# CFD Analysis of the Hydrogen/Steam Behavior in the OECD-NEA THAI Test HM-2 experiment

Se-Hong Oh [a], Yong-Jin Cho [b], Seongnyeon Lee [b], Jung-Jae Lee[b], Choengryul Choi [a*]
[a]*ELSOLTEC, 2806 U-Tower, 120 Heungdeokjungang-ro, Giheung-gu, Yongin-si, Gyeonggi-do 16950, Korea*
[b]*Korea Institute of Nuclear Safety, 62 Gwahak-ro, Yuseong-gu, Daejeon 34142, Korea*
[*]*Corresponding author: crchoi@elsoltec.com*

## 1. Introduction

Hydrogen could be generated by active reactions of fuel-cladding and steam in the reactor vessel during a severe accident of a nuclear power plant, and released into the atmosphere inside the containment [1-3]. A local concentration of hydrogen which is higher than a flammability limit could lead to hydrogen combustion inside the containment. Therefore, it is important to predict local hydrogen concentration distribution for assessment of hydrogen combustion, deflagration and detonation risks.

When mixture of hydrogen, steam and non-condensable gases is released at a high energy level, very complex behaviors and phenomena occur, which include steam condensation and evaporation. In CFD (computational fluid dynamics) analysis, numerical modeling for condensation and evaporation phenomena is important to predict flows and local hydrogen concentration accurately.

In this study, a three-dimensional CFD analysis is carried out and compared with the results of the OECD-NEA THAI Test HM-2 experiment in order to verify adopted numerical models including condensation and evaporation models.

## 2. OECD-NEA THAI Test HM-2 experiment

OECD-NEA performed THAI (Thermal hydraulics, Hydrogen, Aerosol and Iodine) Project from 2007 for three years to address open questions concerning the behavior of hydrogen, iodine and aerosols in the containment of water cooled reactors during severe accidents [4-7]. In order to investigate the erosion of a stable atmospheric stratification layer by a buoyant plume from below, which has a higher density than the stratification layer, the experiment HM-2 in the THAI containment test facility was run and selected as subject of a code benchmark. A detailed evaluation of the experiment, the results of the blind benchmark calculations and a short description of open post calculations are given in [5-7].

"The HM-2 experiment was carried out in the THAI-facility (Fig. 1), which is operated by Becker Technologies in Eschborn, Germany. The cylindrical containment has a height of 9.2 m, a diameter of 3.2 m and a volume is 60 m³. The thickness of the steel walls is generally 0.022 m, at the top cover it is 0.12 m. The facility is insulated by rockwool with a thickness of 0.12 m. Important internal structures are the inner cylinder (diameter 1.4 m) and the four condensate trays at the elevation of 4 m. The inner cylinder is open at both ends and forms an annular gap with the vessel wall. The condensate trays form a mid floor, blocking 2/3 of the horizontal flow area of the annular room [7]".

The test procedure began with ambient conditions (1 bar, 21 °C) and covered the following phases (Fig. 2):

① Time 0 - 4320 s (Phase 1): Hydrogen injection (rate 0.286 g/s) from a pipe with a diameter of 0.0285 m in the annular gap, directed vertically upward, at the elevation of 4.8 m.
② Time 4200 - 4320 s: There were no injections.
③ Time 4320 - 6820 s (Phase 2): Steam injection (rate 24.1 g/s) from a nozzle with a diameter of 0.138 m below the inner cylinder, directed vertically upward, at the elevation of 1.8 m.

