THAI-HM2 Benchmark Study with STAR-CCM+ Code Simulation

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1. Introduction

After Fukushima's nuclear accidents, an interest in the nuclear safety has been increased around the world and researches. For this reason, for a maintenance and an enhancement of the nuclear containment, all of the nuclear power plant in Korea has been emphasized that it should be set up systems to guard against a destruction of the containment barrier by an over-pressure from a regulatory authority.
The Filtered Containment Venting System (FCVS) has been emphasized that it should passively retain fission product releases to environment and control the hydrogen produced in a severe accident. It is possible to have combustion or explosion of hydrogen by a convection flow, a diffusion process, and a condensation or a change of vapor and hydrogen in the local and global region of containment. When a FCVS is operating, *i.e.*, exhausting the containment atmosphere, it needs to check the gas components and hydrogen risk. However, it is hard to study a hydrogen risk in the containment scale because it has many complex phenomena and takes a long time to calculate.
Therefore, before predict a hydrogen risk of the nuclear containment scaled case, many researchers performed analyses with their codes for the THAI-HM2 experiment [1-2]. THAI Project is an experiment about Thermal hydraulics, Hydrogen, Aerosols, and Iodine by OECD/NEA organization from 2010. From among the series of THAI experiments, HM-2 experiment focused on the behaviors of hydrogen in the steam-air environment [3]. In this study, thus, the hydrogen mixing behavior is studied with the STAR-CCM+ code while validating the code to the THAI-HM2 experiments, in order to find out a best practice model for physics models such as condensation, turbulence, and gas models as well as mesh structures.
The rest of this paper is organized as follows: In the next section, a brief scheme of Computational Fluid Dynamics (CFD) code simulations using a STAR-CCM+ code is introduced. Next, our simulation results especially focused on the behaviors of the pressure and the mole fraction of hydrogen. Conclusions are discussed in the last section.

2. Simulation Scheme

In order to validate the code with the benchmark study about the THAI-HM2 experiments, we performed Computational Fluid Dynamics (CFD) code simulation using a STAR-CCM+ code [4] that is developed in the CD-adapco (Siemens PLM software) Inc.

2.1 Design, Mesh, and Initial Conditions

The schematic initial conditions for the THAI-HM2 simulation described in Fig. 1 and Table. I. The THAI-vessel is structured with a height of 9.2 m and a diameter of 3.2 m. The total free volume of the THAI vessel is 60 m3. While the tetrahedral mesh with near 150,000 EA about half geometry is used in advanced study, the trimmed cell mesh with 171,570 EA about full geometry is used in this study (for reference in Fig. 2). A simulation is done with the time step as 0.1 sec, turbulent model as k-w (SST) and k-e model, and an equation of states as an ideal and real gas property (Redlich-Kwong model). With these initial condition, simulations are consist of 2 phases. In the phase 1, hydrogen mixture is injected at 4.8 m in upward direction from 0 sec to 4200 sec and it has break-time during 120 sec. In the phase 2, Steam is injected at 1.8 m in upward direction from 4320 sec to 6820 sec.

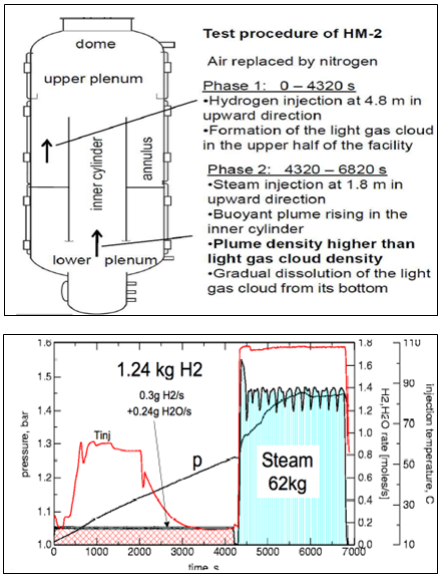

Fig. 1. Schematic initial conditions of THAI-HM2 simulation.

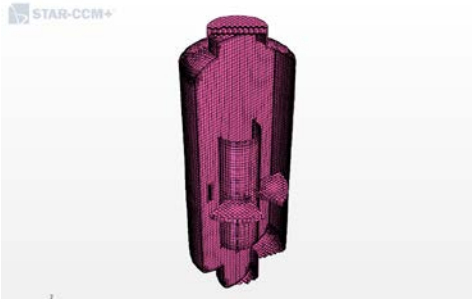

Fig. 2. Mesh structure (Trimmed cell mesh, 171,570 EA).

