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Numerical Methods for an Analysis of Hydrogen Behaviors Coupled with Thermal Hydraulics in a NPP Containment

Jongtae Kim [a*], Rae-Joon Park [a], Seong-Wan Hong [a], Gun-Hong Kim [b]

[a] *Severe Accident & PHWR Safety Research Division, KAERI, Daeduk-daero 989-111, Daejeon, Korea*
[a] *Kyung-Won E&C, Seongnam, Korea*
[*] *Corresponding author: ex-kjt@kaeri.re.kr*

1. Introduction

During a severe accident with a core damage in a water-cooled nuclear reactor, a large amount of steam and hydrogen is released into the reactor containment. The hydrogen is generated by an oxidation of a heated core in a very high rate during a severe accident. Hydrogen safety in a reactor containment is very important because the integrity of the reactor containment can be threatened by an explosive combustion of the hydrogen. The released hydrogen is mixed with steam and air in the containment. When it is well mixed with other gases, hydrogen concentration becomes leaner and finally a probability of hydrogen explosion may be reduced. On the contrary if mixing of the released hydrogen is limited and a highly-concentrated hydrogen mixture cloud is developed in a certain region of a containment, it is very probable that hydrogen flame undergoes DDT (deflagration to detonation transition) locally or globally in the containment. Hydrogen distribution in a containment is also affected by steam condensation and evaporation. If steam is condensed on a cold wall in a containment, the hydrogen concentration near the wall can be increased. If steam in a hydrogen mixture cloud is condensed and becomes fog, the density of the hydrogen cloud containing the fog becomes high, and the cloud may descend in the atmosphere of the containment.

In a containment safety analysis, multi-dimensional characteristics in thermal hydraulics are very important because the flow paths are not confined in a large free volume of the containment. The analysis is difficult because of a difference in length scales between a characteristic length of the flow and representative length of the containment.

In order to simulate hydrogen and steam behaviors in a containment during postulated severe accidents, the GASFLOW [1] code as a multi-dimensional analysis tool for NPP containment has been used for years because of its computational efficiency. Though GASFLOW is well developed for a real NPP containment analysis, there exist shortcomings in nodalization, two-phase and turbulence models. It is based on a Cartesian or cylindrical coordinate mesh, so it is impractical to refine a mesh locally in a region with a physical or geometrical complication. Recently it is known that jet flow of a released gas from a RCS (reactor cooling system) strongly affects initial distribution and mixing of hydrogen. If the turbulent convection of the released gas augmented by jet momentum and buoyancy force is not well resolved, then the hydrogen distribution during an accident may not be conservative.

In order to overcome shortcomings of the GASFLOW code, it is necessary to develop a new generation code founded on modern CFD technology for containment safety analysis. The new code is based an open-source CFD library OpenFOAM [2]. It is programmed by C++ language in an object-oriented paradigm. One of main reasons choosing the OpenFOAM library is easy modification and addition of physical models such as turbulence.

In this paper, recently conducted research for the development of a hydrogen safety analysis code is introduced.

2. Development of Numerical Methods

2.1 Physical Models for hydrogen safety analysis

Hydrogen behaviors during a severe accident in an NPP containment are strongly dependent on thermal hydraulics in the containment. Important thermal hydraulic physics which must be considered are buoyant jet flow, turbulent mixing, gas species diffusion by concentration gradients, steam condensation, thermal radiation, structure heat transfer, condensed/sprayed droplet flow, combustion of hydrogen, and et al. Active or passive devices installed in a containment in order to control a containment atmosphere must also be modeled. Among them PAR, igniter, fan/cooler and passive heat removal system considerably affects hydrogen behaviors in a containment.

Implementation of all the physical models in a single code makes it complicated and heavy to run for a long-term accident scenario. Modulization of an analysis code is a commonly used technology to keep the code manageable. Fig. 1 shows physical models grouped by modules required to simulate hydrogen safety in a NPP containment. Each module will be separately managed and easily coupled with other modules.

An analysis tool for hydrogen behavior in a containment is udder development based on the OpenFOAM library which supplies mudulized numerical and physical models by using classes and namespaces.

