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COMPUTATIONAL FLUID DYNAMICS ANALYSES ON VERY HIGH TEMPERATURE REACTOR AIR INGRESS

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ABSTRACT

A preliminary computational fluid dynamics (CFD) analysis was performed to understand density-gradient-induced stratified flow in a Very High Temperature Reactor (VHTR) air-ingress accident. Various parameters were taken into consideration, including turbulence model, core temperature, initial air mole-fraction, and flow resistance in the core. The gas turbine modular helium reactor (GT-MHR) 600 MWt was selected as the reference reactor and it was simplified to be 2-D geometry in modeling. The core and the lower plenum were assumed to be porous bodies. Following the preliminary CFD results, the analysis of the air-ingress accident has been performed by two different codes: GAMMA code (system analysis code, Oh et al. 2006) and FLUENT CFD code (Fluent 2007). Eventually, the analysis results showed that the actual onset time of natural convection (~160 sec) would be significantly earlier than the previous predictions (~150 hours) calculated based on the molecular diffusion air-ingress mechanism. This leads to the conclusion that the consequences of this accident will be much more serious than previously expected.

INTRODUCTION

The potential for air ingress into the VHTR vessel stems from consideration of postulated loss of coolant accidents (LOCAs). The VHTR is located in a reactor cavity that is filled with air under normal operational conditions. If a LOCA

occurs, air may be given the opportunity to move into the reactor vessel. It is presently thought that the worst-case scenario will occur if a double-ended guillotine break is postulated in the hot duct. The hot duct is a large pipe (exact dimensions presently not defined, but the outer diameter is over a meter) that connects the reactor vessel with the vessel housing the power conversion equipment.

For a postulated double-ended guillotine rupture, the transient will commence with a depressurization from operating pressure (assumed to be approximately 7 to 9 MPa) as helium is discharged into the reactor cavity. During the depressurization phase, hot helium from the vessel will mix with the air in the reactor cavity. Hence, a helium-laced air mixture will be available to move into the reactor vessel once the break is unchoked and the flow behavior at the break changes from momentum-driven flow from the reactor vessel into the reactor cavity to density-gradient driven stratified countercurrent flow with helium moving into the reactor cavity and helium-laced air moving into the reactor vessel from the reactor cavity.

The potential for density-gradient governed stratified air ingress into the VHTR following a large-break LOCA was first described in the Next Generation Nuclear Plant (NGNP) Methods Technical Program [1] based on stratified flow studies performed with liquid (Liou et al. 1997, 2005). Studies on density-gradient-driven stratified flow in advanced reactor systems has been the subject of active research for well over a

decade because density-gradient dominated stratified flow is an inherent characteristic of passive systems used in advanced reactors.

The work done on Generation III+ systems, although for light water reactors, is conceptually identical and directly applicable to the phenomenological behavior that occurs in the NGNP. Even though the earlier studies were based on Generation III+ systems using water as the working fluid, the governing equations are identical. The boundary conditions change to reflect the differences in the working fluid and the reactor vessel geometry. Recently, a simple computational fluid dynamic calculation was made to mimic the LOCA between two tanks filled with helium and oxygen, respectively. The scenario is depicted in Figure 1.

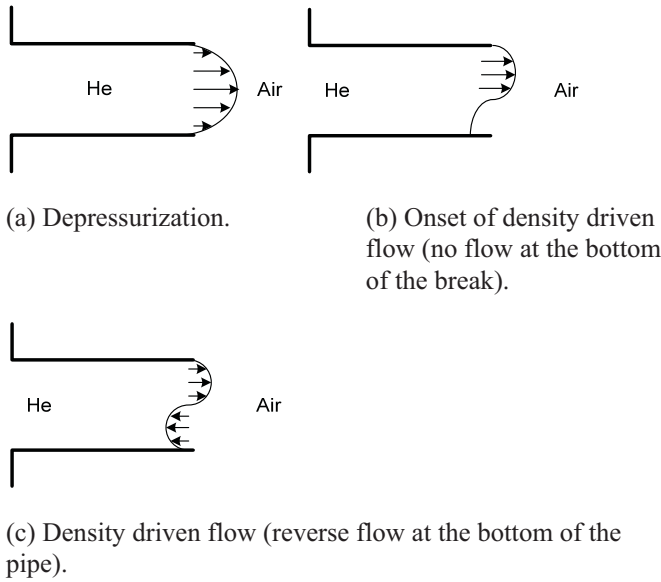


Figure 1. Density-driven induced stratified flow.