Table I: Initial conditions of THAI-HM2 simulation

	Value
Pressure	1.008 bar
Mean Wall / Gas Temp.	21 C 20 C
Initial Gas Composition	N2 : 0.977 O2 : 0.011 Steam : 0.012
Phase 1 Inj. Rate / Temp.	0.3 g/s (H2) + 0.24 g/s (Steam) ~ 45 C
Phase Inj. Rate / Temp.	24.1 g/s (Steam) ~ 107.5 C

2.2 The Bulk Condensation Model

The bulk condensation phenomenon is occurred when the partial vapor pressure is larger than the saturation pressure. In this study, the bulk condensation is modelized with field functions of STAR-CCM+ code. A process of the bulk condensation model is as follows. First, the partial vapor pressures P_{vap} and the saturation pressures P_{sat} of each cells are calculated as follows, and compared.

$$P_{vap} = \${AbsolutePressure} \times \${MoleFractionH2O}[Pa]$$

$$P_{sat} = \exp\left(20.386 - \frac{5132}{T_g}\right)[Pa]$$

when the partial vapor pressure P_{vap} is larger than the saturation pressure P_{sat}, the bulk condensation occurs with the condensation heat Q and the condensation mass $\dot{m}_{con}$ is as follows,

$$Q = \frac{\rho c_{p,g}(T_{eq} - T_g)}{\tau}$$

$$\dot{m}_{con} = \frac{\rho c_{p,g}(T_{eq} - T_g)}{(H_v - H_{eq,l})\tau} = \frac{Q}{H_v - H_{eq,l}}$$

where ρ is the density of the mixture gas, $c_{p,g}$ is the specific heat of the mixture gas, T_{eq} is the temperature in the equilibrium state (*i.e.*, the boiling temperature with the current partial vapor pressure), T_g is the temperature of the mixture gas, τ is the time coefficient (*i.e.*, the implicit unsteady time step), H_v is the vapor enthalpy with T_g, and $H_{eq,l}$ is the enthalpy in liquid state with T_{eq}, respectively.

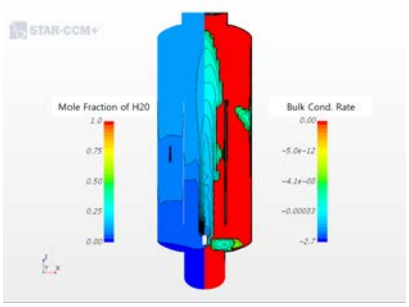

Fig. 3. The mole fraction of H20 and the bulk condensation rate at 5,700 sec. The bulk condensation is occurred at not only the ideal bulk region and but also layers that is close to an wall surface.

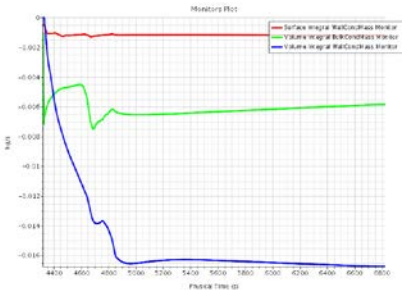

Fig. 4. The temporal evolution of the each condensation rate: the ideal wall condensation (red line, ~2.5 kg), the ideal bulk condensation (green line, ~15 kg), and the quasi-wall condensation (blue line, ~42 kg).

These calculated condensation heat Q and the condensation mass $\dot{m}_{con}$ are adjust with the source term of the energy equation and the continuity equation. In this case, the condensation mass $\dot{m}_{con}$ is just minus from the vapor mass of the control volume, and it is not assumed behaviors and the mass of the liquid.

However, this model has several weakness. As shown in Fig. 3, the bulk condensation is occurred at not only the ideal bulk region that is closed to the injected steam portion but also the layers that is closed to the wall surface. Therefore, we separated the bulk condensation at the cells within 0.3 m closed to the wall surfaces from the ideal bulk condensation as the quasi-wall condensation. (For reference in Fig. 4)

2.3 Wall Condensation Model

While the wall condensation of advanced study with an ANSYS-CFX code is modelized with an internal developed model, our wall condensation is modelized with field functions of STAR-CCM+ code like the preceding bulk condensation model.

