifts. Green (2006) describes a model that addresses all of the physical processes expected to occur in these cases. The computing algorithm described by Green (2006) was programmed in accordance with the logical framework of the FLOW-3D computer program. The moisture transport module added to FLOW-3D is capable of modeling

- Water evaporation from saturated surfaces into the air when the surface temperature is above the local dewpoint
- Water condensation to surfaces from the air when the surfaces are at a temperature less than the local dewpoint
- Re-evaporation of water from surfaces on which water had been previously condensed
- Local condensation of liquid water as a mist in the bulk of the flow domain when heat transfer cools the air to the local dewpoint

It is noted that one limitation of this moisture transport model is that any water condensed as a mist will not coalesce and rain (i.e., it is assumed that the mist diffuses and advects much like an atmospheric fog).

Likewise, the basic FLOW-3D code cannot account for radiation heat transfer between solid surfaces. This heat transfer process can be a significant portion of the overall heat transfer in a repository where natural convection and conduction are the only other means of energy transport between waste packages and the drift walls. The computing algorithm described by Green (2006) was programmed in accordance with the logical framework of the FLOW-3D computer program. The capabilities and features of this module are as follows:

- All surfaces are assumed to be diffuse and gray
- The moist air in the drift does not affect the surface-to-surface thermal radiation
- Solid obstacles may be subdivided so that radiation heat transfer can vary depending on the location and orientation with respect to the other surfaces
- Radiation configuration factors are computed for the radiation-active surfaces or can be provided by the user in the problem input specifications

3.3 Hardware

The program can be run on computers running the Windows or Linux/UNIX operating systems as described in the FLOW-3D manual.

4 PREREQUISITES

Users should be trained to use FLOW-3D and have experience in fluid mechanics and heat transfer.

5 ASSUMPTIONS AND CONSTRAINTS

None.

6 NATURAL AND FORCED CONVECTION TEST CASES

6.1 Laminar Natural Convection on a Vertical Surface, Test Case 1

Analytical results and experimental data for laminar natural convection on a flat-vertical surface provide a method to validate the accuracy of FLOW-3D for natural convection. The analytical solution documented by Incropera and Dewitt (1996) provides an expression for the local Nusselt number and the average Nusselt number for laminar flow cases (Rayleigh number, $Ra < 10^9$). The Nusselt number is a dimensionless temperature gradient at a surface and provides a measure of the efficiency of convection for heat transfer relative to conduction. The empirical correlation of Churchill and Chu (1975) provides an improvement to the analytical solution for average Nusselt numbers at lower Rayleigh numbers. For this validation test case, the local and average Nusselt numbers will be compared to the FLOW-3D results and these published analytical and empirical correlations.

The calculated range of Rayleigh numbers for natural convection in the Yucca Mountain drifts is 5×10^8 to 1×10^{10}, depending on rock temperatures and air properties (Scientific Notebook #536E). Accordingly, test cases for the validation of the computational fluid dynamics results for natural convection flows were chosen for the laminar flow ($Ra < 10^9$) regime to the low speed turbulent regime ($Ra \sim 10^{10}$).

6.1.1 Test Input

A FLOW-3D input file (prepin.*) will be developed to model the vertical flat plate natural convection. The model will be developed with an isothermal vertical wall with a temperature of 340 K [152 °F]. The fluid will be air with a free stream temperature set to 300 K [80 °F]. The case will be modeled as two-dimensional with an incompressible fluid and the Boussinesq approximation to capture the thermal buoyancy effects. No turbulence model will be used.

Two different grid resolution cases will be analyzed. A refined mesh will be developed to support a grid sensitivity analysis. This mesh should provide more accurate results as well as the accuracy limits of FLOW-3D for this particular test case. A coarse mesh with grid resolution similar to what is expected to be practical for future modeling of the full-scale Yucca Mountain drifts will be also be tested to determine its accuracy level.

6.1.2 Test Procedure

FLOW-3D will be run with the input file, as described in the previous section. The output of the wall heat transfer rates will be used to calculate the local and average Nusselt numbers for comparison to the benchmark correlations.

6.1.3 Expected Test Results

Based on a review of the data presented in Churchill and Chu (1975), the approximate uncertainty of the correlation fit to the available experimental data is ± 25 percent in the range of interest for the Rayleigh number (i.e., Ra ~ 10^9). This is larger, but still consistent with the general statement that uncertainties for Nusselt number measurements in heat transfer experiments should be in the range ± 15 percent (e.g., Incropera and DeWitt, 1996, pp. 487–490). Consequently for this test case, the acceptance criteria for the computational fluid dynamics results should be that the benchmark and average Nusselt numbers on the vertical wall will agree within ± 25 percent. Local Nusselt numbers will be held to a tighter criteria. The local Nusselt number for the region from 10 to 90 percent of the length (i.e., the entry 10 percent and exit 10 percent should be neglected) should agree within 10 percent.

6.2 Turbulent Natural Convection in an Air-Filled Square Cavity, Test Case 2

An experimental study conducted by Ampofo and Karayiannis (2003) provides good benchmark data to evaluate the accuracy of FLOW-3D for natural convection in low-level turbulence. The two-dimensional experimental work was conducted on an air-filled square cavity {0.75 × 0.75 m [2.5 × 2.5 ft]} with vertical hot and cold walls maintained at isothermal temperatures of 50 and 10 °C [122 and 50 °F]. These conditions resulted in a Rayleigh number of 1.58×10^9, which is within the range of Rayleigh numbers for natural convection expected for the Yucca Mountain drifts (5×10^8 to 1×10^{10}, depending on rock temperatures and air properties). For this validation test case, the local and average heat transfer rates described by the Nusselt number, the local velocities, and temperature profiles will be compared between the FLOW-3D and experimental results.

6.2.1 Test Input

A FLOW-3D input file (prepin.*) will be developed to model the square cavity experiment. The experiment will be modeled as two-dimensional with an incompressible fluid and the Boussinesq approximation to capture the thermal buoyancy effects. The large eddy simulation model in FLOW-3D will be used to model the fluid turbulence. The model geometry, fluid properties, and boundary conditions will match (as closely as practical) the experimental apparatus described by Ampofo and Karayiannis (2003).

Two different grid resolution cases will be analyzed. A refined mesh will be developed to support a grid sensitivity analysis. This mesh should provide more accurate results as well as the accuracy limits of FLOW-3D for this particular test case. A coarse mesh with grid resolution similar to what is expected to be practical for future modeling of the full-scale Yucca Mountain drifts also will be tested to determine its accuracy level.