Earlier studies of the mechanisms leading to air ingress into the reactor vessel were focused on diffusion [2,3,4,5] as described by Fick's Law and ignored the effects of density gradients on the interactions between helium (low density) and air or helium-laced air (high density) flow.

Air ingress into the reactor vessel stemming from density-gradient-driven stratified flow occurs in a much quicker time scale than diffusion, resulting in a depressurized conduction cooling scenario with a different set of boundary conditions than previously assumed. Hence experiments are needed to study these phenomena as noted in the NGNP Methods Thermal-Fluids Experiment Plan (Schultz et al. 2006). Subsequent to the break in the hot duct hypothesized in depressurized conduction cool-down, air present in the reactor cavity will enter the reactor vessel, and because of the significantly higher molecular weight and lower initial temperature of the reactor cavity air, the air-helium mixture in the cavity is always heavier than the helium discharging from

the reactor vessel through the break into the reactor cavity. Once the air-helium mixture enters the reactor vessel, it will pool at the bottom of the lower plenum. It will move from the lower plenum into the core via diffusion and density-gradients induced by heating. When density-gradient-driven stratified flow is considered as a contributing phenomenon for air ingress into the reactor vessel for a large pipe size, the following factors contribute to a much earlier natural circulation-phase in the reactor vessel: (a) density-gradient-driven stratified flow is a much more rapid mechanism (at least one order of magnitude) for moving air into the reactor vessel lower plenum than diffusion, and consequently, (b) the diffusion dominated phase begins with a much larger flow area and a much shorter distance for air to move into the core than earlier scenarios, which attribute all air ingress from the reactor cavity into the core to diffusion only.

In essence, the stratified flow assumption is based on the formation of a wedge of air at the lower portion of the hot duct break that will advance into the reactor vessel as a function of the density-gradients when the blowdown has become unchoked. Such flows are well characterized by the densimetric Froude number F , which correlates the densities of helium and the air mixture to a constant value representative of the flow condition at different times in the scenario.

$$F = \frac{u}{\sqrt{g'd}} \quad (1)$$

where u = discharge velocity of air, d = hydraulic depth of air, and g' = reduced gravity defined by

$$g' = \frac{g(\rho_2 - \rho_1)}{\frac{\rho_2 + \rho_1}{2}} \quad (2)$$

The buoyancy induced by the density difference of the two fluids necessitates the usage of reduced gravity g' instead of the standard gravity g . The magnitude of F indicates the magnitude of inertia force relative to the buoyancy created by stratification, and is a controlling parameter in stratified flows. This idea and experimental confirmation can be found in References [6,7].

A stratified flow experiment is required to better understand this phenomenon and provide data for code validation because the codes will be used in conjunction with systems analysis codes to model this inherently multidimensional phenomenon. It is expected the densimetric Froude number will be found to be a function of

$$F = f\left(\alpha, L / D, \frac{V_{vessel}}{V_{vault}}, P_R, R\right) \quad (3)$$

where α = orientation of the break with respect to the vertical,
 L = length of the separated hot duct on the reactor vessel side,
 D = diameter of the hot duct, V = volume, Pr = Pressure coefficient, and R = Reynolds number.

Thus, as shown above in Figure 1(a), outward flow of helium into the reactor cavity from the reactor vessel continues until the reactor pressure is sufficiently reduced to unchoke the blowdown flow. Thereafter, air starts to intrude into the pipe through the lower portion of the break as depicted in Figure 1(b) and Figure 1(c). In a rectangular flow cross section, it can be shown theoretically that the volumetric flow rate of the two fluids through the break is the same [6]. Therefore it is assumed that the helium volumetric flow and air volumetric flow are equal. The heavy air will enter the vessel and collect (allowing dome turbulent mixing) at the bottom of the VHTR and air will penetrate the VHTR lower plenum and core through the diffusion. The diffusion will trigger a natural circulation in the reactor, resulting in graphite oxidation, which will be detrimental to VHTR safety. If the stratified air flow induces the natural circulation flow to begin earlier than previously thought, the time frame for graphite oxidation will occur earlier and at a more rapid rate. Earlier predictions from the GAMMA code [5] predict oxidation between 150 and 200 hours following pipe rupture, depending on the initial air volume in the containment. Calculations using MELCOR predict that oxidation begins at 220 hours [7] following pipe rupture. However, recent CFD calculations [8] using the stratified flow approach predict that natural circulation commences much earlier than 150 hours. Hence, the need to clarify the understanding of this phenomena and its effect on the progression of the scenario are quite important.