The wall condensation mass $\dot{m}''$ on the wall is as follows,

$$\dot{m}'' = h_{m,0} \ln \frac{Y_{nc,b}}{Y_{nc,i}}$$

where $Y_{nc,b}$ and $Y_{nc,i}$ are the mass fraction of the non-condensable gases evaluated in the bulk region and the interface, respectively. $h_{m,0}$ is the mass transfer coefficient when the condensation mass flux tends to zero, and defined as follows,

$$h_{m,0} = Sh \frac{\rho_{m,b} D_{v:m,b}}{l}$$

where Sh is the Sherwood number that is calculated from the analogy using the McAdams correlation for the heat transfer under the turbulent natural convection as follows,

$$Sh = 0.13 Gr^{0.33} Sc^{0.33}$$

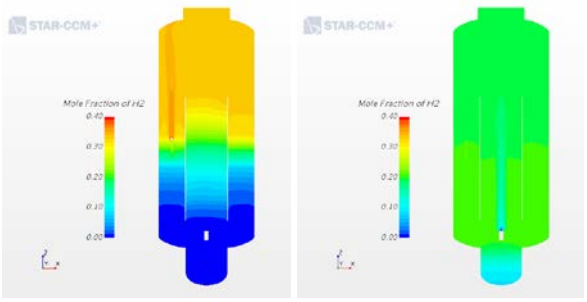

Fig. 5. The mole fraction of hydrogen at t = 4,000 s (left) and at t = 6820 s (right). There are the hydrogen stratification phenomenon in the phase 1 and an erosion phenomenon of such stratificated layers in the phase 2.

The Grashof and Schmidt numbers are calculated as below,

$$Gr = \frac{g(\rho_{m,b} - \rho_{m,i})l^3}{\rho_{m,b}\nu_{m,b}^2}$$

$$Sc = \frac{\nu_{m,b}}{D_{v:m,b}}$$

where g is the gravity acceleration, $\rho_{m,i}$ is the density of the gas mixture evaluated at the interface, $\nu_{m,b}$ is the kinematic viscosity of the gas mixture evaluated in the bulk region. The density of the gas mixture evaluated at the interface is calculated using the ideal gas law, assuming that the water is at saturation and extrapolating the relative concentrations of the non-condensable gases from the bulk region.

3. Simulation Results

In THAI-HM2 experiments, there are the hydrogen stratification phenomenon in the phase 1, and the erosion phenomenon of such stratificated layers in the phase 2. For benchmark study with STAR-CCM+ code, as shown in Fig. 5, these phenomena are well simulated.

3.1 The Mesh and Time step Dependences

In the advanced study, as shown in Fig. 6, their results are well estimated by control of the mass transfer coefficient of the wall condensation model of MELCOR code, *i.e.*, by over-estimating about the wall condensation phenomenon. Therefore, they are concluded that ANSYS-CFX code are under-estimated about the wall condensation phenomenon.

However, in our simulation, as shown in Fig. 7, well-estimated results are obtained by using STAR-CCM+ code. Compared with the advanced study, there are only one difference on the mesh structure; whether the tetrahedral mesh or the trimmed cell mesh. That is, the poor-estimated results of the advanced study are because not an under-estimation of the code internal condensation model, but numerical errors. There are not a great dependence about time-step.

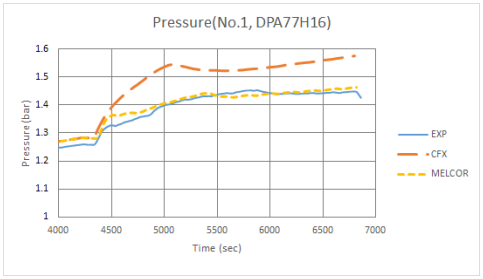

Fig. 6. The temporal evolution of the pressure of an advanced study [2]; experimental result (blue line), result using ANSIS-CFX code (orange line), result using MELCOR code with controlling mass transfer coefficient (yellow line).

3.2 The Turbulent Model Dependence

In our simulation, simulations with k-w (SST) turbulent model is set as base case and simulations with k-e model are additionally checked. In the simulations with k-w (SST) turbulent model, as shown in Fig. 8, the erosion time is reveal early in the phase 2. However, with k-e turbulent model, this erosion problem is eased off.

