# Simulations of a Hydrogen Combustion at Wet Condition using OpenFOAM

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## 1. Introduction

In this study, the propagation rate and pressure of premixed hydrogen flames were calculated to ensure the safety of NPP containment from hydrogen flames with various water vapor concentrations, and is based on an experiment conducted by the OECD THAI program as a benchmark. In the situation of a NPP accident, it is difficult to predict the environment inside the containment because it varies from completely dry condition to saturated due to water vapor leakage. The THAI-HD test series [1] was conducted to understand the behavior of a deflagrating hydrogen flame with varying amounts of water vapor. The experimental cases in which the simulation was conducted are shown in the table below.

Table I: Experimental Cases

| Case | HD-15 | HD-22 | HD-24 |
|---|---|---|---|
| $H_2$ vol % | 9.9 | 9.9 | 9.8 |
| $H_2O$ vol % | 0 | 25.3 | 48 (saturated) |
| Equivalent ratio | 0.26 | 0.36 | 0.55 |
| Pressure | 1.504 bar | 1.487 bar | 1.472 bar |
| Gas temperature | 92.5 ℃ | 91.9 ℃ | 90.3 ℃ |

The hydrogen combustion experiments in Table 1 were performed in the vessel in Figure 1. All three experiments ignite at the bottom of the vessel and the flame propagates upwards. Before ignition, the recirculation fan is removed from the vessel.

## 2. Methods and Results

The simulation was performed with XiFoam, a solver that modified the radiation effect and laminar flame speed in OpenFOAM-v1906 [2]. The flamelet based combustion model has been applied to XiFoam. See the following reference for details on this combustion model and for calculation of laminar flame speed [3, 4].

### *2.1 Simulation set-up*

The 3D mesh created using the OpenFOAM utility-snappyHexMesh consists of 936,246 hexahedral cells (Figure 2). Simulations were performed in OpenFOAM-v1906 with XiFoam, a modified solver for radiative effects, laminar flame velocity and mass fraction of water vapor [4, 5]. The models used in the simulation are summarized in Table 2.

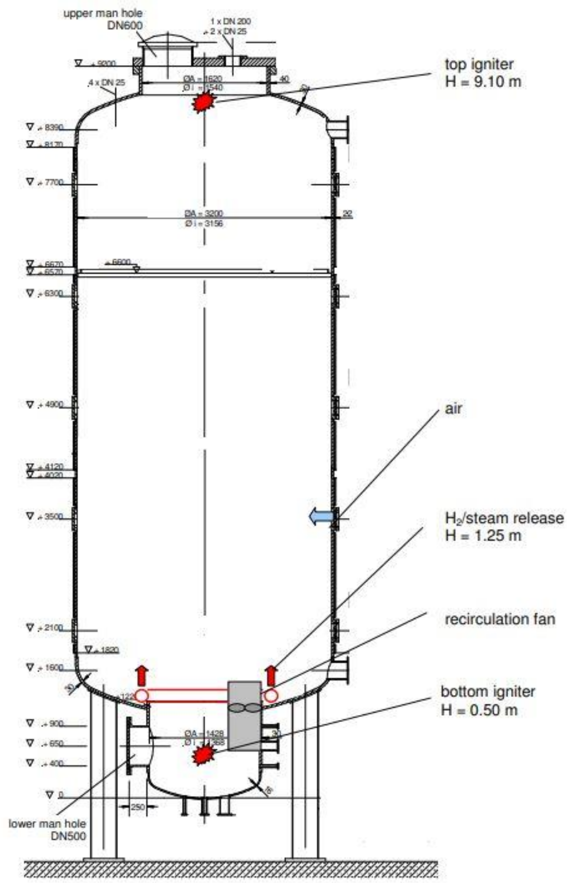


Fig. 1. THAI-HD test facility

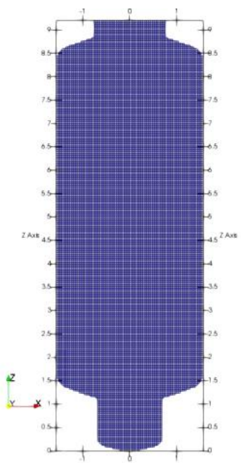

Fig. 2. Generated mesh of THAI-HD test facility

Table II: Simulation set-up

| Solver | XiFoam |
|---|---|
| Combustion model | Flamelet |
| Turbulent model | k-omega SST |
| Radiation model | P1 |
| Cells in mesh | 936,246 (100% Hexahedral) |
| Unit cell size | 40 mm |

### *2.2 Flame propagation rate*

Figure 2 shows the contours of the flame over time measured in the experiment. The time at each location is the moment the flame reaches. Based on this, the time recorded at each height and the CFD results are shown in a graph in Figure 3.

