SOFTWARE VALIDATION PLAN AND REPORT FOR

FLUENT® VERSION 6.2.16

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SOFTWARE VALIDATION REPORT FOR FLUENT VERSION 6.2.16

FLUENT® is a computational fluid dynamics computer code that numerically solves governing equations for momentum, mass, and energy balance for a given system. The software was developed by FLUENT, Inc. The software is ISO-9001 certified. The certificate is attached at the end of the report. The software is routinely used by the automobile industry, aircraft manufacturers, the oil and gas industry, and the microprocessor manufacturing industry. FLUENT uses control volume formulation to solve the governing equations and posseses capabilities to simulate laminar and turbulent flow fields, and buoyancy-driven natural convection of fluids. The software can also model conductive, convective, and radiative heat transfer in a given system.

The software will be used to determine the thermal behavior of the spent nuclear fuel HI-STAR 100 storage/transportation cask system (HI-STAR 100 Final Safety Analysis Report, 2002). The cask system consists of two components: a small multipurpose cylindrical canister and a large cylindrical multiwalled canister called a overpack. The multipurpose canister is placed inside the overpack. Bare fuel assemblies are stored in a fuel basket, which is placed inside the multipurpose canister. The fuel basket has square shape compartments for storing fuel assemblies. The fuel basket is made of Alloy X (Holtec International has proposed to use carbon steel for the fuel basket panel). An MPC-24 fuel basket can host 24 pressurized water reactor fuel assemblies. During the dry storage, the HI-STAR 100 system is filled with pressurized helium that is approximately six times more thermally conductive than air. When the HI-STAR 100 system is closed, the heat generated by the fuel assemblies is passively rejected into the atmosphere. The heat transfer is assisted by a higher helium thermal conductivity. HOLTEC International has reported the thermal analysis of the closed cask in the HI-STAR 100 Final Safety Analysis Report. For a closed HI-STAR 100 system containing 24 pressurized water reactor fuel assemblies, the maximum estimated temperature is reported to be 648 K. The software will be used to verify the thermal analysis of the closed cask as reported by HOLTEC International. In addition, thermal analysis of the HI-STAR 100 system will be performed when the cask is open and bare fuel assemblies are in contact with ambient air.

The thermal analysis of the HI-STAR 100 cask system using computational fluid dynamics requires models for natural convection, conduction, and radiation. The heat generated by the spent fuel creates temperature gradients in the fluid adjacent to fuel assemblies. As a result, the fluid convects due to buoyancy force. Because of temperature gradient between fuel assemblies and internal surfaces of the cask system, the heat is also dissipated from fuel assemblies by radiation heat transfer. The heat transfer from overpack external surface to ambient also take place by natural convection and radiation. Therefore, buoyancy-driven natural convection and radiation heat transfer models are needed to develop a thermal model for the cask system.

1 SCOPE OF THE VALIDATION

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. The scope of the validation study is limited to evaluate FLUENT's ability to model laminar and turbulent natural convection, conduction, and radiation heat transfer. 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. This test case evaluates FLUENT's capability to model natural convection in a closed domain. The experimental results reported by Kuehn and Goldstein (1978, 1976) 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.

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3 ENVIRONMENT

3.1 Software

FLUENT Version 6.2.16 runs in a Microsoft® Windows environment (98, ME, NT, 2000, and XP). The validation tests are conducted in Windows XP. The FLUENT graphical user interface is started by clicking the executable file that appears on the desktop window as the FLUENT trademarked icon. The input mesh files for both test problems are generated using the preprocessor GAMBIT. These files are then imported into FLUENT where fluid flow models, heat transfer models, boundary conditions, and physical properties of fluid and solid are defined. The information is saved in a file, and the FLUENT solver is executed. The analysis of the computed results is carried out using point and click menus embedded in FLUENT graphical user interface.

3.2 Hardware

The software was installed on a computer with an AMD 64 Athelon microprocessor. The Microsoft Windows operating version of the software can also be installed on personal computers with the Intel Pentium® 4 processor, and 512 MB of random access memory. The actual memory required for a particular application depends on the size of the mesh, the physical models that are enabled, and the complexity of the domain.

4 PREREQUISITES

The user must be trained to use GAMBIT and FLUENT and also be familiar with theory of fluid mechanics and heat transfer.

5 ASSUMPTIONS AND CONSTRAINTS

None.