The turbulent Schmidt number is one of the controlling parameter in the CFD codes. It is defined as follows,

$$\frac{\partial(\rho_m x_i)}{\partial t} + \nabla \cdot (\rho_m \vec{v} x_i) = \nabla \cdot \left(\rho_m D_{L,i} + \frac{\mu_t}{Sc_t}\right)\nabla x_i + S_{x_i}$$

where ρ_m is the density of mixture gas, x_i is the mass fraction, $D_{L,i}$ is the laminar diffusion coefficient, μ_t is the turbulent viscosity, Sc_t is turbulent Schmidt number, and S_{xi} is the mass source term. In this case, the turbulent diffusion coefficient $D_{t,i}$ is defined as μ_t/Sc_t. If the turbulent diffusion coefficient is larger than the laminar diffusion coefficient, this value could have a significant role. This value has a default as 0.9 in STAR-CCM+, as 0.7~0.8 in ANSYS-CFX, and as 0.6 in FLUENT code. As shown in Fig. 9, this value make tiny difference in the THAI-HM2 conditions and the erosion problem is little eased off.

Whether the equation of state is the ideal gas property or the real gas property (Redlich-Kwong model) also did not make differences. (For reference in Fig. 10).

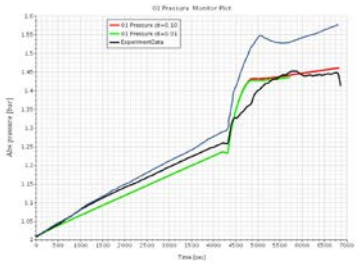

Fig. 7. The temporal evolution of the pressure; an experimental result (black line), an result using STAR-CCM+ code with dt = 0.1 s (red line), an result using STAR-CCM+ with dt = 0.01 s (green line), an result of the advanced study using ANSIS-CFX code (blue line). Compared with the advanced study, well-estimated results are obtained.

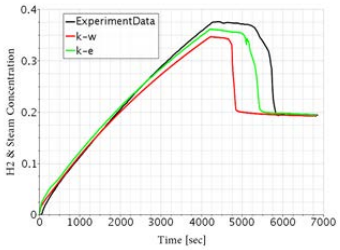

Fig. 8. The temporal evolution of the hydrogen concentration; a result using the k-w (SST) model (red line), a result using the k-e model (green line). With k-e turbulent model, the erosion problem is eased off.

3. Conclusions

THAI-HM2 benchmark studies are performed with STAR-CCM+ code, focusing on the mesh structures, turbulent models, and gas models. Numerical errors by a mesh type was found quite important, and controlling turbulent model could ease off the erosion problem. Whether the equation of state is the ideal gas property or the real gas property (Redlich-Kwong model) did not make differences.

With these insights, in the study about nuclear containment scaled cases, the polyhedral mesh is recommended because the heat transfer between solid structure and fluid flow region is significantly occurred. Also, such case could be that turbulent diffusion coefficient is larger than laminar diffusion coefficient, *i.e.*, the turbulent Schmidt number could have a significant role.

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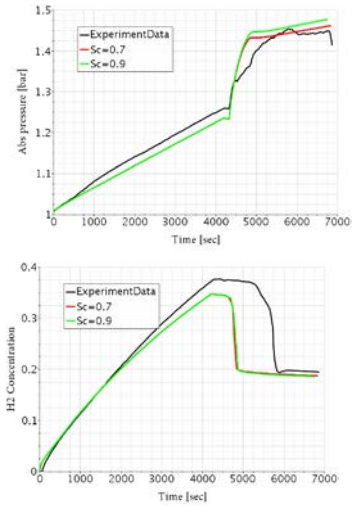

Fig. 9. The temporal evolution of (a) the pressure (b) hydrogen concentration; results using the turbulent Schmidt number as 0.7 (red line) and as 0.9 (green line). It make a tiny difference and the erosion problem is little eased off.

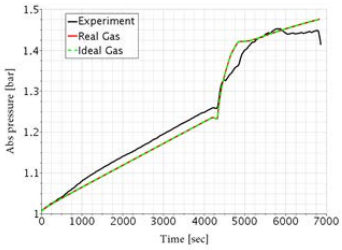

Fig. 10. The temporal evolution of the pressure; results using the equation of state as an real gas property (Redlich-Kwong model, red line), results using the equation of state as an ideal gas property (green line). Whether the equation of state is ideal or real has not differences.

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