PRELIMINARY CFD CALCULATIONS

Problem Description

Preliminary calculations were performed using commercial CFD code FLUENT 6.3 [9] in order to estimate the air ingress that stems from density-gradient driven stratified flow. A short description of the underlying assumptions is given below. The FLUENT code has been used to model the hot duct and reactor vessel of the gas turbine modular helium reactor (GT-MHR) 600 MWt [10]—a General Atomic, Inc., (GA) design with a prismatic core. Figure 2 shows the reactor configuration; overall size and dimensions are specified here.

For the first simulation, the reactor core was highly simplified because the detailed geometry of the reactor is too complicated to be rigorously modeled. For simplification, the core, reflector and lower plenum were considered as porous bodies. The simplified geometry is illustrated in Figure 3. The flow path between the cavity and the core (the break) includes only the core and a portion of the reactor cavity. The volume

of the containment was not taken into consideration for these preliminary calculations. The fluid region was divided into five zones: Zone 1 represents the core, Zone 2 represents the lower plenum, Zone 3 represents the hot duct, Zone 4 represents the vessel inside, and Zone 5 represents the reactor cavity.

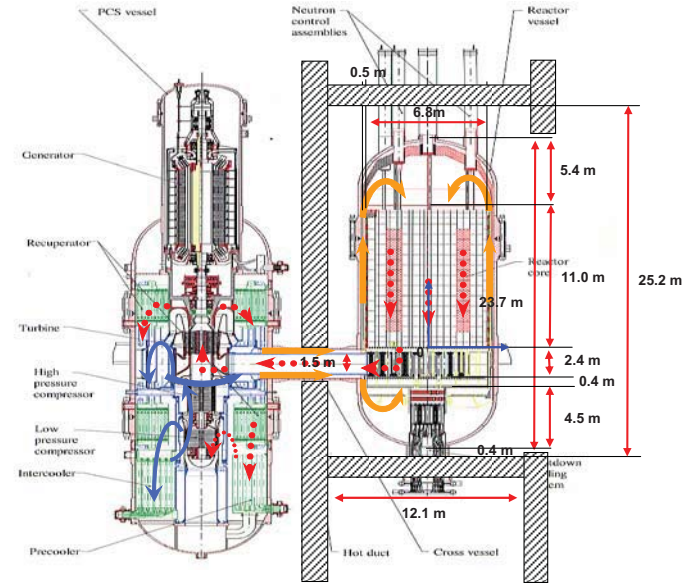


Figure 2. Geometry and size of GT-MHR 600 MWt reactor.

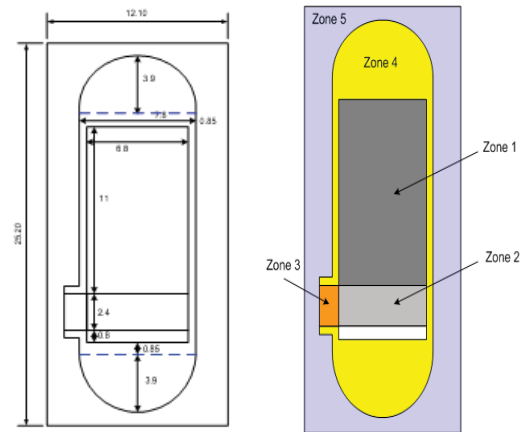


Figure 3. Simplified 2-D geometry of GT-MHR 600 MWt for preliminary stratified flow simulation.