6 TEST CASES

6.1 TEST CASE 1: Natural Convection in an Annulus Between Horizontal Concentric Cylinders

The first test case considers natural convection between two isothermal concentric horizontal cylinders. This test case simulates the experimental study conducted by Kuehn and Goldstein (1978, 1976). A two-dimensional model is developed to model natural convection in the annulus for different conditions. The geometric dimensions of the model is same as one used by Kuehn and Goldstein (1978) for the experimental study. The diameters of the inner and outer cylinders are 3.56 cm and 9.25 cm, respectively, and length of both cylinders is unity. The annular space between the two cylinders is filled with nitrogen. The experimental studies were also conducted with nitrogen between cylinders. 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. In the experimental study, Kuehn and Goldstein (1976, 1978) measured 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.

The experimental results are reported in terms of equivalent thermal conductivity k_{eq}, defined as

$$k_{\text{eff}} = \frac{Q \ln\left(D_o / D_i\right)}{2\ \pi \Delta Tk} \tag{2}$$

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, k_{eq}, using Eq. (2), and calculated values are compared to the experimental values.

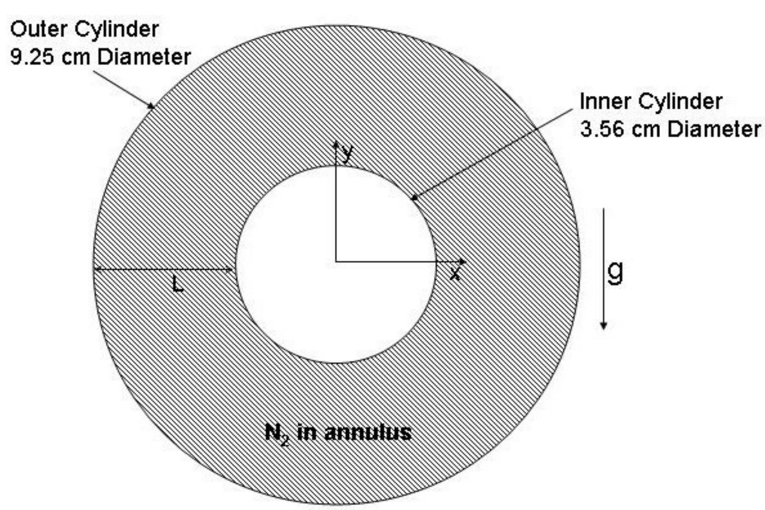

Figure 6-1. Schematic of Concentric Cylinders for Natural Convection Study. The Gravitational Acceleration Is 9.81 m/s^2 Along $-y$ Direction.

6.1.1 Test Input

The input files for different flow conditions are developed for 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.

6.1.2 Test Procedure

FLUENT Version 6.2.16 is executed using identical grid resolution for six different test conditions. The simulation results are used to compute the equivalent thermal conductivity for comparison to the experiment results of Kuehn and Goldstein (1978).

6.1.3 Expected Test Results

The acceptance criterion for the simulated equivalent thermal conductivity will be a deviation of no more than 25 percent of the measured value.

6.1.4 Test 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 6-1. The properties of nitrogen (Green, et al., 2005) at the selected conditions are listed in Table 6-2.

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 intervals on the circumference of each cylinder and 40 intervals 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.

Table 6-1. Selected Experiments for FLUENT Version 6.2.16 Simulations			
Ra	**P** **atm**	**ΔT** **°C**	**½(T_i + T_o)** **°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 6-2. Properties of Nitrogen for FLUENT Version 6.2.16 Simulation Conditions						
Ra	**ρ** ***kg/m*³**	**β** **1/*K***	**μ** ***Pa*×sec**	**C_p** ***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
6.60×10^7	38.07	3.185×10^{-3}	1.916×10^{-5}	1,040.67	0.02874	K-G_Ra6-6e07.cas

A sample of the fluid flow field with temperature distribution predicted by FLUENT Version 6.2.16 is shown in Figure 6-2. These results are for the case of *Ra* = 6.6×10^7. 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.

The FLUENT Version 6.2.16 postprocessor provides the total heat transfer rate from solid objects to the fluid. The calculated heat transfer rate is the value of *Q* in Eq. (2) to compute the k_{eq}. These calculations were performed in Excel as explained in Scientific Notebook 704E.