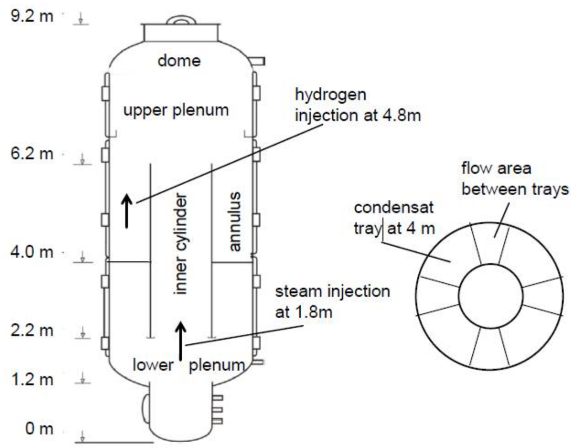



Fig. 1. THAI vessel, configuration of HM tests.

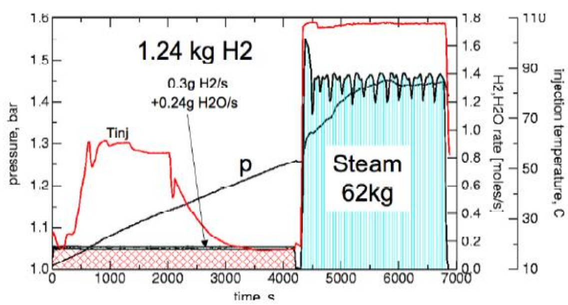



Fig. 2. Test procedure of HM-2.

## 3. Numerical Methods and Conditions

*2.1 Numerical Method*

A three dimensional transient calculation is carried out in a commercial CFD software, CFX version 5 (ANSYS Inc.) [8]. Fundamental governing equations are the continuity equation, momentum equations and energy equation. To consider turbulent effects, the SST (Shear Stress Transport) model is included. Mixing of species (nitrogen, hydrogen, oxygen, and vapor) and multi-phase flows are additionally handled with the species transport equation and the algebraic slip model (ASM), respectively. Compressibility effect of gases and buoyancy are included in this analysis.

*2.2 Treatment of Steam Condensation/Evaporation*

2.2.1 Bulk Condensation

Bulk condensation is modeled as follows.

① Calculates saturated pressure ($P_{sat}$) at each cell by Antoine equation

$$p_{sat} = p_{\text{scale}} \exp\left(A - \frac{B}{T_P + C}\right)$$

② Calculates partial vapor pressure at each cell
$P_{partial,vapor}$=$P_{abs}$*Vapor Molar Fraction

③ Compares $P_{sat}$ and $P_{partal,vapor}$
$P_{partail,vapor}$>$P_{sat}$: condensation

④ If condensation occurs, calculates mass and heat(energy) transfer rates due to the condensation by the heat balance equation

$$m_{vap} = \frac{\rho c_{pmix}\left(T_{eq} - T_{gas}\right)}{H_{VT} - H_{LT_{eq}}}$$

$$Q = \rho\, c_{pmix}\left(T_{eq} - T_{gas}\right)$$

⑤ The calculated mass transfer rates are treated as a sink for steam and as a source for liquid droplet phase. The latent heat due to the phase change is considered a source in the energy equation.

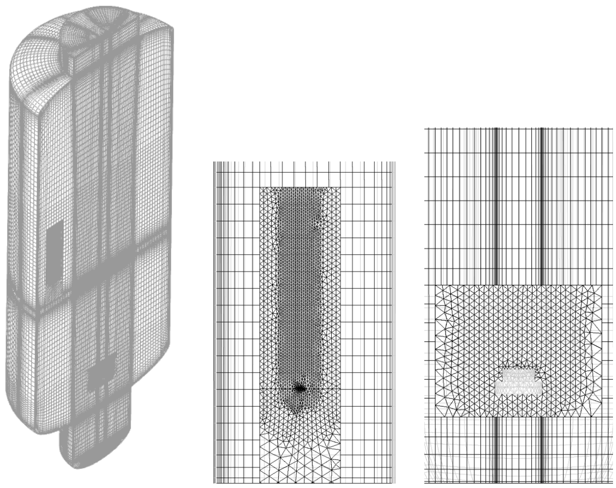
2.2.2 Wall Condensation

Wall condensation phenomenon of steam (vapor) has been modeled with a wall condensation model loaded in CFX as follows [8].