Solver and Model Setup

The solver and model set-up of this first calculation are as follows:

- Solver
 - 2-D (hexagonal mesh (31,232 cells))
 - Segregated solver
 - First order implicit

- Unsteady
- Noniterative time advancement
- Absolute velocity formulation
- Cell-based gradient
- Energy Equation
- Viscous Model
 - Laminar/Turbulence (k-ε or Reynolds stress model [RSM])
 - Standard k-ε
 - Standard wall function
- Species Model
 - Species transport equation
 - 2 gas species: Air/Helium.

This simulation adapts a noniterative time-advancement scheme. The traditional iterative time-advancement scheme requires considerable computational effort because of a large number of outer iterations performed for each time-step.

Boundary conditions

For the first calculation, the operating pressure was set equal to be 1.0 atm (101,325 Pa) in all the fluid zones. Gravity force (acceleration of gravity = 9.8 m/s^2) was defined in the negative y-direction in order to consider the density driven force. All the initial conditions to Fluent following the depressurization were calculated using the GAMMA code [3].

Air and helium were the two gas species considered. The detail mixture model is summarized as follows:

- Mixture species: air/helium
- Density calculation: incompressible ideal gas law
- Heat capacity calculation: mass weighted mixing law
- Thermal conductivity calculation: mass-weighted mixing law
- Viscosity calculation: ideal gas mixing law
- Mass diffusion calculation: constant dilute approximation.

The property model of each species was set using National Institute of Science and Technology's (NIST's) chemistry Web book (2008) as a form of a polynomial function.

Turbulence Models

Currently, no single turbulence model is universally accepted as being superior for all classes of problems. The choice of turbulence model will depend on considerations such as the physics encompassed in the flow, the established practice for a specific class of problem, the level of accuracy required, the

available computational resources, and the amount of time available for the simulation.

In the stratified flow, the driving force is the density difference between air and helium, so the flow velocity is not very fast. For this reason, it is expected that the flow has a low Re number. However, because of the large pipe diameter and the low viscosity, it is not clear if the flow is within a laminar regime or a low Reynolds number turbulent regime.

This study considered the following turbulence models (the below summary refers to the FLUENT user's guide [9]).

- Laminar model
- Standard k-ε model
- RNG k-ε model
- Realizable k-ε model
- k-ω model
- Reynolds stress model

RESULTS

Grid Sensitivity

The grid sensitivity was checked. Figure 4 shows the calculated average air mole fractions at each zone for two different meshes; the computational mesh is composed of 31,232 numbers of grid points, and the finer mesh is composed of 53,601 numbers of grids. The lines represent the normal mesh scheme, and the points represent the fine mesh scheme. As a result, the differences between the two mesh sizes were very slight to be negligible within the maximum error of 3%.

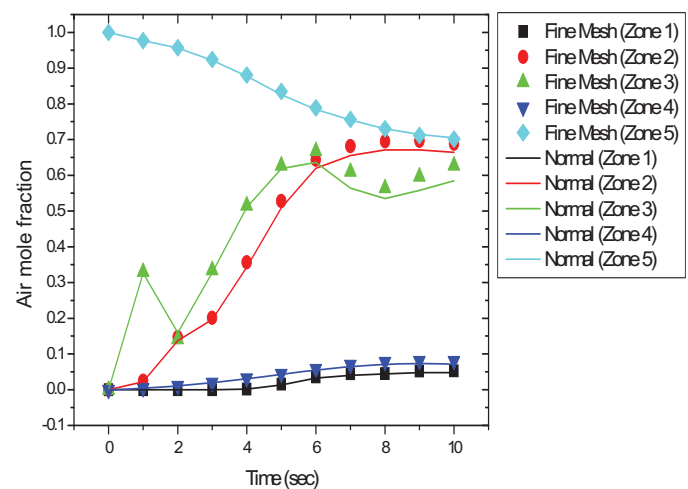


Figure 4. Grid sensitivity (31,232 meshes vs. finer 53,601 meshes).

CFD Results

The stratified flow was first calculated using GT-MHR design. The calculated results are expected to be conservative because the initial air-mole fraction in the reactor cavity was assumed to be 1.0, which maximizes the initial density gradient. In the real accident, the mole fraction is usually much less than 1.0 by mixing of the discharged helium coolant and the air in the containment. The actual air-mole fraction in the reactor cavity depends on the reactor design, containment (or confinement) geometry, and size.