The measured values of k_{eff} reported by Keuhn and Goldstein (1978) are compared to the values predicted by FLUENT Version 6.2.16 in Table 6-3. The percent deviation ranges from −6.8 percent at low *Ra* to +14.48 percent at high *Ra*. The deviation in equivalent thermal conductivity for all *Ra* numbers is within the established acceptance criterion.

6.2 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.

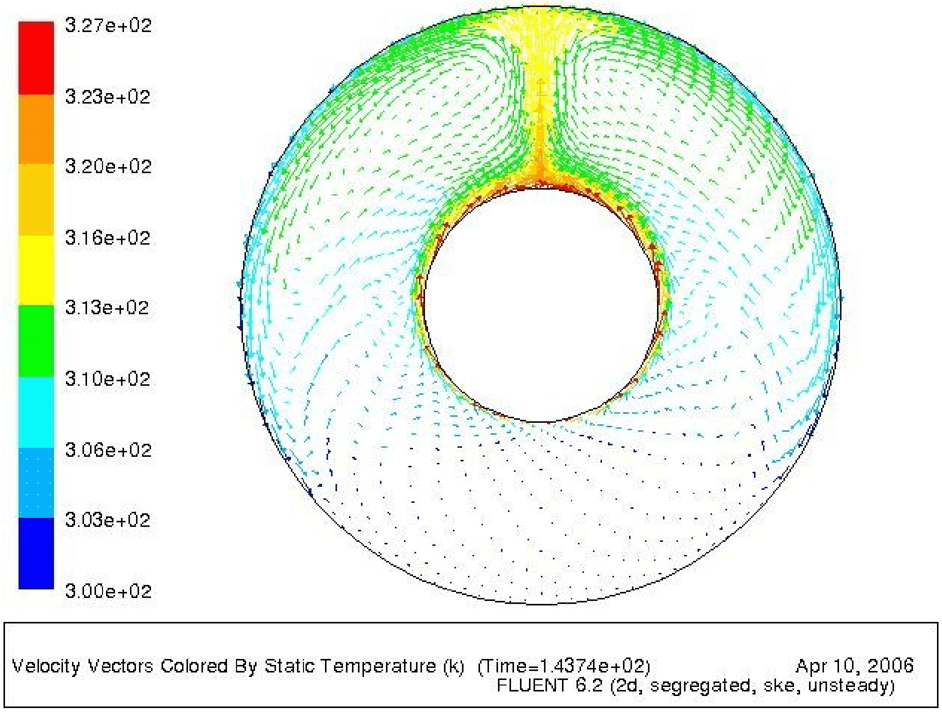

Figure 6-2. Predicted Fluid Temperature and Velocity Vectors for Natural Convection Between Cylinders. The Rayleigh Number Is 6.6 × 10^7.

Table 6-3. Equivalent Thermal Conductivity k_{eq} From Experiments and Simulations			
Ra_L	k_{eq} **experiment**	k_{eq} **FLEUNT® Version 6.2.16**	**Percentage Deviation**
1.31×10^3	1.14	1.09	−4.6
6.19×10^4	3.32	3.1	−6.8
6.81×10^5	5.6	5.81	3.8
2.51×10^6	7.88	8.03	1.9
1.90×10^7	13.27	14.53	9.5
6.60×10^7	18.65	21.35	14.48

A schematic diagram of the problem is presented in Figure 6-3, where the right side wall is maintained at temperature T_h equal to 2,000 K and the left side wall is maintained at temperature T_c equal to 1,000 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 6-4. 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

$$\tau = (\mathrm{K} + \sigma)\mathrm{L} \tag{3}$$

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, Nu_R. The overall *Nu* is defined as

$$Nu = \frac{\overline{q}L}{k(T_h - T_c)} \tag{4}$$

Table 6-4. Physical and Thermal Properties of Fluid Used in the Square Enclosure Test Case

Property	Value
Density ρ	1000 kg/m^3
Heat capacity C_p	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 m^{-1}
Scattering coefficient σ	0.0 m^{-1}
Optical thickness τ = (K+σ)L	1.0, 5.0, and 0.2

where

$\bar{q}$	—	average heat flux at the hotter wall
k	—	conductivity of the gas

The Nusselt number for radiation heat transfer, Nu_R, 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 Nu_R are compared to those reported by Yücel, et al. (1989) using S8 linear quadrature for discrete ordinates method.