$$M_B = W_B J_B = m_B \ln\left(\frac{1 - X_B(\delta)}{1 - X_B(0)}\right)$$

$$m_B = \frac{W_B}{W_m}\frac{D_{AB}\rho_m}{\delta}$$

In this model, the condensation near the walls is assumed to occur within only one grid layer adjacent to the walls and the mass and energy sink due to the condensation are implemented within the layer. The mass and energy of condensed water are not treated and



(a) all (0.15 millions) (b) $H_2$ injection nozzle (c) Steam injection nozzle
Fig. 3. Mesh system.

a condensed film is not considered [1,8].

2.2.3 Evaporation

Evaporation is modeled as follows.

① Calculates saturated pressure ($P_{sat}$) and temperature ($T_{sat}$) at each cell by Antoine equation

$$p_{sat} = p_{\text{scale}} \exp\left(A - \frac{B}{T_P + C}\right)$$

② Calculates partial vapor pressure at each cell
$P_{partial,vapor}$=$P_{abs}$*Vapor Molar Fraction

③ Estimates whether evaporation occurs
$P_{partail,vapor}$<$P_{sat}$ & $T_{gas}$ < $T_{sat}$ : evaporation

④ If evaporation occurs, calculates mass and heat(energy) transfer rates due to the evaporation by the mass transfer equation

$$\frac{dm_P}{dt} = \pi\, d_P\, \rho\, D\, \text{Sh}\, \frac{W_C}{W_G} \ln\left(\frac{1 - X_s^V}{1 - X_{\text{vap}}^V}\right)$$

$$\frac{dS}{dt} = -\frac{dm_P}{dt}$$

⑤ The calculated mass transfer rates are treated as a source for steam and as a sink for liquid droplet phase. The latent heat due to the phase change is considered a heat sink at each cell.

*2.3 Geometry and Initial/Boundary Conditions*

The calculation model including mesh system is shown in Fig. 3, which is based on the THAI-facility shown in Fig. 1. Smaller meshes are inserted around the injection nozzles and walls. Initial and boundary conditions are listed in Table 1, which are identical with the HM-2 experiment conditions, but the injection rate and temperature curves of $H_2$ and steam are slightly simplified [5,7].

Table 1. Initial and boundary conditions

| | | |
|---|---|---|
| I/C | - | ･Pressure: 1.008bar<br>･Temperature<br>- Gas: 20.7 ℃<br>- Wall: 21.7 ℃<br>･Concentration<br>- Nitrogen: 97.7 vol%<br>- Vapor: 1.2 vol%<br>- Oxygen: 1.1 vol% |
| B/C | $H_2$ injection nozzle | ･Time: 0 s ~ 4,200 s<br>･Injection rate<br>- $H_2$: 0296 g/s<br>- Steam: 0.24 g/s<br>･Temperature: 45 ℃ |
| | Steam injection nozzle | ･Time: 4,320 s ~ 6,820 s<br>･Injection rate<br>- $H_2$: 0 g/s<br>- Steam: 24.1 g/s<br>･Temperature: 107.5 ℃ |
| | Walls | ･Temperature<br>- Wall: 21.7 ℃<br>･No-slip |

## 3. CFD Results

A three-dimensional CFD analysis is carried out based on the geometry and test conditions of OECD-NEA THAI Test HM-2 experiment. The flows and local distributions of H2, vapor and temperature inside the vessel are shown in Fig. 4. As shown in Fig. 4(b), hydrogen accumulated in the top of the vessel at 4,000 sec and 4,500 sec. The concentration of hydrogen increases according to the elevation. The concentration of steam increases gradually after 4,500 sec. Also, the erosion of a stable atmospheric stratification layer is found during this period due to a buoyant plume from below.