Figure 5 shows the calculated air distributions in the reactor core and the cavity for different times. An initial air mass fraction in the confinement was used as 0.5 that was calculated by the GAMMA code [3]. Figure 5 also shows rapid air intrusion into the reactor core along the hot duct and lower plenum. In this calculation, flow transition was very fast, and all the bottom part of the reactor core was filled up with air very rapidly. After the ingress of air, some heated air migrated into the reactor core by thermal expansion, and some air rebounded back to the reactor cavity. A series of snapshots of the FLUENT simulation in which the natural convection was initiated about 2–3 minutes after the stratified flow started. And, after 4 minutes, the whole reactor core and vessel was filled with air. It is much quicker than the previous predictions (~150 hrs) using the diffusion driven flow assumption [2, 3]. For CFD calculations in Figure 5, air volume in the vault was used as 25,708 m³ close to that of GT-MHR [8].

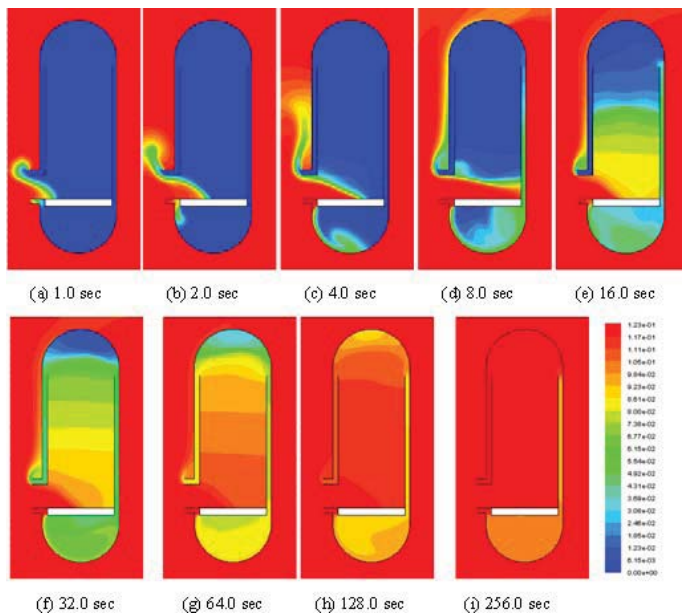


Figure 5. Variations of calculated air concentrations.

Figure 6 shows calculated air mole fractions in five different zones defined in Figure 3. Instead of using a large vault volume used for CFD calculations in Figure 5, only the core and a portion of cavity were used to see the air concentration using a number of various turbulence models as part of the sensitivity study shown in Figures 6 and 7. The air concentration that was assumed to be 1 as part of parametric studies decreases in the cavity while air concentration (oxygen is only 21% of air) in zone 1 increases up to 10 seconds and reaches a steady-state value.

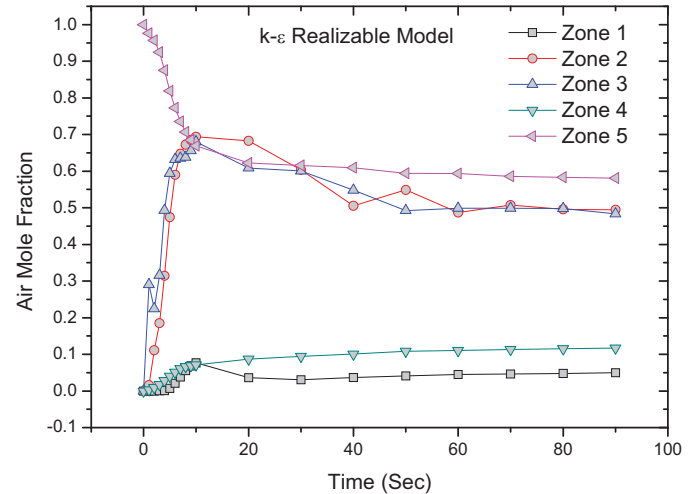


Figure 6. Variations of averaged air mole fractions.

As mentioned, the flow regimes are not clear in the first stage of the air ingress accident, and therefore the effects of turbulence models were estimated in this section. Four different models (laminar, k-ε, k-ω, and RSM) were taken into consideration for isothermal conditions. The laminar option is the most conservative because of no mixing associated with dissipations.

