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Addition of Diffusion Model to MELCOR and Comparison with Data

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INTRODUCTION

A chemical diffusion model was incorporated into the thermal-hydraulics package of the MELCOR Severe Accident code (Reference 1) for analyzing air ingress events for a very high temperature gas-cooled reactor.

MATHMATICAL MODEL

The differential equation expressing conservation of mass for the i^{th} material solved by MELCOR for the atmospheric phase of the fluid flow is:

$$\frac{\partial \rho^i_A}{\partial t} + \nabla \bullet (\rho^i_A \mathbf{v_A}) = \Gamma^i_A \qquad (1)$$

where
ρ^i_A - atmosphere material density (kg/m^3)
v_A – atmosphere flow velocity (m/s)
Γ^i_A - atmosphere material source term (kg/m^3-s)

Equation 1 was modified by adding a gaseous diffusion term that obeys Fick's Law of diffusion as follows:

$$\frac{\partial \rho^i_A}{\partial t} + \nabla \bullet (\rho^i_A \mathbf{v_A}) = \nabla \bullet \rho_A D^i_A \nabla \omega^i_A + \Gamma^i_A \qquad (2)$$

where
D^i_A – mass diffusivity (m^2/s) for the i^{th} material diffusing through the atmosphere phase (A) of the fluid flow
ω^i_A - mass fraction of the i^{th} material = ρ_i/ρ_A

In MELCOR these equations are solved for control volumes (volumes defined by average material properties such as rooms) that are interconnected by flow paths (connections between volumes such as piping). After integrating Equation 2 over the j^{th} control volume, the result is as follows:

$$\frac{\partial M^i_{j,A}}{\partial t} = \sum_k \sigma_{j,k}\, \alpha_{k,A}\, \rho^{i,d}_{k,A} v_{k,A} F_k A_k + \sum_k \rho_{k,A} D^i_{k,A} \left(\frac{\omega^i_{m,A} - \omega^i_{j,A}}{L_k} \right) \alpha_{k,A} F_k A_k + \dot{M}^i_{j,A} \qquad (3)$$

Here, as described in Reference (1), M is the total mass; subscript k refers to a given flow path, with $\sigma_{j,k}$ accounting for the direction of flow in flow path k with respect to volume j; $\alpha_{k,A}$ is the volume fraction of the atmospheric phase in flow path k; superscript d denotes "donor", corresponding to the control volume from which the material is flowing; A is the flow path area; F is the fraction that the flow area is open; L_k is the length of flow path k; subscript m refers to the volume connected to volume j by flow path k, and $\dot{M}$ includes all sources of mass. The diffusion coefficients for Equation 3 are calculated by the MELCOR as described in Reference (2).

The diffusive term of Equation 3 is evaluated explicitly in time prior to each time advancement by MELCOR. Because an explicit update of the diffusive term has an upper stability limit regarding time interval size, defined per flow path as $L_k^2/D^i_{k,A}$, the maximum allowed time interval is determine for all flow paths and if the MELCOR adopted time interval exceeds this diffusive limit then the calculation is terminated with an error message stating that the maximum diffusive time step size has been exceeded. The remaining terms of Equation 3 are advanced in time as described in Reference (1).

The equation expressing conservation of energy for the atmospheric phase in the j^{th} control volume is derived in a similar manner. The conservation equation, written neglecting potential and kinetic energy, is as follows:

$$\frac{\partial E_{j,A}}{\partial t} = \sum_k \sigma_{j,k}\, \alpha_{k,A} \left(\sum_i \rho^{i,d}_{k,A} h^{i,d}_{k,A} \right) v_{k,A} F_k A_k + \sum_k \rho_{k,A} \left(\sum_i D^i_{k,A} \left(\frac{\omega^i_{m,A} - \omega^i_{j,A}}{L_k} \right) \right) h^d_{k,A}\, \alpha_{k,A} F_k A_k + \dot{H}_{j,A}$$

(4)

where, E is the total internal energy, "i" represents the summation over all species in the atmosphere phase, h^i is the specific enthalpy of specie "i", h is the total specific enthalpy for the atmosphere in the volume attached to the j^{th} control volume by the k^{th} flow path, and $\dot{H}$ is the non-flow energy sources related to the mass sources of Equation 3.

RESULTS OF VALIDATION

In order to validate the diffusion model incorporated into MELCOR, we compared the results from MELCOR with the inverse U-tube experimental data from Takeda (Reference 3). The experiment consisted of a reverse U-shaped inconel tube containing a 450 mm in length graphite sleeve. Both ends of the tube are attached to a tank containing helium and air. The tube is initially isolated from the tank by valves located at the ends of the tube. One side of the U-shaped tube is heated and the other side is cooled.

A MELCOR model of the experimental configuration was constructed and preliminary MELCOR results are compared to the experimental results as shown below in Figures 1 and 2. Figure 1 is a plot of the mixture (N_2, O_2, He, CO_2, and CO) density as a function of time and location in the pipe. The solid lines are MELCOR results and the experimental results are represented by symbols. In Figure 2 the mole fraction of O_2 is shown for the same locations as Figure 1. The preliminary results from MELCOR appear to show good agreement with the experimental results.

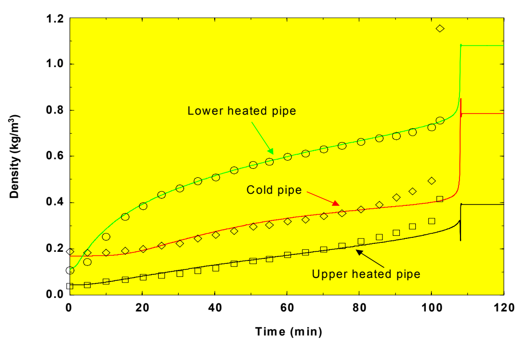

Figure 1. Comparison of density change of mixtures.

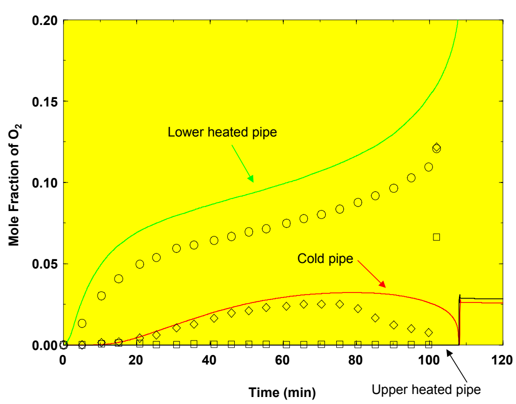

Figure 2. Comparison of oxygen mole fractions.

REFERENCES

1. MELCOR Computer Code Manuals, “Thermal Hydraulic (CVH and FL) Packages”, NUREG/CR-6119, Vol. 2, CVH/FL-RM-17, May 2000.

2. MELCOR Computer Code Manuals, “Material Properties (MP) Package”, NUREG/CR-6119, Vol. 2, MP-RM-55, May 2000.

3. TAKEDA, M. HISHIDA, Studies on molecular diffusion and natural convection in a multicomponent gas system, *Int. J. Heat Mass Transfer,* 39, No.3, pp.527-536, 1996.