6.2.2 Test Procedure

FLOW-3D will be run with the input file, as described in the previous section. The output of the wall heat transfer rates, temperature and velocity profiles, and the mid-width and mid-height will be compared to the experimental benchmark data.

6.2.3 Expected Test Results

For the refined mesh, the experimental and numerical simulation average Nusselt numbers on the horizontal and vertical walls should agree within ± 20 percent. As discussed in Section 6.1.3, Nusselt number errors in this range are generally considered acceptable, especially when considering the added complexity of test case 2 over test case 1. Also, for the Yucca Mountain drift scale, an error of 25 percent in the Nusselt number would lead to an error of approximately 0.4 K [0.7 °F] in the temperature difference between the drift wall and the waste package, assuming there is no drip shield. The temperature difference is the driving force for convection between the waste package and the drift wall. The Nusselt number criteria, the fluid temperature, and velocity profiles will be compared graphically to the measured values. The trends of the profiles will be compared for overall goodness of fit.

For the coarse mesh, the experimental and simulation average Nusselt numbers on the horizontal and vertical walls should agree within ± 25 percent. The fluid temperature and velocity profiles will be compared graphically to the measured values. The trends of the profiles will be compared for overall goodness of fit.

6.3 Natural Convection in an Annulus Between Horizontal Concentric Cylinders, Test Case 3

Kuehn and Goldstein (1978) conducted experiments on the temperature and heat flux measurements of the thermal behavior of a gas in an annulus between concentric and circular cylinders. This is a widely referenced article for empirical correlations and validations of computational fluid dynamics calculations of natural convection flows. The experimenters used nitrogen at subatmospheric and high pressures to create flow field regimes ranging from pure conduction to laminar flow to turbulent flow. The annulus was constructed of cylinders with diameters of 3.56 and 9.25 cm [1.4 and 3.6 in] and had a length of 20.8 cm [8.2 in]. The inner cylinder was heated to a nearly uniform temperature with electric heaters while the outer cylinder was cooled by water. The experimenters accounted for the effects of end losses and radiation to estimate the heat transfer by convection. The test results are summarized in the form of an equivalent thermal conductivity as if the heat transfer is solely by conduction across the radial gap between the cylinders.

The equivalent thermal conductivity of the annulus gas is defined as

$$k_{eq} = \frac{Q \ln(D_o/D_i)}{2\pi Z \, \Delta T} \tag{1}$$

where

Q	—	heat transfer rate at the inner cylinder
D_o	—	inner diameter of the outer cylinder
D_i	—	outer diameter of the inner cylinder
Z	—	length of the annulus
ΔT	—	temperature difference between cylinders

For pure conduction, k_{eq} = 1, and k_{eq} increases to nearly 20 for the most turbulent flow reported by Kuehn and Goldstein (1978).

The results are correlated by the Rayleigh number for gap width

$$Ra_L = \frac{\rho^2 g \beta}{\mu^2} \Delta T \, L^3 \, Pr \tag{2}$$

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 delineated by the diameters of the cylinders
Pr	—	gas Prandtl number

6.3.1 Test Input

FLOW-3D input files will be developed for the cases described by Kuehn and Goldstein (1978) or $Ra_L = 6.19 \times 10^4$, $Ra_L = 2.51 \times 10^6$, and $Ra_L = 6.60 \times 10^7$. These represent laminar, transitional, and fully turbulent flow. Note that the transition values for Rayleigh numbers are approximate and dependent on the geometric configuration of the flow domain.

6.3.2 Test Procedure

FLOW-3D will be run using an identical grid resolution for all three test flows. In addition, the flow with the greatest Rayleigh number will be simulated with a finer grid resolution to demonstrate that the simulation results are approximately grid-independent. The FLOW-3D results will be used to compute the effective overall equivalent thermal conductivity for comparison to the experiment results of Kuehn and Goldstein (1978). The calculated fluid temperature profiles across the gap will be compared to the available experiment results.

6.3.3 Expected Test Results

The acceptance criterion for the simulated overall equivalent thermal conductivity will be a deviation of no more than 25 percent of the measured value. The fluid temperature profiles across the gap will be compared graphically to the measured values. The trends of the profiles will be compared for overall goodness of fit.

6.4 Natural Convection Inside a Ventilated Heated Enclosure, Test Case 4

Test case 4 compares FLOW-3D results against measured data from a natural ventilation experiment (Dubovsky, et al., 2001) and against results from a different numerical model created in FLUENT Version 4.52, a widely recognized and employed computational fluid dynamics code. Because of widespread usage of FLUENT by industry, the published FLUENT Version 4.5.2 simulation results (Dubovsky, et al., 2001) are considered a good metric for assessing FLOW-3D results, particularly when they are both compared against measured data.

The enclosure for test case 4 has an inlet, an outlet, and one interior wall partially blocking direct flow from the inlet to the outlet. This test, while computationally intensive, will allow examination of the interaction between the air flow and the solid wall object. Measured data from thermocouples installed within the enclosure will be used to validate the computational results for test case 4. The simulation will also allow for confirmation of thermal properties as suggested by the experiments.

This scaled room-like natural convection experiment includes a portion of the ceiling heated by a boiling water tank and two ceiling sections open for natural ventilation through an inlet and an outlet for air flow. Figure 1 contains a schematic of the experiment. 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 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 of 100 °C [212 °F] was experimentally verified and shown to be constant and uniform. The box acting as the experimental room had the length, height, and width dimensions of 60, 30, and 24 cm [24, 12, and 9 in]. Along the top of the box, two 5-cm [2-in] openings running the entire width of the box act as the air inflow and outflow regions. Also, there is an interior wall that runs from the air inflow edge to 5 cm [2 in] above the bottom of the box.