6.2.1 Test 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.

6.2.2 Test Procedure

FLUENT Version 6.2.16 is executed using a uniform grid resolution for the four test conditions. The simulation results are used to compute average wall heat flux and the overall Nusselt number, Nu, and the radiation Nusselt number, Nu_R. The computed values of Nu and Nu_R are compared to the values reported by Yücel, et al. (1989).

6.2.3 Expected Test Results

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).

6.2.4 Test Results

The details of this validation test are described in Scientific Notebook 704E. The test results are summarized below.

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, Nu_R, 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, Nu_R, is listed in Table 6-6. The values of Nu_R are also with five percent of reported results by Yücel, et al. (1989).

Table 6-5. Comparison of Overall Nusselt Numbers, *Nu*, of the Hot Wall for Test Case 2 for Different Radiation Conditions			
Test Condition	***Nu*** **(Yücel, et al., 1989)**	***Nu*** **(FLUENT Version 6.2.16)**	**Percentage Deviation**
Nonradiating	13.76	14.30	−3.90
$\tau = 1$	38.93	37.88	2.71
$\tau = 5$	31.76	31.68	0.26
$\tau = 0.2$	46.11	44.68	3.09

Table 6-6. Comparison of Radiation Nusselt Numbers, *Nu*, of the Hot Wall for Test Case 2 for Different Radiation Conditions			
Test Condition	Nu_R **(Yücel, et al., 1989)**	Nu_R **(FLUENT Version 6.2.16)**	**Percentage Deviation**
$\tau = 1$	31.28	30.42	2.75
$\tau = 5$	23.64	24.05	1.74
$\tau = 0.2$	37.40	35.93	3.93

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.

7 INDUSTRY EXPERIENCE

FLUENT Version 6.2.16 has been used in several industrial applications including automobile, aerospace, and nuclear systems. The software was previously used to model spent nuclear fuel storage cask systems (Walavalkar, et al., 2004; Lee, et al., 2005). For example, Walavalker, et al. (2004) reported the thermal analysis of the VCS-17 cask system using FLUENT. In another study, Lee, et al. (2005) also used FLUENT to conduct the thermal analysis of a storage cask with 24 pressurized water reactor fuel assemblies.

8 NOTES

None.

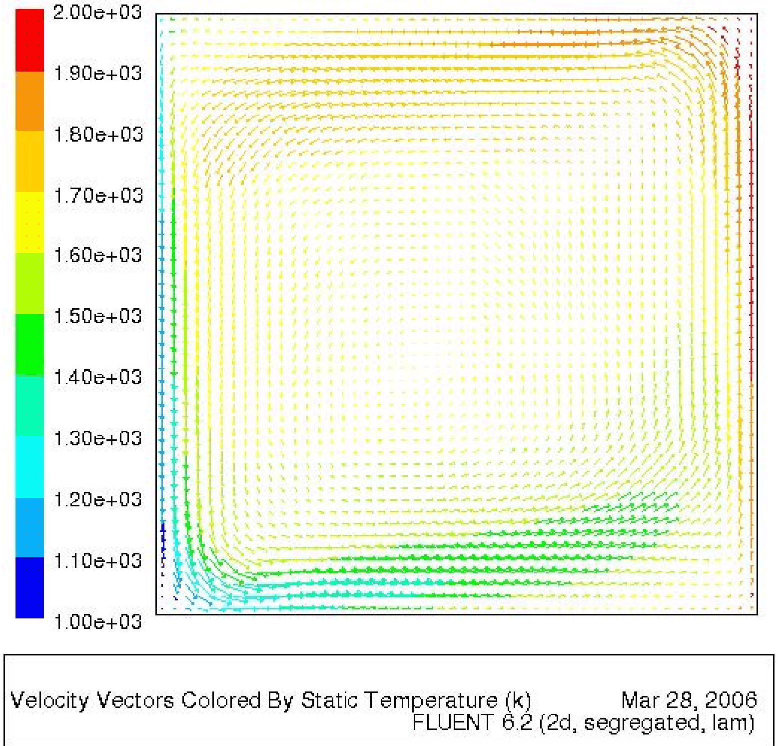

Figure 6-4. Calculated Flouid Flow Field Vectors Colored by Fluid Temperature for Natural Convection and Radiation in the Square Enclosure for Fluid With Optical Thickness Equal to 1.0.