Numerical Simulation of Hydrogen Behavior in the OECD-THAI HM-2 Experiment with Commercial Code

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1. Introduction

During severe accidents, chemical reaction between steam and zirconium produces hydrogen which is release into containment. If hydrogen concentration is higher than 4 % in containment then combustion is possible, and its concentration is higher than 10 % then detonation can occur which could threat the integrity of containment.

According to chapter 16 of Regulatory Guide, hydrogen concentration shall be lower to avoid wide flame acceleration and deflagration-to-detonation transition in containment.

Safety analysis to check the satisfaction of the Regulatory Guide have been conducted by Lumped Parameter code such as MAAP and MELCOR. However, it is questionable that it is enough to check if flame acceleration and deflagration-to-detonation transition occur only by LP code methodology.

For example, maximum cell size used in MAAP simulation of APR1400 Shin-kori unit 3 safety analysis is about 20,000 m3 in which hydrogen concentration is assumed to be uniform. However, it has not proven that the uniform hydrogen concentration in that large size cell is reasonable. It cannot completely rule out the possibility that LP simulations say the hydrogen concentration meets the regulatory guide but its concentration in the cell is actually locally so high that detonation could be possible. Therefore, we think that high resolution analysis methodology for hydrogen distribution is needed as supplement mean in safety analysis.

This is a preliminary study to examine the feasibility to use a three-dimensional CFD (Computational Fluid Dynamics) tool in safety analysis of full-scale nuclear power plants. As the first step, hydrogen distribution behavior of the OECD-THAI HM-2 experiment is calculated and compared with the data.

2. OECD-THAI HM-2 Project

The THAI project is carried out by Becker Technologies in Germany. The HM-2 experiment in THAI-vessel is run using hydrogen as a working fluid. Also HM-experiment is compared with one-dimensional LP code and a three-dimensional CFD code. THAI-vessel is stainless steel construction had a height of 9.2 m, a diameter of 3.2 m, a volume of 60 m^3.

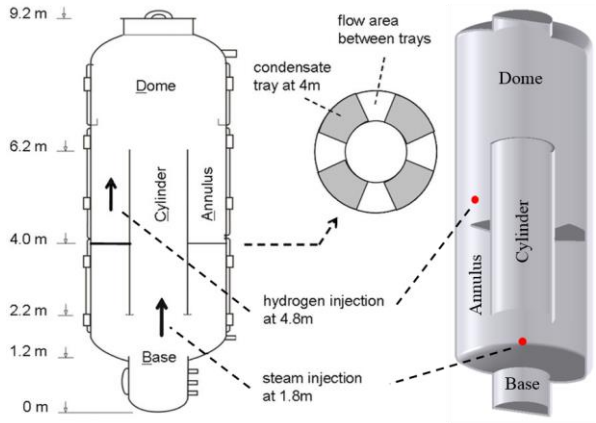

Fig. 1. THAI-vessel configuration of HM test and three-dimensional geometry applied in the numerical simulation

THAI-vessel configuration is shown in Fig. 1. Internal structures are inner cylinder of a diameter 1.4 m and the four condensate trays at the elevation of 4 m. The inner cylinder is open at both side [1].

At the start of the HM-2 test, the vessel atmosphere consists of 98 vol% nitrogen gas, 1 vol% oxygen and 1 vol% steam at ambient conditions (1 bar, 21 ◦C). The HM-2 test is run following two phases:

• Phase-1: hydrogen/steam injection and formation of a stable stratified hydrogen-rich gas layer in the upper part of the vessel (0–4300 s).

• Phase-2: steam injection, dissolution of the stratified hydrogen-rich gas layer and mixing of the atmosphere in the vessel (4300–6860 s).

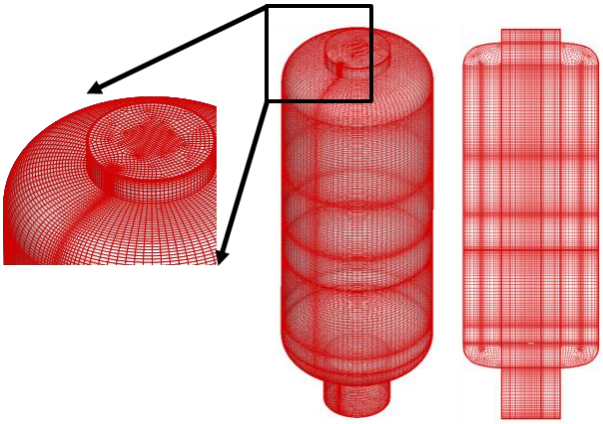

Fig. 2. The mesh system for numerical simulation of THAI-vessel

3. Numerical Simulation

2.1 Numerical Method

A commercial code is used for the three dimensional transient calculation in a grid system of the THAI-vessel model that is constructed by another commercial preprocessor software. The computation domain contained approximately 880,000 cells and the mesh system is shown in Fig. 2. This simulation is carried out with standard k-ε turbulence model with EWT and full buoyancy. For the pressure-velocity coupling, the SIMPLE algorithm is used. Continuity, momentum and energy equation are used as governing equations. Mixing of species is handled with species transport equation.