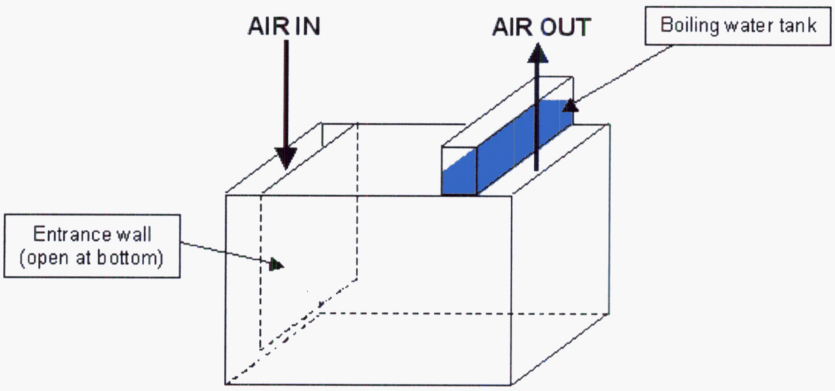

Figure 1. Experimental Apparatus Used in Test Case 4

All walls of the box in the experiment are thermally insulated with a 0.2-cm [0.08-in] layer of insulation. The convective heat transfer coefficient measured outside the box was 10 to 12 W/m^2-°C [1.8 to 2.1 BTU/h-ft^2-°F] (Dubovsky, et al., 2001, p. 3,158). The convective heat transfer coefficient assumed inside the box was 2 to 5 W/m^2-°C [0.35 to 0.88 BTU/h-ft^2-°F]. The heat transfer coefficient based on the thermal resistance of the wall and the convective resistance outside the box was obtained as 0.07 W/m^2-°C to 0.09 W/m^2-°C [0.012 BTU/h-ft^2-°F to 0.016 BTU/h-ft^2-°F] with an uncertainty of 15 percent. The heat transfer coefficient for the heated plate was found to be 5 W/m^2-°C [0.88 BTU/h-ft^2-°F] with a 20-percent uncertainty.

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 than a 0.2-°C [0.4-°F] deviation from a previous measurement was made for all thermocouples in the system. Typical times to reach steady state were on the order of 2 hours.

A more detailed accounting of the test fixture and experimental method can be obtained in Dubovsky, et al. (2001).

6.4.1 Test Input

A comparison of the measured data with results derived from numerical model simulations using the computational fluid dynamics code FLUENT Version 4.52 is provided in Dubovsky, et al. (2001). Specifically, they compare (i) a steady-state case when the whole system is sealed, (ii) a ventilated steady state when the entrance and exit windows are open, and (iii) the early transient between state (i) and state (ii). A two-dimensional grid evaluation study using FLUENT Version 4.52 was described in Dubovsky, et al. (2001) that used 60 × 30 (length × height) and 120 × 60 grid cells to determine whether temperature effects were significant. There was little difference in the comparative runs, so the coarser mesh was extended to three-dimensional calculations. The reported three-dimensional FLUENT 4.52 simulations used a grid defined as 60 × 30 × 8 (length × height × width) cells, where each cell was 1 × 1 × 3 cm [0.4 × 0.4 × 1.3 in]. A grid refinement study was conducted for one case utilizing 60 × 30 × 24 cells. Differences between results for the grids were within experimental error, so the coarser grid was maintained for the rest of the calculations.

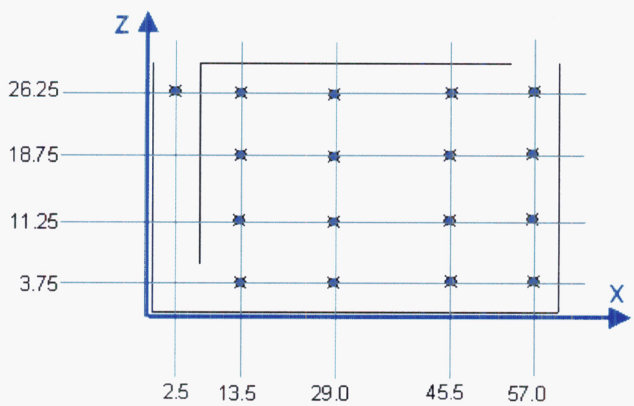

Figure 2. Thermocouple Placement Along Midline (Depth) of System. Left and Lower Inside Walls Shown at the Zero Axes Location. Offset Given Is in cm.

The FLOW-3D model will use the same grid scale as the coarse FLUENT grid, but additional cells will be added for the walls. Thus, the FLOW-3D Version 9.0 model will employ 64 × 34 × 12 grid cells to include the physical nature of the walls and insulation materials of the test fixture. The original FLUENT Version 4.52 model simplified these boundaries as mesh boundaries with generalized wall properties. The boundary that incorporated the inflow/outflow condition was given properties such that the pressure derivative equaled zero, which is the same as the continuative condition that will be employed in the FLOW-3D Version 9.0 model. The thermal properties used in the FLOW-3D model will match those of the FLUENT model.

6.4.2 Test Procedure

First, the simulated system will be 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 will be evaluated using the temperature at history points within the system at locations shown in Figure 2. When no change in local temperature is observed (aside from normal and regular numerical oscillation), the system will be deemed steady. Then, the side vents of the system will be opened and the transient behavior observed and compared to FLUENT results. After reaching steady state, simulated temperature results will be compared to the measured data.

6.4.3 Expected Test Results

Two-dimensional plots of FLOW-3D results at different times during the transient period when the vents are open will be plotted for comparison with FLUENT results. Flow patterns should visually match between the results from FLOW-3D and FLUENT. There should be less than a 1 percent difference in aggregated velocity results for zones within the domain for the steady-state condition.

Simulated temperature profiles will track relative changes in measured profiles and will not differ by more than 5 percent. Some variation in temperature values may occur because slightly shifted flow patterns between the experiment and the numerical model can lead to markedly different temperatures. The locations to be tracked are the same as those illustrated in Figure 2 along the mid-line of the system.

6.5 Forced Convection Inside a Confined Structure, Test Case 5

This test case involves forced convection in a room when the fluid (air) is assumed to be compressible. A comparison of velocity and mass flow rate at the inlet and outlet of the system at steady state will be used to confirm that the boundary condition and overall mass balance implementation in the code are sufficient.

To accomplish this check, a room having length, depth, and height dimensions of 4, 2, and 3 m [13, 6.5, and 10 ft] with a single source of forced ventilation and a single exit for natural exhaust will be simulated (Figure 3). Forced ventilation will be through a 0.4 × 0.4 m [1.3 × 1.3 ft] rectangular vent. Exhaust will be through a similarly sized vent in the ceiling. The model will be maintained at a constant temperature and pressure. Any variation in these parameters is an artifact of the compressibility of the gas employed, which in this case will be air.