The pressure, H2 concentration and temperature variations monitored at the monitoring points (for the point locations, Ref. [5] and Ref. [7]) during the CFD simulation are plotted in Fig. 5 with the HM-2 experiment data. The comparison between the CFD results and HM-2 experiment data has shown a good reasonable agreement physically.

## 4. Conclusions

In this study, a three-dimensional CFD analysis has been carried out and compared with the OECD-NEA THAI Test HM-2 experiment in order to verify adopted numerical models including condensation and evaporation models. This CFD simulation has predicted flows, temperature, pressure, species concentrations and so on inside the THAI vessel. The comparison between the CFD results and HM-2 experiment data has shown a good reasonable agreement physically. The numerical models adopted in this CFD simulation would be applicable for further study.

## REFERENCES

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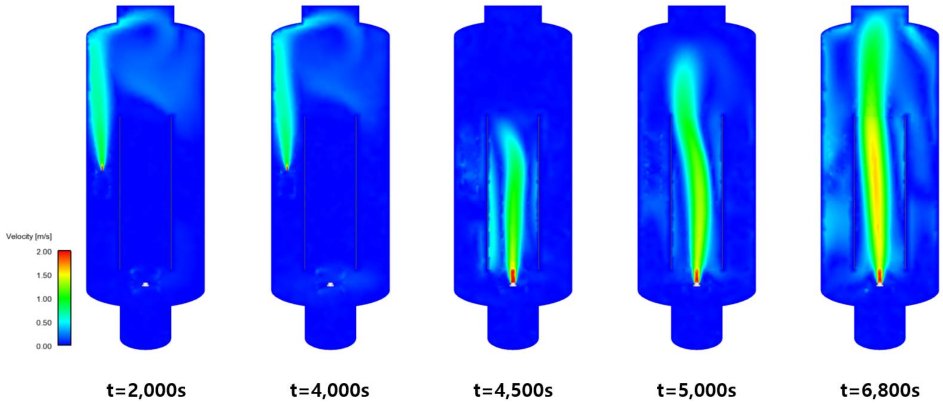
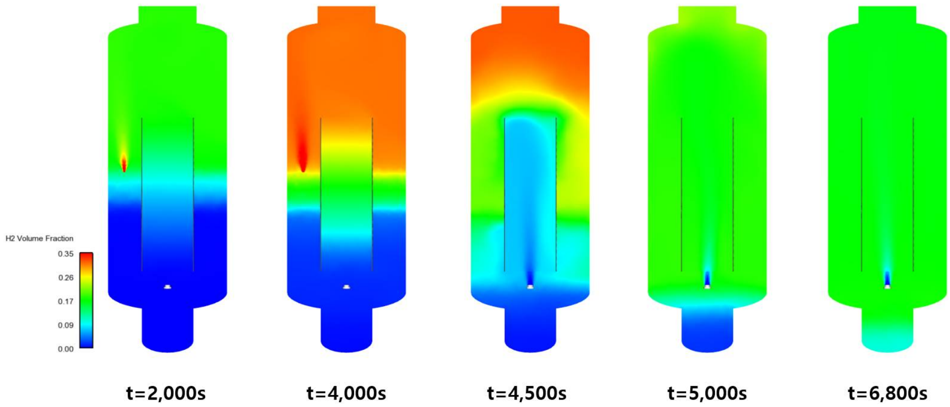
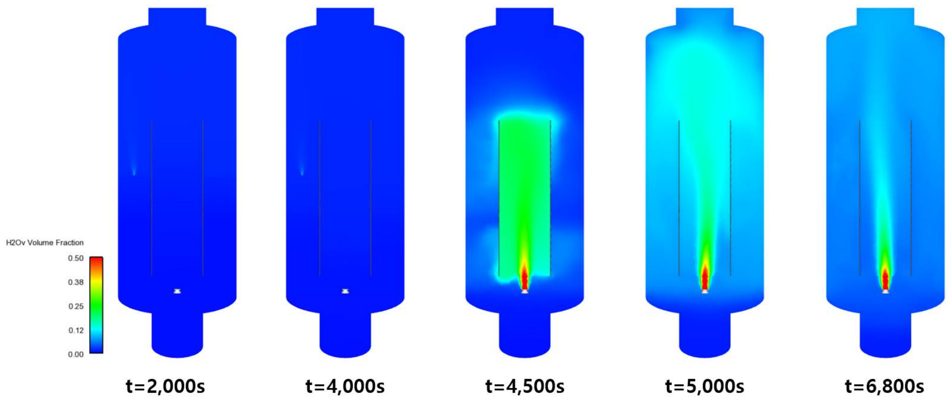
[8] CFX manual, ANSYS CFX, version 5