2.2 Bulk Condensation Model

The applied bulk condensation model in this study take into the following processes:

1) Calculate partial pressure of vapor at each cell

$$P_{sat} = P_{cell} \times mole\ fraction\ of\ vapor$$

2) Calculate saturated temperature (T_{sat}) at each cell by Antoine equation using UDF. A, B, C is Antoine equation coefficient.

$$T_{sat} = \frac{B}{A - \ln P_{sat}} - C$$

3) Compare T_{sat} and T_{cell}.

$$T_{sat} > T_{cell} : Condensation$$

4) If condensation occurs, mass sink is calculated by Lee model [2]. Coff is time relaxation parameter and α is mole fraction.

$$Mass\ Sink[{}^{kg}/_{s \cdot m^3}] = coff \cdot \alpha_v \rho_v \frac{(T_{sat} - T_{cell})}{T_{sat}}$$

5) Calculate heat generation by phase change.

$$Heat\ Generation = Mass\ Sink \times Latent\ Heat$$

Lee model is included for multi-phase simulation in commercial code. However, this condensation model for single-phase flow is adapted by means of user-defined-functions (UDF). In this equation, Coefficient needs to be tuned and can be interpreted as a relaxation time. But Coefficient is usually not very well known. So coefficient can be properly tuned to match experimental data. Generally, the coefficient for condensation is 0.1 [4].

2.3 Geometry, Initial and Boundary Condition

The calculation model is based on the THAI-facility shown in Fig. 1**.** The applied initial conditions and boundary conditions are specified by existing study and listed in Table I [3]. Injection rate and temperature during phase-1 and phase-2 of the HM-2 test is extracted using digitizer. Extracted value is shown in Fig. 2. Then, Profile created from extracted value used as mass-flow-rate boundary condition in commercial code.

Table I. Initial and Boundary Conditions

Initial Condition	-	• Pressure : 1.008bar • Temperature - Gas: 20.7 ℃ - Wall: 21.7 ℃ • Composition - Nitrogen: 98 vol% - Vapor: 1 vol% - Oxygen: 1 vol%
Boundary Condition	Phase 01	• Time : 0 s ~ 4,200 s • Injection rate & Temperature - Fig. 3.
	Phase 02	• Time : 4,200 s ~ 6,820 s • Injection rate & Temperature - Fig. 3.
	Walls	• Temperature - 21.7 ℃ • No-slip

4. Numerical Simulation Results

Numerical simulation is conducted using geometry in Fig. 1. Comparison of HM-2 experiment and numerical simulation is shown in Fig. 4-5. Mutually, difference of HM-2 experiment and numerical simulation caused by condensation in phase-1 isn't indicated because vapor is very lower. However, different results is shown in phase-2. Mass of vapor and hydrogen in closed vessel is injected so pressure is steadily increased. However, pressure of numerical simulation is less than HM-2 experiment because condensation isn't sufficiently demonstrated. Similarly concentration of hydrogen in Fig. 5 is lower than HM-2 experiment. Similar tendency is indicated from comparison of HM-2 experiment and simulation.

5. Conclusions

In this study, a three-dimensional numerical simulation using commercial code is conducted and compared with the THAI HM-2 experiment in order to check the feasibility of CFD methodology in safety analysis of hydrogen distribution.

Similar tendency is indicated from the comparison between HM-2 experiment and current simulation. In the future, study will be continued improvement of Lee model and compare with another condensation model.

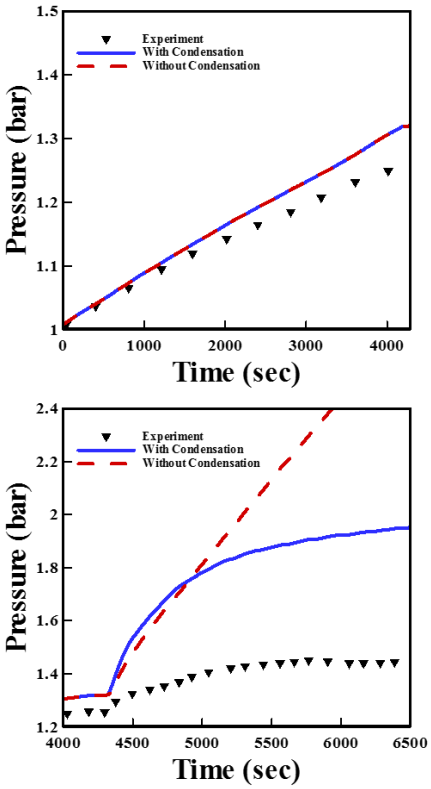

Fig. 4. Comparison of HM-2 experiment and numerical simulation during phase-1 (top) and phase-2 (bottom) in the THAI-vessel

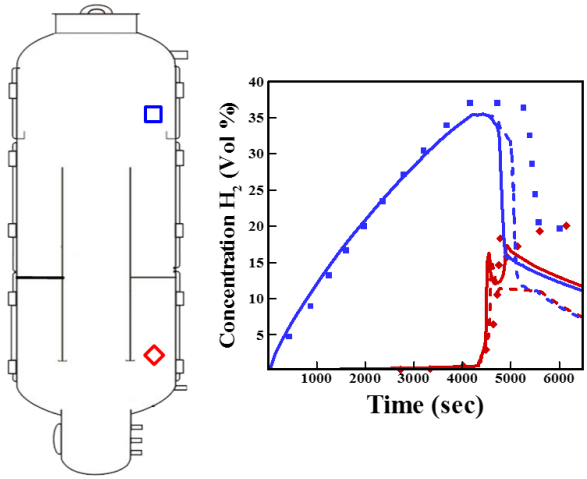

Fig. 5. Hydrogen concentrations in the THAI-vessel during 0-6,500 s as HM-2 experiment (symbols) and numerical simulation with condensation (solid lines) and without condensation (dashed lines)

REFERENCES

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