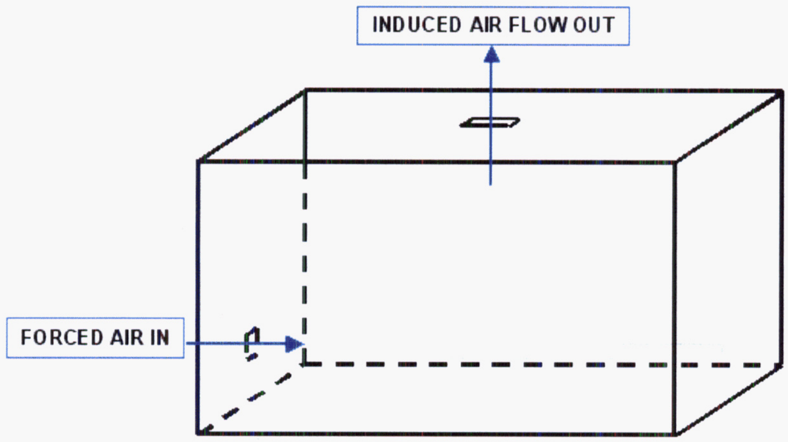

Figure 3. Schematic of Experimental Apparatus Used for Test Case 5

Conservation of mass 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: (i) the flow is normal to the boundary at locations where mass enters or exits the control volume and (ii) all intensive properties (e.g., velocity and density) are uniform with position over each inlet or exit area through which matter flows (e.g., Moran and Shapiro, 2000). In particular, when flow is considered one dimensional, the mass flow rate ($\dot{m}$) at the inlet and outlet is defined by $\dot{m} = \rho A V$, where ρ is density, A is the cross-sectional area, and V is velocity. Steady state, therefore, in these situations is often regarded as mass in equals mass out.

Given the construct of this validation test case and the definition of one-dimensional flow, both constant velocity and density are expected at the inlet and outlet. This validation run evaluates this physical phenomenon and ascertains whether or not FLOW-3D Version 9.0 accurately predicts the outcome.

6.5.1 Test Input

The computational model will be generated based on the physical model described above. Interior dimensions of the room will be 4 × 2 × 3 m [13 × 6.5 × 10 ft]. Computational walls with a thickness of 0.2 m [8 in] will be applied in each direction to simplify visualizations and restrict inflow and outflow properly. Vents will be created as 0.4 × 0.4 m [1.3 × 1.3 ft] openings through their respective boundaries. The full model will utilize a mesh of 44 × 24 × 34 with a uniform grid of individual block size 0.1 × 0.1 × 0.1 m [0.3 × 0.3 × 0.3 ft]. An additional run at double the resolution will also be completed to support the coarse grid results.

A forced air in-flow condition equivalent to the application of a constant velocity of 0.25 m/s [0.8 ft/s] will be applied to the in-flow vent as shown in Figure 3. A continuative condition will be applied on the outflow boundary, which indicates that FLOW-3D will extrapolate local data upstream into appropriate conditions through the boundary. Zero normal derivatives for all quantities are implemented for continuative boundary conditions in FLOW-3D Version 9.0.

The fluid will be air having the following properties at 293.15 K [68 °F]:

Viscosity	=	1.86×10^{-5} kg/m-s [1.25×10^{-5} lbs/ft-s]
Specific heat	=	1883.7 m^2/s^2-K [1.126×10^4 ft^2/s^2-°F]
Thermal conductivity	=	0.0264 kg-m/s^3-K [9.86×10^4 lbs-ft/s^3-°F]
Gas constant	=	287.0 m^2/s^2-K [1720 ft^2/s^2-°F]
Density	=	1.2 kg/m^3 [0.075 lbs/ft^3]

The gas will be assumed compressible so that the physical sensitivities of pressure and velocity can be included in the calculations.

6.5.2 Test Procedure

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

To ascertain an average velocity across both the inflow and outflow boundary, the magnitude of total velocity will be evaluated as an integral over the cross sectional area of each vent. Simulation data will be taken at a distance of one grid plane from boundary; this gives a more accurate representation of velocity through the opening instead of at a discrete boundary.

6.5.3 Expected Test Results

The simulated velocity at the inflow and outflow vents should be within 5 percent of the intended ventilation flow rate. The mass flow rate at the inlet and outlet should not differ by more than 2 percent. This acceptance criterion is adequate for simulations of compressible flow at steady state.

7 MOISTURE TRANSPORT TEST CASES

7.1 Conduction Heat Transfer and Vapor Diffusion

This test case is depicted schematically in Figure 4. Two large flat plates are separated by a gap filled with moist air. The left plate is held at constant temperature, and the right plate is held at a lower temperature. Both surfaces provide a stationary film of water that can exchange mass with the water vapor in the air gap between the plates. It is assumed that there is no convection in the air gap. The following parameters define the necessary geometric and physical properties of the system:

Gap thickness, L	=	0.1 m [0.3 ft]
Fluid thermal conductivity	=	k_g = 0.026 W/(m-K) [0.015 BTU/h-ft-°F]
Left surface temperature	=	T_h = 320 K [116 °F]
Right surface temperature	=	T_c = 280 K [44 °F]
Pressure	=	1 atm [2,116 psf]

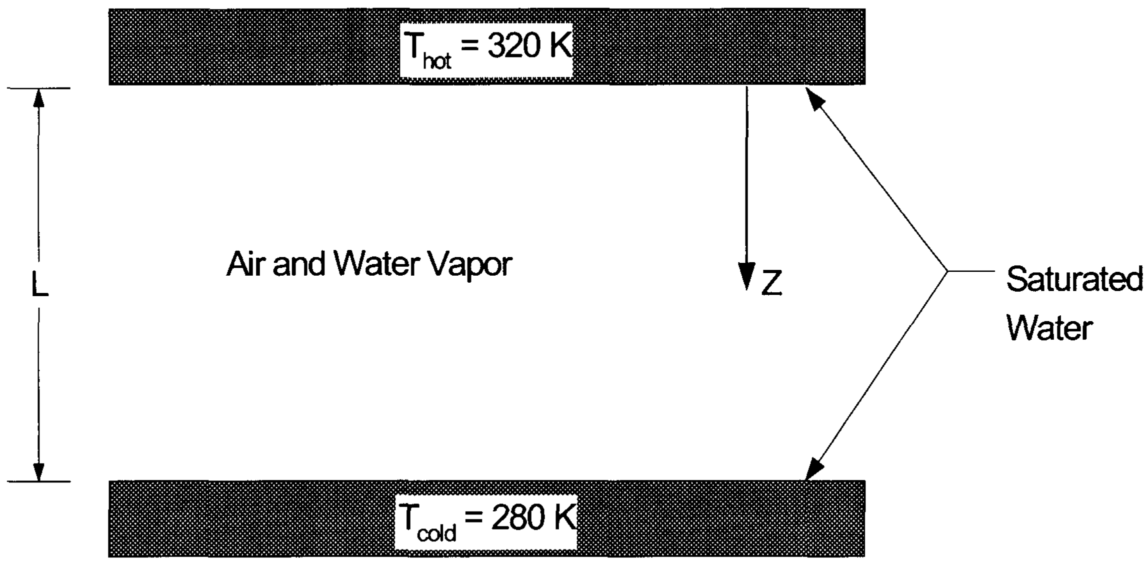

Figure 4. Schematic for Heat Conduction and Species Diffusion Between Surfaces

The equations describing the diffusion of thermal energy and water vapor across the gap are described by Bird, et al. (1960).