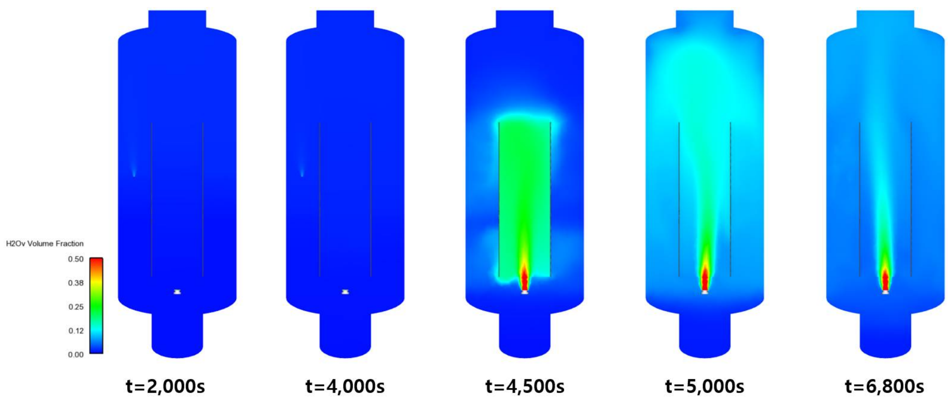

(a) Velocity magnitude




(b) $H_2$ distribution



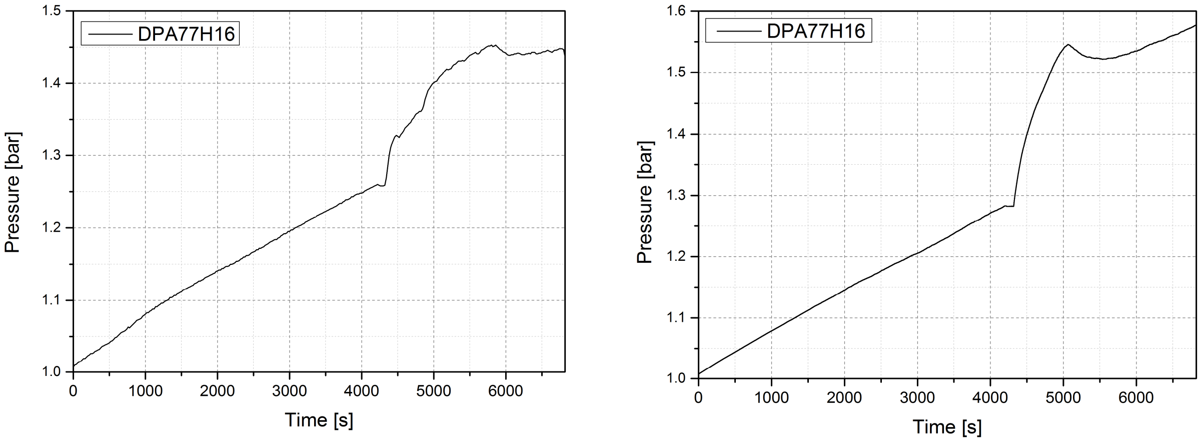

(c) Vapor distribution



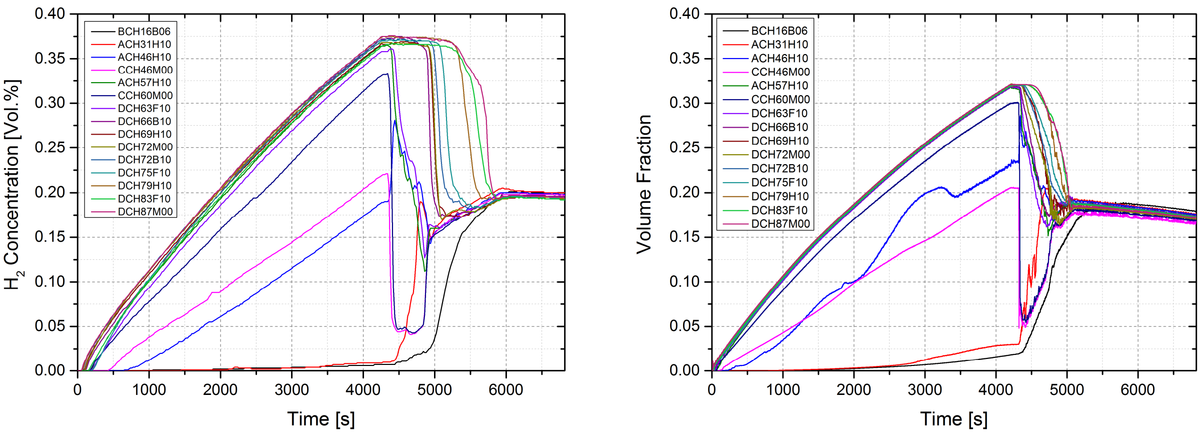

(d) Temperature distribution

Fig. 4. Calculation results (CFD).