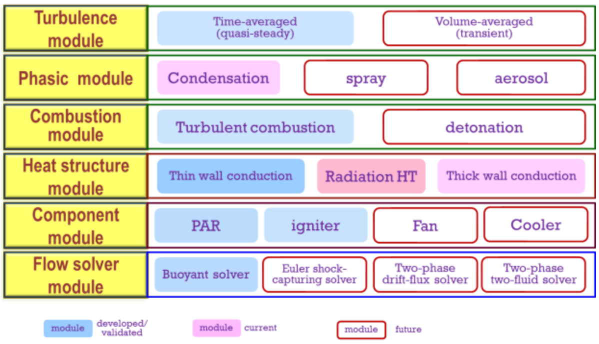

Fig. 1. Physical models needed for hydrogen behavior analysis

2.2 Current Development of Analysis Modules

1) Buoyant jet model

During a severe accident, hot steam and hydrogen are released into a containment as a jet flow through a break or a pressure relief valve of a reactor coolant system. Because of lower density of the released steam and hydrogen compared to the containment atmosphere, the jet flow easily becomes a buoyant jet or plume when it loses its momentum by a jet impingement on an obstacle or compartment wall. The turbulent buoyant flow of the steam and hydrogen has an important contribution to distribution of hydrogen in the containment. For example, a turbulent buoyant flow of steam enhances mixing of a highly concentrated hydrogen mixture cloud which could be developed in the upper region of a containment, which is called an erosion of a stratified hydrogen mixture. This phenomenon has been studied in the frame work of international collaboration research HYMERES [3] operated by PSI and CEA.

In a simulation of a transient turbulent buoyant jet flow, a turbulence modeling plays a major role. Because there still exists a computing resource problem in application of a large eddy simulation (LES) to a simulation of a long-term hydrogen safety analysis, a RAS (Reynolds averaged simulation) model is preferred. A standard k-ε turbulence model chosen for an analysis of hydrogen mixing by a buoyant jet is modified to consider generation of kinetic energy by buoyancy and prevention of kinetic energy build-up at a stagnation point. Buoyancy generation term originated from body force of a momentum equation is approximated by Boussinesq's simple gradient diffusion hypothesis (SGDH) as shown in Eq. (1).

$$G = \overline{\mathbf{U}'\rho'} \cdot \mathbf{g} = -\frac{\nu_t}{\mathrm{Pr}_t} \nabla \rho \cdot \mathbf{g} \quad (1)$$

The term is added in k and ε equations. In order to prevent a build-up of turbulent kinetic energy at a stagnation point, a term proposed by Mentor[4] is implemented in the k-ε turbulence model

$$\tilde{P} = \min(P, 10\rho\varepsilon) \quad (2)$$

, where P is a production of turbulence and $\tilde{P}$ is a limited value of the production.

Recently, a blind benchmark of a Helium mixing by a buoyant jet (HM1-1) [5] was conducted in the frame of the HYMERES project. The OpenFOAM-based containment analysis code with the modified k-ε turbulence model was applied for the blind benchmark simulation.

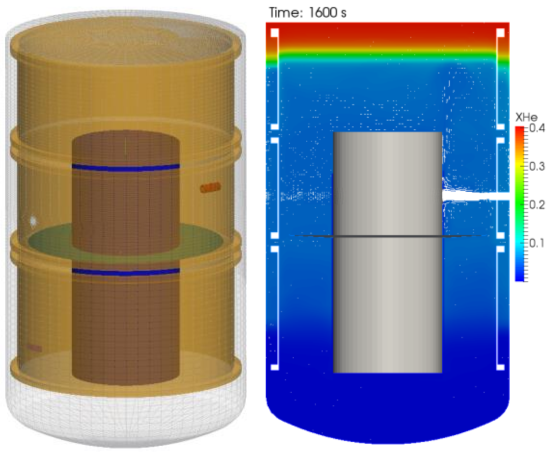

Fig. 2. Left: MISTRA test facility for HM1-1, right: Helium concentration and jet velocity vectors at 1600s.

Hot air jet is injected into the MISTRA vessel and it impinges on the inner cylinder. After losing the momentum of the jet, it moves upward by a buoyancy force and interacts with the Helium cloud. The Helium cloud is slowly diluted by the erosion process. Fig. 3 shows profiles of Helium concentration along vertical center line at 2100s and 3600s. In the experiment, the Helium was fully eroded after 3500s.