7.1.1 Test Input

A FLOW-3D input file (prepin.*) will be developed to model the idealized case of one-dimensional conduction heat transfer and chemical species diffusion through the air gaps. The lateral edges of the computational domain will be specified as adiabatic surfaces. Convection flow will be disallowed in the simulation. This portion of the test input is accomplished with the standard input file procedure of the basic FLOW-3D code.

The standard version of FLOW-3D can simulate the diffusion of chemical species as defined in the idealized case. The unique feature of this problem is that the water (liquid phase) at each surface must be in thermodynamic equilibrium with its vapor. The moisture transport processes will be accomplished by providing the user inputs to the customized portion of the code as described in Scientific Notebook #536E.

7.1.2 Test Procedure

FLOW-3D will be run with the input file as described above until a steady-state condition is achieved. The output of the temperature profiles and water vapor concentration profiles will be compared to the predictions of the analytical solution.

7.1.3 Expected Test Results

The acceptance criterion for this test case is that the local water temperatures and water vapor concentrations predicted by FLOW-3D shall be within 5 percent of the analytical predictions.

7.2 Moisture Transport in a Closed Container

This test case is based on the condensation cell experiment conducted specifically for validating the moisture transport model. The experiments are fully described in Scientific Notebook #643. The experimental setup is depicted schematically in Figure 5. The walls of this container are fabricated primarily of Plexiglas. The aluminum pan is attached to the floor at one end of the box and extends across the width of the box. The entire opposite end of the box is an aluminum plate that is cooled with chilled water flowing through passages machined into plate. The entire container is covered with Styrofoam insulation.

The water pan is maintained at a constant temperature by a heater attached to its bottom. The water is maintained at a constant level by a siphon device between the pan and a water bottle located outside the clear acrylic enclosure. Thermocouples record the temperature at the locations shown in Figure 5. Condensed water is collected in a graduated cylinder. The net condensation rate is estimated by knowing the time period for collecting the observed amount of water.

The laboratory experiment procedure calls for the heater and chiller to be adjusted to provide for constant temperatures measured by thermocouples immersed in the water and attached to the cold plate surfaces. The test is operated for several hours until a steady-state condition is achieved, as shown by the air temperatures and the condensation rate.

Test runs were conducted at several different combinations of heater and chiller temperatures.

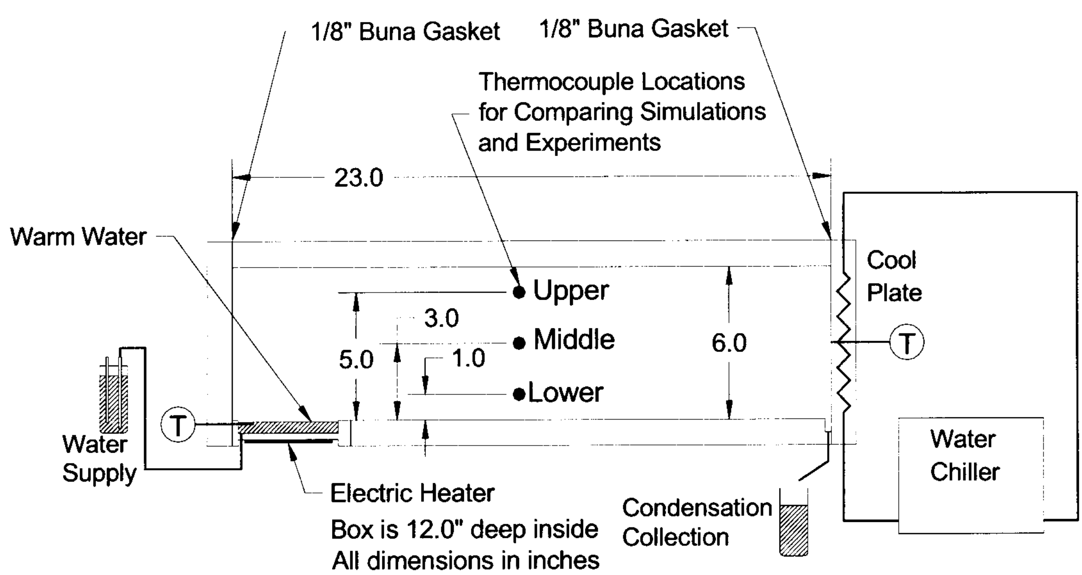

Figure 5. Test Setup for Natural Convection and Water Vapor Transport in a Closed Container

7.2.1 Test Input

A FLOW-3D input file (prepin.*) will be developed to model the idealized case of two-dimensional flow in the vertical symmetry plane of the box. The box is wide enough that very nearly two-dimensional flow will exist in this cross section; therefore, the simulation for this case will be two-dimensional. Boundary conditions and fluid properties will be based on the thermal conditions specific to each experimental test run.

The convection and conduction aspects of the problem are handled by the standard portions of the FLOW-3D code. The simulation of the moisture transport processes will be accomplished by providing the user with inputs to the customized portion of the code as described in Scientific Notebook #536E. Input files describing all of the test runs will be developed.

7.2.2 Test Procedure

FLOW-3D will be run with the input files as described above until a steady-state condition is achieved. The output of the temperatures at the center of the container will be compared to the test measurements. Likewise, the output of the condensation rate at the chilled plate will be compared to the test measurements.

7.2.3 Expected Test Results

The acceptance criterion for temperature predictions is that the air temperatures at the selected locations should be within 20 percent of the measured values. Similarly, the acceptance criterion for condensation rate is that the predicted condensation rate should be within 20 percent of the measured value. These levels of error are consistent with generally accepted errors for turbulent convection heat transfer experiments and correlations [e.g., Incropera and DeWitt (1996)].

8 THERMAL RADIATION TEST CASES

8.1 Thermal Conduction and Radiation Between Two Surfaces

This test case is depicted schematically in Figure 6. Two large flat plates are separated by a gap. The upper plate has internal heat generation so that the heat flux at its lower surface is 255 W/m^2 [80.9 $BTU\text{-}h\text{-}ft^2$]. The bottom of the lower plate is held at a lower temperature. It is assumed that there is no convection in the air gap.

