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

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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, incompressible and compressible flow, and laminar and turbulent flows. The code 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.

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 into 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 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.

1.0 SCOPE OF THE VALIDATION

FLOW-3D® is capable of simulating a wide range of mass transfer, fluid flow, and heat transfer processes. Its capabilities only in the area of natural and forced convection processes are considered in this validation exercise. 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 last two 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.

- The first test case is 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) and 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.
- The second test case is that of 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.
- The third test case is that of natural convection between two concentric cylinders. The experiment results reported in Kuehn and Goldstein (1978) are used here to validate FLOW-3D®.
- The fourth test case involves 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 in Dubovsky, et al. (2001). In addition to a comparison against the measured data, FLOW-3D® results will be compared against the results of another widely used computational fluid dynamics code, Fluent Version 4.52.
- The fifth test case is 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.

2.0 REFERENCES

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3.0 ENVIRONMENT

3.1 Software

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. While the original code was a general purpose computational fluid dynamics package that could simulate the effects of irregular solid objects, 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 post-processing.

3.2 Hardware

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

4.0 PREREQUISITES

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

5.0 ASSUMPTIONS AND CONSTRAINTS

None.

6.0 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 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 in 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 between 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. 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~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 and provide 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 is ± 25 percent in the range of interest for Rayleigh Number (i.e., $Ra \sim 10^9$). 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 the 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 of dimension 0.75 m × 0.75 m [2.5 ft × 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 (LES) 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 and provide 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.

6.2.2 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 and 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 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 inner cylinder
D_o = inner diameter of the outer cylinder
D_i = outer diameter of the inner cylinder
Z = length of 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 = $0.5(D_o\text{-}D_i)$ = 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) for $Ra_L = 6.19 \times 10^4$, $Ra_L = 2.51 \times 10^6$, $Ra_L = 6.60 \times 10^7$. 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 will be a comparison of 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, outlet, and one interior wall partially blocking direct flow from inlet to outlet. This test, while computationally expensive, 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, an interior wall, running from the air inflow edge to 5 cm [2 in] above the bottom of the box exists.

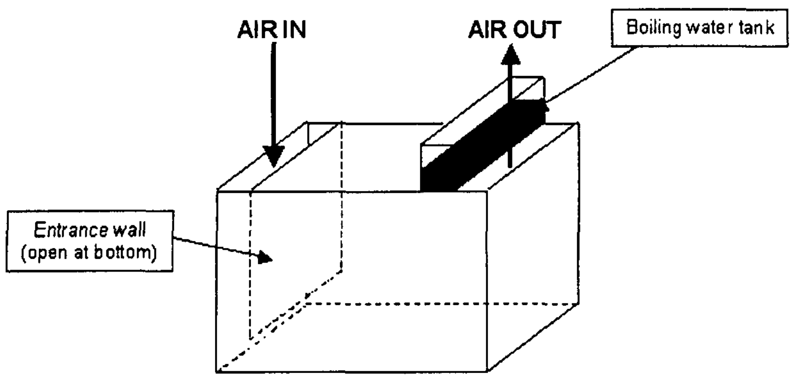

Figure 1. Experimental Apparatus Used in Test Case 4

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 0.08 W/m^2-°C [0.014 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 that 0.2-°C [0.4-°F] 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 Dubovsky, et al. (2001).

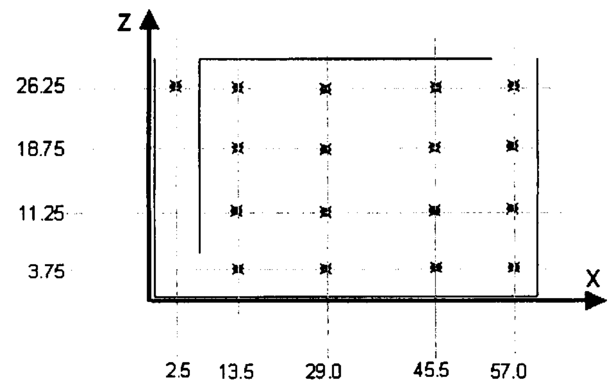

Figure 2. Thermocouple Placement Along Midline (Depth) of System. Left and Lower Inside Walls Shown at the Zero Axes Location. Offset Given Is in cm.

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 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 if 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 cm × 1 cm × 3 cm [0.4 in × 0.4 in × 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.

The FLOW-3D® model will use the same grid scale at 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 4.52 model simplified these boundaries as mesh boundaries with generalized wall properties. The boundary that incorporated the inflow/outflow condition was given the property 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, 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 rectangular vent of size 0.4 m × 0.4 m [1.3 ft × 1.3 ft]. Exhaust will be through a similarly sized vent in the ceiling. The model will be 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 will be air.

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, such as velocity and density, are uniform with position over each inlet or exit area through which matter flows (e.g., Morin and Shapiro, 2000). In particular, when flow is considered one-dimensional, the mass flow rate ($\dot{m}$) at inlet and outlet is defined by $\dot{m} = \rho AV$, 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 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. Therefore, this validation run evaluates this physical phenomenon and ascertains whether or not FLOW-3D® Version 9.0 accurately predicts the outcome.

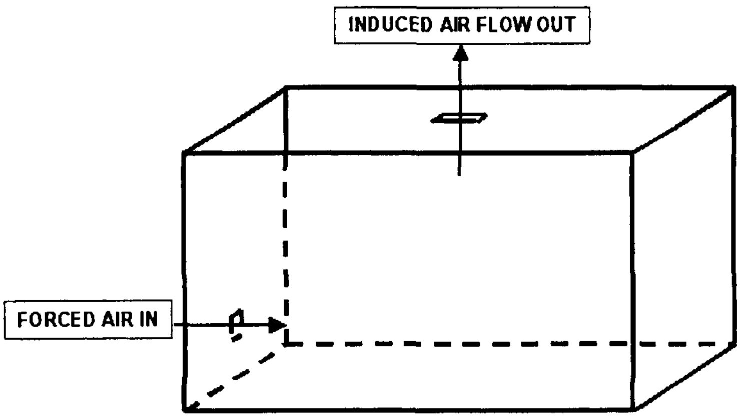

Figure 3. Schematic of Experimental Apparatus Used for Test Case 5

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 m × 2 m × 3 m [13 ft × 6.5 ft × 10 ft]. Computational walls of thickness 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 m × 0.4 m [1.3 ft × 1.3 ft] openings through their respective boundaries. The full model will se a mesh of 44 × 24 × 34 with a uniform grid of individual block size 0.1 m × 0.1 m × 0.1 m [0.3 ft × 0.3 ft × 0.3 ft]. An additional run at double the resolution also will 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 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 = 1,883.7 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 [1,720 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 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 criteria is acceptable for simulations of compressible flow at steady state.

7.0 INDUSTRY EXPERIENCE

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

8.0 NOTES

None.