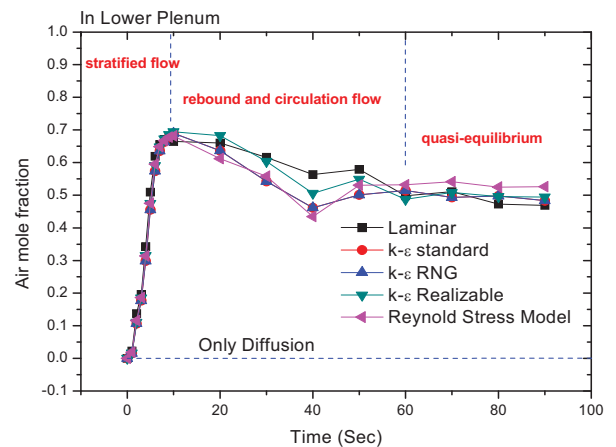


Figure 7. Average mole fractions in the lower plenum.

In the isothermal condition shown in Figure 8, the air distribution in the equilibrium appears sensitive to the turbulence models. As shown, the laminar model predicts that the largest amount of air is ingressed into the reactor core. The main reason is that the laminar model has no additional mixing terms, which are considered in all the other viscous models. The mixing terms in the turbulence models diminish the density gradient, leading to a decreased driving force. In this work, the practical two-equation turbulence models were compared to the RSM, which can theoretically provide the most realistic results for highly anisotropic and complicated turbulent flow as in this case. Among the turbulence models, the k- ϵ realizable model shows the most similar results to the RSM.

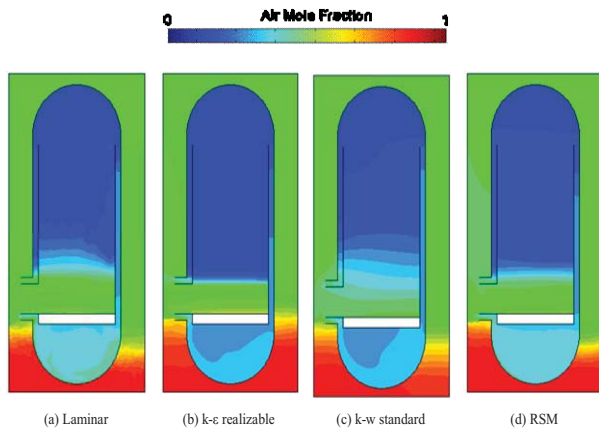


Figure 8. Quasi-equilibrium states for different turbulent models.

Duncan and Toor's Two Bulb Experiment

The second case of CFD calculations was made on "two bulbs" experiment conducted by Duncan and Toor [11]. The experimental apparatus consists of two bulbs separated by a small horizontal capillary tube. The bulbs had volumes of 77.99 cm³ and 78.63 cm³, respectively. The capillary tube joining them was 85.9 mm long and 2.08 mm in diameter. The bulbs were initially isolated by a stopcock installed at the center of the capillary tube. The entire device was maintained at a temperature of 35.2°C in atmospheric pressure.

In a previous study [3], the GAMMA code was used to compare with the experimental results. The 1-D GAMMA results were in good agreement [3]. In this paper, the 2 mm pipe size was changed to 16 mm while other initial conditions and the geometry including the pipe length remained the same as the experiment. Figure 9 shows the two 3-D CFX models [12]. The bulb 1 shown in the left side in Figure 9 contains CO₂ and nitrogen initially while bulb 2 in the right is initially filled with hydrogen and nitrogen.

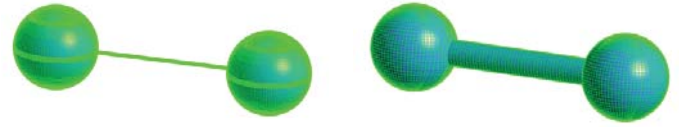


Figure 9. CFX Models of Duncan Experiment (2 mm horizontal pipe (left) vs. 16 mm horizontal pipe (right)).

The initial conditions used for CFX simulations are 0.499 mole fraction CO₂ and 0.501 nitrogen in Bulb 1, and 0.501 mole fraction hydrogen and 0.489 mole fraction nitrogen in the Bulb 2.