The following parameters define the necessary geometric and physical properties of the system:

Gap thickness, t_g	=	0.1 m [0.3 ft]
Plate thickness, t_1	=	t_2 = 0.02 m [0.06 ft]
Emissivity, ε_1	=	ε_2 = 0.9
Gap thermal conductivity	=	k_g = 0.1 W/(m-K) [0.05 BTU/h-ft-°F]
Plate thermal conductivity, k_1	=	k_2 = 1 W/(m-K) [0.57 BTU/h-ft-°F]
Upper surface heat flux	=	Q_{gen} = 255 W/m^2 [80.8 $BTU/h\text{-}ft^2$]
Lower surface temperature	=	T_c = 300 K [80 °F]

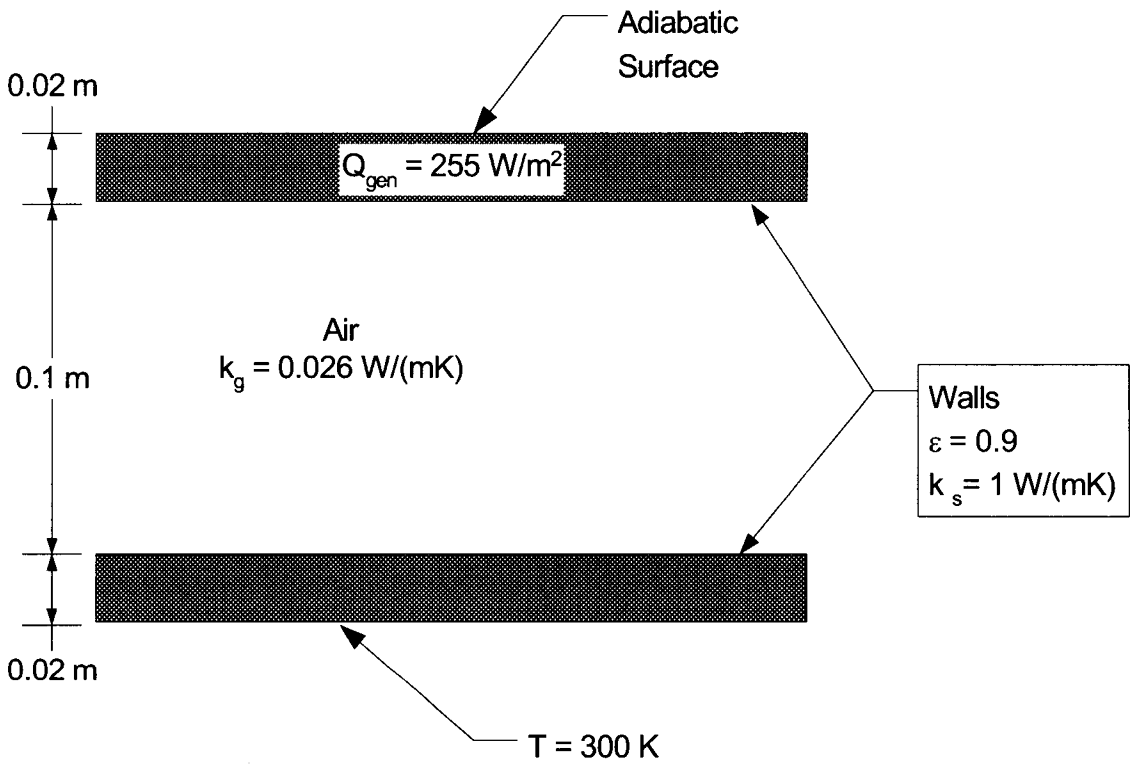

Figure 6. Schematic for Thermal Conduction and Radiation Between Opposing Surfaces

The radiation and conduction heat transfer processes will be modeled by the appropriate exact one-dimensional equations for this case.

8.1.1 Test Input

A FLOW-3D input file (prepin.*) will be developed to model the idealized case of one-dimensional conduction heat transfer through the three objects. The lateral edges of the computational domain will be specified as adiabatic surfaces. Air movement will be disallowed in the simulation. This portion of the test input is accomplished with the standard input file procedure of the basic FLOW-3D code.

The radiation heat transfer simulation will be accomplished by providing the user inputs to the customized portion of the code as described in Scientific Notebook #536E. Because this is an idealized one-dimensional case, the radiation configuration factors will be

$F_{1\text{-}1} = F_{2\text{-}2} = 0$
$F_{1\text{-}2} = F_{2\text{-}1} = 1$

8.1.2 Test Procedure

FLOW-3D will be run with the input file as described above until a steady-state condition is achieved. The output of the temperature profiles will be compared to the predictions of the mathematical analysis. The output temperature profiles will be used to compute the overall heat transfer rate for comparison to the analytical solution.

8.1.3 Expected Test Results

The acceptance criterion for this test case is that the local temperatures predicted by FLOW-3D shall be within 5 percent (relative to the overall temperature difference between the two isothermal surfaces) of the analytical predictions. Similarly, the overall heat transfer rates should be within 5 percent of the analytical prediction.

8.2 Thermal Radiation Configuration Factors

This test case demonstrates the computation of configuration factors, which is a part of the overall radiation module created for FLOW-3D. There will be two scenarios in this test case.

The first scenario is the two-dimensional geometry of concentric cylinders (Figure 7). The outer cylinder has an inner diameter of 0.5 m [1.6 ft], and the inner cylinder has an outer diameter of 0.3 m [0.98 ft]. In this scenario, each of the cylinder surfaces is divided into four subsurfaces of equal size for which the configuration factors are to be computed. The Hottel method [as described by Siegel and Howell (1992)] will be used to compute the configuration factors between each pair of surfaces for this case. In the radiation module, the radiative exchange from one part of a sector to another part of the same sector is neglected; consequently, these self-referenced configuration factors will be neglected. The essential point to this scenario is to test the capability of the radiation module to account for blockages between surfaces so that the configuration factor is less than for the condition in which the surfaces.

The second scenario is the radiation within a three dimensional enclosure (Figure 8). This enclosure is 2 × 1 × 0.5 m [6.6 × 3.3 × 1.6 ft]. (Configuration factors are dimensionless so the units of these dimensions are, in fact, not relevant). The exact configuration factors can be computed from published literature for this geometry (e.g., Howell, 1982).

8.2.1 Test Input

FLOW-3D input files (prepin.*) will be developed to model the idealized cases described above. The radiation heat transfer simulation will be accomplished by providing the user inputs to the customized portion of the code as described in Scientific Notebook #536E. Only the configuration factors are to be validated; therefore, the description of the fluid and other heat transfer related parameters is not necessary.