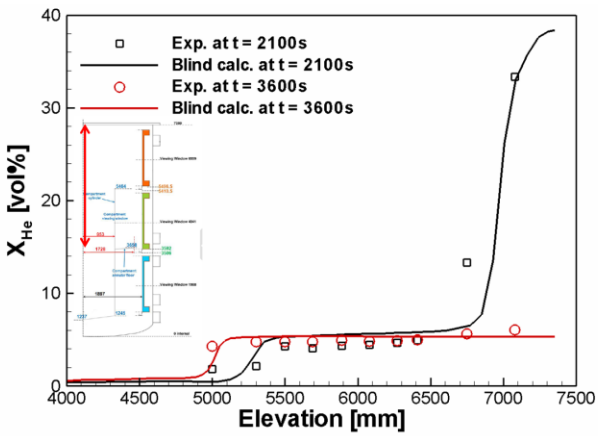

Fig. 3. Profiles of Helium concentration

2) Species diffusion model

Hydrogen mixing with steam and air in a containment during a severe accident is very important in view of a hydrogen safety. A local accumulation of hydrogen in a containment is highly prohibited in order to keep the integrity of the containment. Mixing of gas species is governed by convection and diffusion. The diffusion of gas species is depending on strength of turbulence in the convective flow. In a laminar flow, molecular diffusion by gradients of gas species concentrations is dominant, but as turbulence in a gas flow becomes stronger, turbulent eddies augment the diffusive mixing of gas species. Because of a complicated geometry inside an NPP containment, the characteristics of local compartment flows are varying from laminar to turbulent flows. So in a laminar flow region, the gas mixing by molecular diffusion becomes very important. The current version of OpenFOAM only considers diffusion by turbulence. So a molecular diffusion modeled is implemented in the code.

$$\dot{\mathbf{m}}''_{i,diff} = \mathbf{J}_i = \rho Y_i \mathbf{v}_i = \rho D_{im} \nabla Y_i \qquad (3)$$

Mass flux by a molecular diffusion is described by Fick's law and it can be written as Eq. (3), where Y_i and x_i are mass and molar fractions of specie i. Diffusion velocity of i-specie ($Y_i \mathbf{v}_i$) is depending on concentration gradient and diffusion coefficient (D_{im}) of i-specie. D_{im} for diffusion of i-specie to mixture is calculated from binary diffusion coefficients as follows.

$$D_{im} = \frac{\sum_{j \neq i} x_j}{\sum_{j \neq i} x_j / D_{ij}} = \frac{1 - x_i}{\sum_{j \neq i} x_j / D_{ij}} \qquad (4)$$

The current module of the diffusion model has diffusion coefficient models of binary diffusion and constant diffusion coefficients.

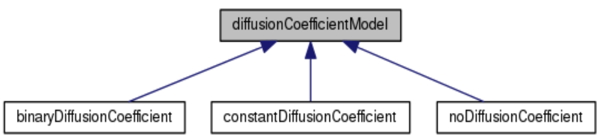

Fig. 4. Class inheritance diagram for diffusion coefficient model.

Molecular diffusion model was tested by solving diffusion of helium stratified in the SPARC vessel [6] with 9.532 m height. Initially, gas mixture with 30 vol% of Helium concentration is filled in upper plenum. As time goes on, Helium is diffused into the quiescent air in the vessel. Fig. 5 shows Helium distributions in the vessel initial and final states (48 hours after diffusion starts). Fig. 6 is a comparison of vertical profiles of Helium concentrations at 0, 12 and 48 hours, which depicts that the molecular diffusion is a very slow mixing mechanism.