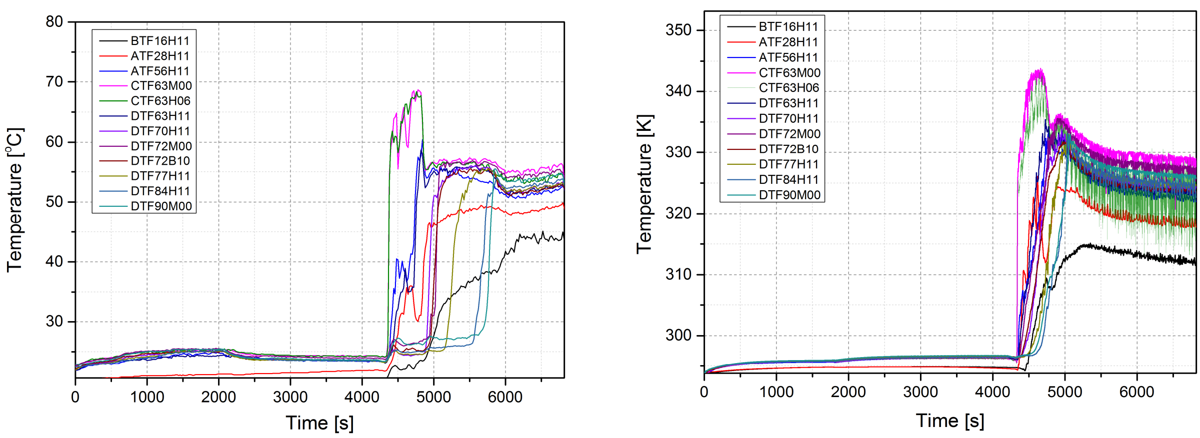
**Experiment HM-2** **CFD (Current Study)**




(a) Pressure




(b) $H_2$ concentration




(c) Temperature

Fig. 5. Comparison between HM-2 experiment and CFD *.

* The locations of the monitoring points are listed in Ref. 5 and 7.