8.2.2 Test Procedure

FLOW-3D will be executed as required for only two time steps to allow the radiation module initialization to be executed. The computed configuration factors are recorded to a file as part of

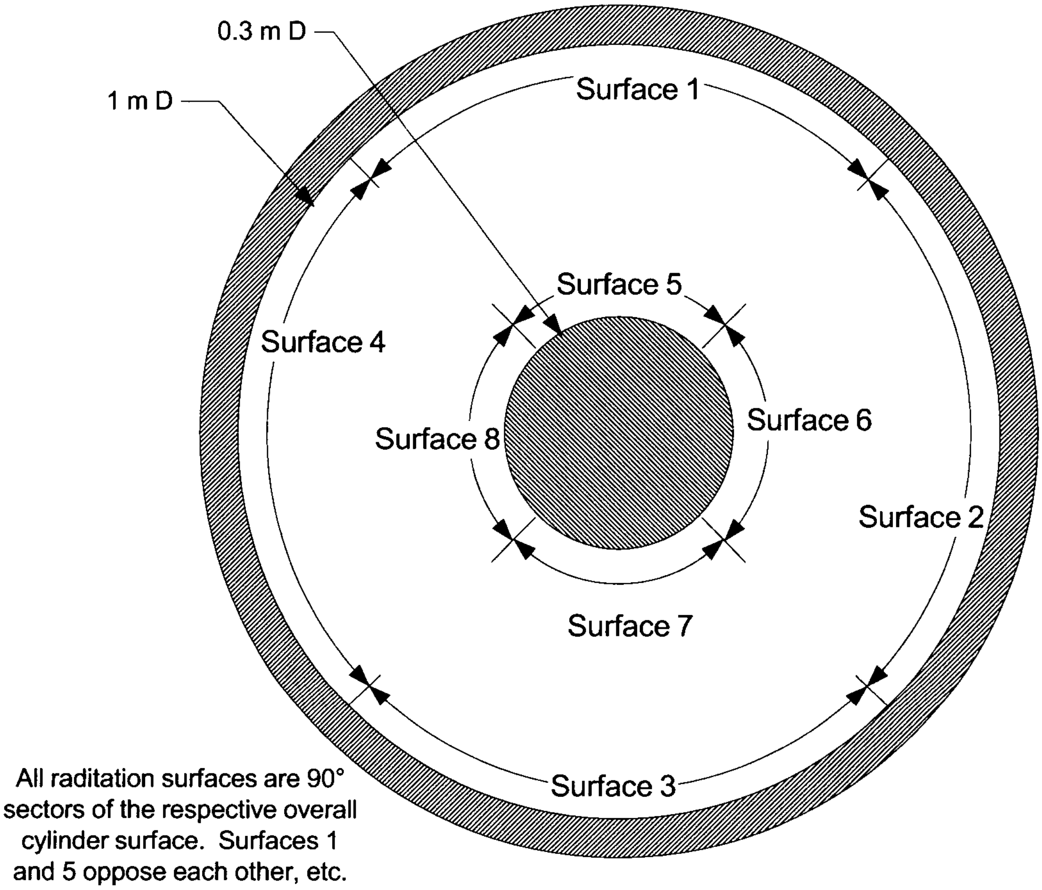

Figure 7. Schematic for Thermal Radiation in an Annular Gap

the initialization sequence. These values will be compared to the exact values computed for the respective scenarios.

8.2.3 Expected Test Results

The acceptance criterion for this test case is that the configuration factors predicted by FLOW-3D shall be within 5 percent of the analytical predictions.

9 COMBINED HEAT TRANSFER TEST CASE

9.1 Convection, Radiation, and Moisture Transport in an Enclosure

The heat transfer by a combination of convection, radiation, and water vapor transport is considered in this test case. A two-dimensional enclosure measuring 0.1 × 0.1 m [0.3 × 0.3 ft] is depicted in Figure 9. The left vertical wall is 0.025 m [0.08 ft] thick and has an internal heat generation rate such that the heat flux at the inner surface is 200 W/m^2 [63.4 BTU/h-ft-°F]. The

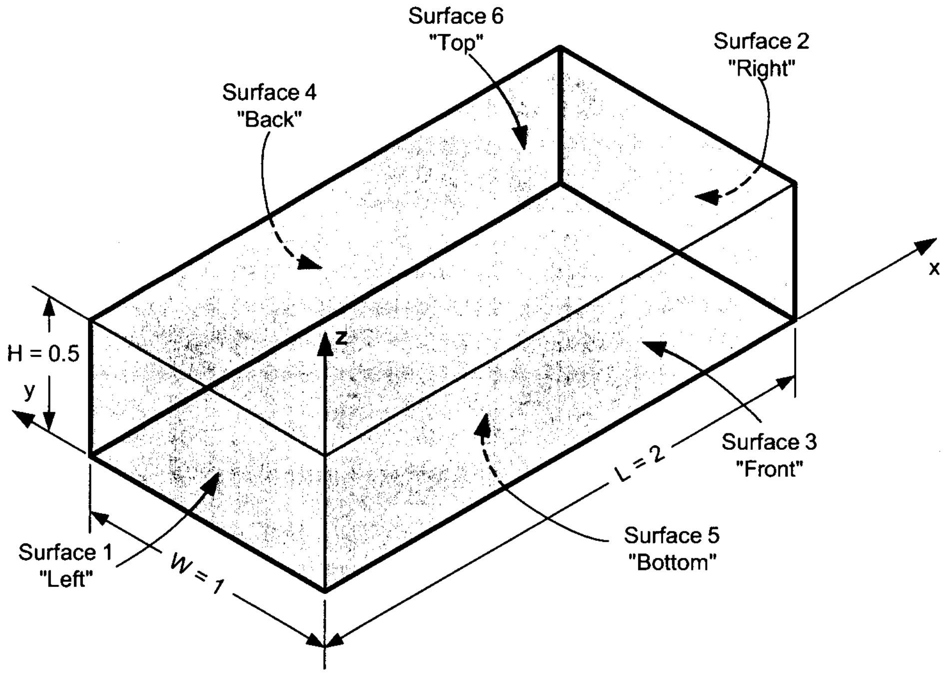

Figure 8. Schematic for Thermal Radiation in a Three-Dimensional Enclosure

outer surface of this wall is adiabatic. The right vertical wall is 0.025 m [0.08 ft] thick, and its outer surface is held constant at 300 K [80 °F]. The emissivity of both the left and right walls is 0.9. The vertical walls are assumed to provide for the evaporation and condensation of water as needed under the existing temperature and concentration conditions in the flow.

The upper and lower walls are adiabatic and do not exchange heat with the vertical walls. These walls are assumed to be transparent to radiation and, therefore, do not interact with the other walls via this mode. Furthermore, these walls are assumed to not be a source or a sink for water. The only interaction of these walls in the problem is to bound the flow and provide for viscous drag.

The acceleration due to gravity is assumed to be only 0.001 g so that the flow field for these geometric and thermal conditions will be laminar. The objective here is to compare the effects of radiation and moisture transport, not to accurately model a turbulent flow scenario.