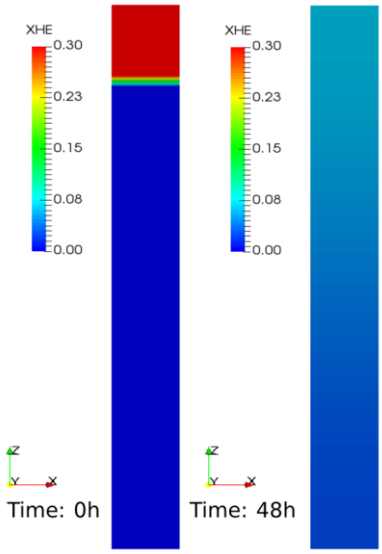

Fig. 5. 1-dimensional analysis of Helium diffusion in a SPARC vessel

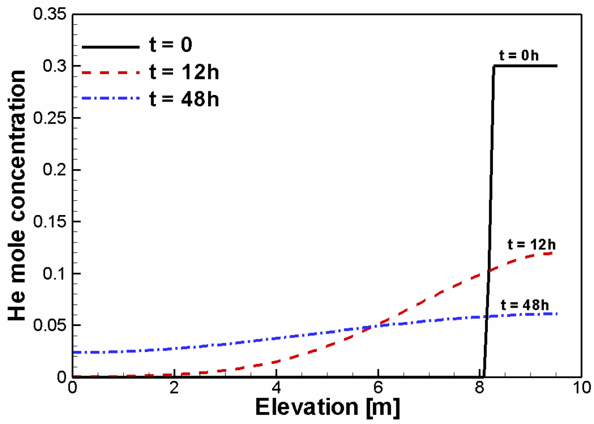

Fig. 6.Variation of vertical Helium distribution along time

3) Solid Heat Transfer model

OpenFOAM already has 3 models implemented for solid structure heat transfer. They are 'thermalBaffle1D' 'thermalBaffle' and 'CHT' (conjugate heat transfer). The 'thermalBaffle1D' is a 1-dimensional steady heat balance model. The 'thermalBaffle' model is a kind of quasi-3D heat conduction model. And the 'CHT' model solves heat conduction equation on a 3-D mesh.

In order to optimize computational costs spent for a NPP containment analysis, it is necessary to carefully control the size of the mesh. So it is decided to add 1-D unsteady heat conduction model in the solid heat transfer module to model so thin heat structure to generate a 3-D mesh. The model is named 'thermalBaffleUnsteady1D' because it solves unsteady heat conduction equation on a virtual mesh for a thin heat structure. The mesh for the 'thermalBaffle-Unsteady1D' model is called virtual because it is generated during a run-time by the model on a patch.

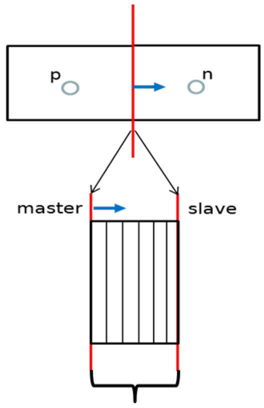

Fig. 7. Virtual mesh for an unsteady 1-D heat conduction model

Fig. 7 shows the virtual mesh on a face of a thermalBaffleUnsteady1D patch. The thin solid of the model is thermally coupled with fluid region. The following 1D heat conduction equation is solved by TDMA (a 3-diagonal matrix solver) for every face on the patch.

$$\rho C_p \frac{(T-T^n)}{\Delta t}\delta = k\left.\frac{dT}{dx}\right|_e - k\left.\frac{dT}{dx}\right|_w \quad (5)$$

The thermalBaffleUnsteady1D model was applied for a 3 mm-thick inner cylinder installed in the MISTRA test facility. Hot air jet in a MISTRA HM1-1 test is directly impinging on the cylinder surface and increasing the surface temperature by a convective heat transfer.

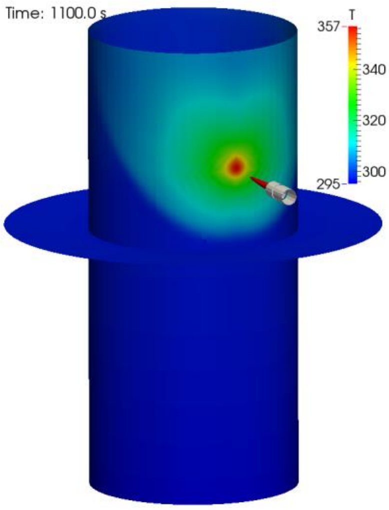

Fig. 8. Surface temperature of an inner cylinder modeled by thermalBaffleUnsteady1D

Fig. 8 shows surface temperature distribution at 1100s. It is clearly seen that a surface region where hot air jet is impinging is very heated compared to the other region.

3. Summary and Future Plan

In this paper, the importance of the hydrogen safety in an NPP containment and requirements of the analysis tool was described. And physical models necessary for the hydrogen safety analysis code were listed.

As a member of international collaborative project HYMERES for containment thermal hydraulics, KAERI is actively participating in an analytic working group. As an analysis tool for blind benchmarkes, the analysis code described in this paper was used. From the blind benchmark analyses, it was found that the code is very promising for hydrogen safety analysis. Currently, it is proposed to develop the code collaboratively in a hydrogen safety community based on an open-source strategy.

It is believed that accurate prediction of a hydrogen behavior during a severe accident in an NPP containment will reduce threat on the containment integrity from a hydrogen explosion.

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