Figure 10 shows the calculated concentration of CO₂ in the two bulbs connected with a 16-mm pipe at 30 seconds. As can be seen, the heavier gas of CO₂ in the left bulb (Bulb 1) flows through the pipe initially as the stratified flow with CO₂ flowing along the bottom and underneath the lighter gas hydrogen.

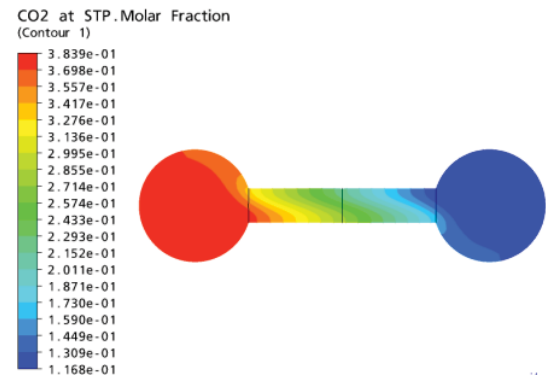


Figure 10. CFX results of two-bulb simulation with 16-mm pipe.

Figure 11 depicts time-dependent gas concentrations from CFX calculations using 2-mm and 16-mm pipes. When 2-mm pipe was used, the gas concentrations of hydrogen in the bulb 2 and CO₂ in bulb 1 are not changed up to 200 seconds by CFX calculations. The test data and GAMMA results show the same trend in the previous study [3].

However, when 16 mm size was used in CFX simulations, as shown in Figure 11, the concentrations of CO₂ in bulb 1 and H₂ in bulb 2 decrease significantly. This indicates that the density-gradient-driven stratified flow is a dominant phenomenon for the gas species transport in a larger size of 16 mm while the molecular diffusion is a dominant phenomenon for gas transport in a small pipe of 2 mm.

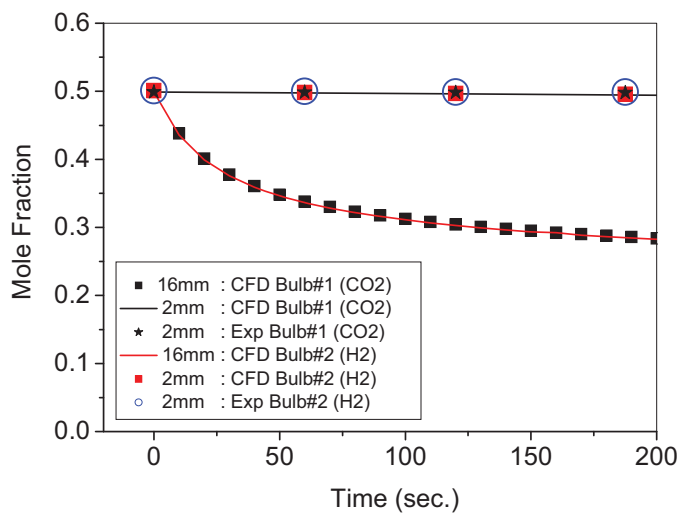


Figure 11. Results of gas species transport in 2-mm vs. a 16-mm pipe.

CONCLUSIONS

The GT-MHR design was selected for the air ingress study. The geometry was simplified to avoid a large CPU time and to understand the air ingress phenomenon until a detailed 3-D model is developed.

Study results showed that the air ingress of the GT-MHR is initiated by the density-gradient-driven stratified flow, which can be found in a certain class of pipe break LOCA in the hot legs of a pressurized water reactor.

A number of various turbulent models in Fluent were used for comparisons in this study to see the effect of the turbulence model on the air ingress. Among the turbulence models, the $k-\epsilon$ realizable model shows the most similar results to the RSM.

CFX simulations on Duncan and Toor's two bulb experiments [11] were conducted with both 2-mm (L/D (length/diameter) = 41.2) and 16-mm (L/D = 5.3) pipes.

Preliminary bounding results indicate that the 16-mm pipe initiated the density-gradient-driven stratified flow in the horizontal pipe and accelerates gas transport much faster than that of molecular diffusion. For the future study, air ingress experiments will be performed at Idaho National Laboratory to investigate this phenomenon further.

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