The FLOW-3D predictions will be compared to the predictions of an engineering analysis of this scenario using a heat transfer empirical correlation approach. This approach is based on the equations described below.

The Nusselt number correlation for natural convection in a two-dimensional square enclosure described by Berkovsky and Poleviko (1977) is a widely used relationship for this case. The net mass transfer rate of water vapor through the enclosure will be estimated using the analogy of heat and mass transfer (Incropera and Dewitt, 1996). This is a common practice that is based

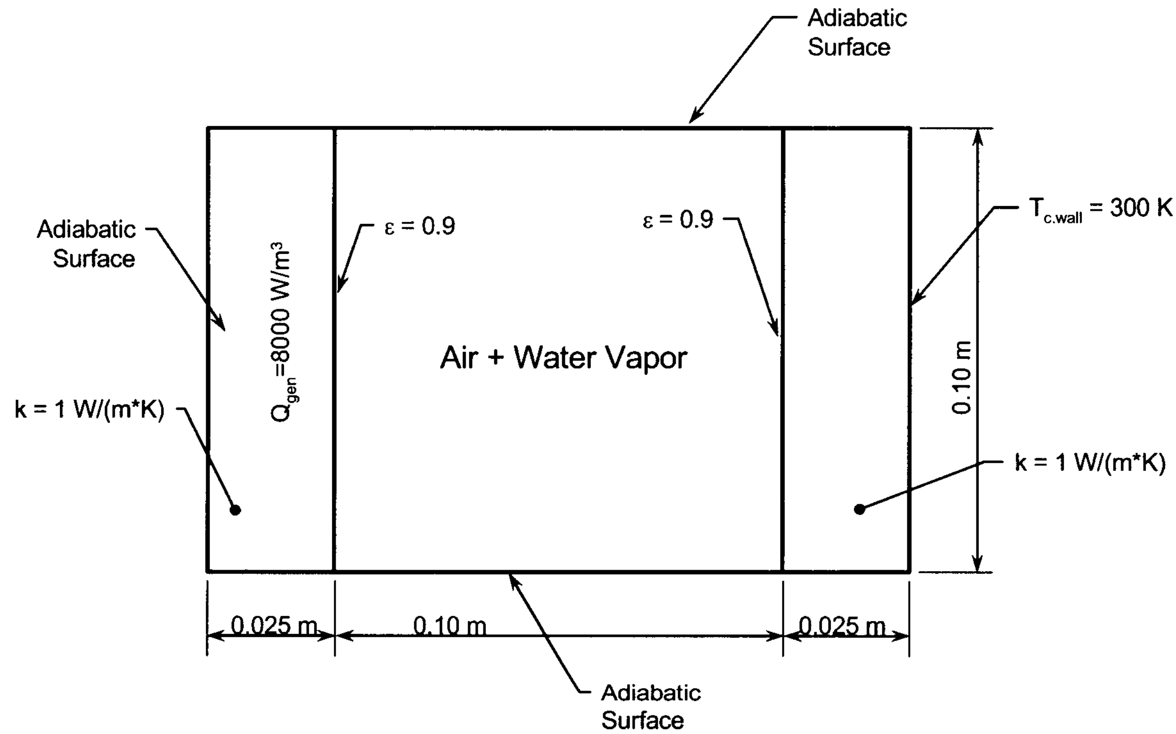

Figure 9. Schematic for Convection, Radiation, and Mass Transfer in a Two-Dimensional Enclosure

on the fundamentals of heat and mass transfer theory and similarity principles. Finally, the radiation heat transfer will be analyzed using the methods of Siegel and Howell (1992) for gray diffuse surfaces in an enclosure.

The following properties are to be used for the fluid and wall:

Viscosity, μ	=	2×10^{-5} Pa-s [0.06 lb/ft-hr]
Fluid thermal conductivity, k	=	0.026 W/(m-K) [0.015 BTU/h-ft-°F]
Air/Vapor diffusivity, D	=	2.6×10^{-5} m²/s [0.00028 ft²/s]
Density, ρ	=	1.169 kg/m³ [0.72 lb/ft³] (nominal value)
Wall thermal conductivity, k_w	=	1 W/(m-K) [0.58 BTU/h-ft-°F]

The density value listed above is used as the nominal density in the conservation of energy equation. In keeping with the moisture transport model, the incompressible ideal gas model is used for this test case for the temperature and concentration dependent density that is used for the momentum equation. The moisture model parameters pertinent to this case are

Water heat of vaporization, u_{fg}	=	2,304,900 J/kg [992 BTU/lb]
Water vapor specific heat, C_{vv}	=	1,370 J/(kg-K) [0.33 BTU/lb-°F]
Water liquid specific, C_{vl}	=	4,186 J/(kg-K) [1.0 BTU/lb-°F]
Water vapor gas constant, R_v	=	416 J/(kg-K) [0.099 BTU/lb-°F]
Air gas constant, R_a	=	289 J/(kg-K) [0.069 BTU/lb-°F]

9.1.1 Test Input

FLOW-3D input files (prepin.*) will be developed to model the idealized cases as follows:

1. Convection only
2. Convection with radiation
3. Convection with moisture transport
4. Convection, radiation, and moisture transport

The convection and conduction aspects of the problem are handled by the standard portions of the FLOW-3D code. The moisture transport and thermal radiation processes will be accomplished by providing the user inputs to the customized portion of the code as described in Scientific Notebook #536E.

9.1.2 Test Procedure

FLOW-3D will be run with the input file as described above until a steady-state condition is achieved. An engineering analysis using the empirical heat and mass transfer correlations will be developed for each of the four scenarios as described above. The output of the heat transfer rates predicted by FLOW-3D will be compared to the predictions of the engineering heat transfer analysis. The average wall surface temperatures predicted by FLOW-3D will be compared to those resulting from the engineering analysis.

9.1.3 Expected Test Results

The acceptance criterion for this test case is that the local temperatures predicted by FLOW-3D shall be within 20 percent (relative to the overall temperature difference between the two isothermal surfaces) of the analytical predictions. Similarly, the overall heat transfer rates should be within 20 percent analytical prediction. This acceptance criterion is acceptable in light of the approximate nature of the available empirical correlations for natural convection heat and mass transfer, especially in combination with radiation.

10 INDUSTRY EXPERIENCE

FLOW-3D is used widely in (i) the casting industry because of its solid-liquid phase change capabilities and (ii) in the aerospace industry for its free surface, surface tension (i.e., zero gravity considerations) and non-inertial reference frame capabilities.

11 NOTES

None.