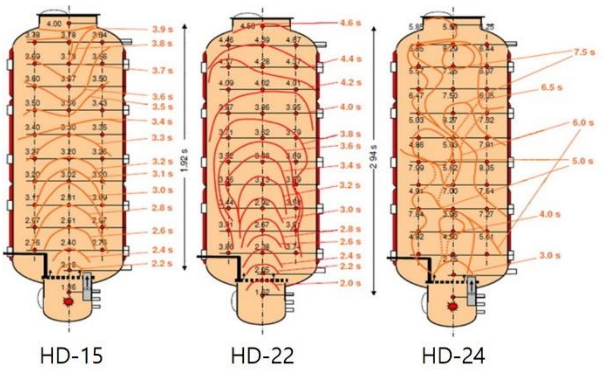

Fig. 2. Contours of flame propagation

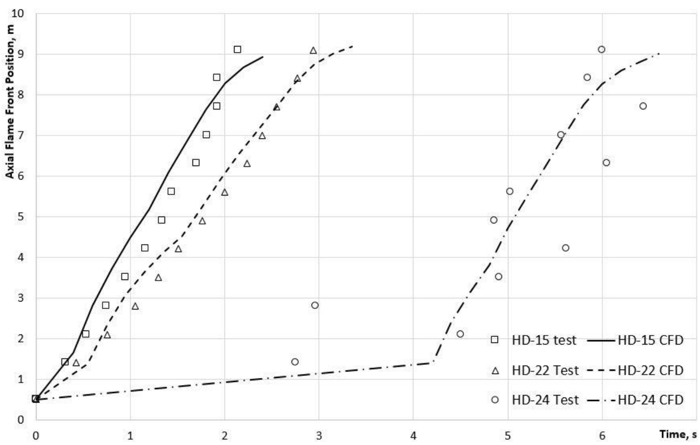

Fig. 3. Flame front propagation

As the content of water vapor increased, the propagation speed of the flame slowed down. This trend is also observed in simulation results using the modified XiFoam.

The result in simulations showed a tendency that the propagation speed of the flame increased until it reached 8 m and then decreased after reaching 8 m.

Compared to the HD-15, HD-22 experiments, the HD-24 showed that the flame propagation was very unstable due to saturated steam. Nonetheless, XiFoam predicted the approximate trend well.

### *2.2 Pressure rise*

The figure 4 is the result of the pressure inside the vessel due to the hydrogen flame.

Like the propagation of the flame surface, the pressure was also affected by the water vapor content. As the amount of water vapor increased, the maximum pressure due to the flame inside the vessel decreased. The general pressure rise trend and maximum pressure were well predicted. But in the simulations of HD-15 and HD-22 cases, the reduction rate after reaching the maximum pressure was smaller. And the maximum pressure in HD-24 was predicted higher than in the experiment. These differences come from the radiating effect of water vapor and heat transfer to the vessel wall. In experiments, it may be that water vapor has absorbed a greater amount of radiation heat than predicted in the simulation.

And in CFD, since the wall condition was fixed with a constant temperature and only convective heat transfer was applied without considering conjugate heat transfer. So the heat loss to the wall was also predicted less than in the experiment.

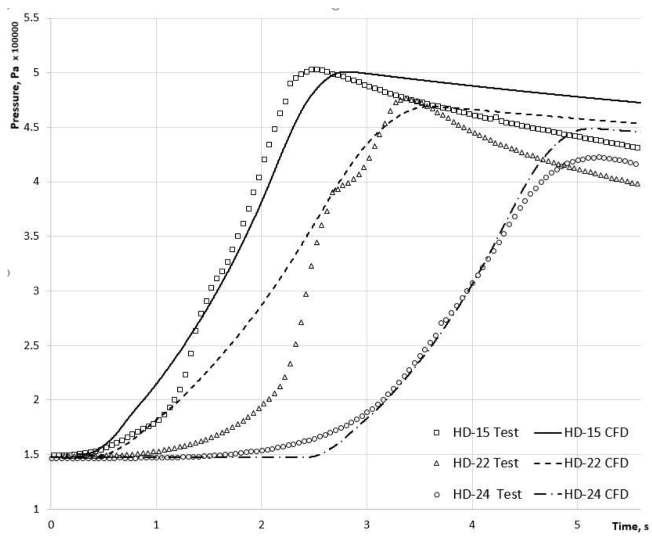

Fig. 4. Pressure rise trend

## 3. Conclusions

As part of a study on hydrogen flame behavior for NPP safety, a benchmark simulations of THAI HD-15, 22 and 24 experiments were performed using the modified XiFoam. Both the flame propagation speed and pressure results of the gas mixed with water vapor and hydrogen showed similar trends to the experiment. However, there was a difference due to the radiation effect and the heat transfer to the wall. The heat transfer area will be improved for more accurate hydrogen combustion simulation.

## REFERENCES

[1] OECD/NEA THAI Project, Hydrogen and Fission Product Issues Relevant for Containment Safety Assessment under Severe Accident Conditions, Final report, NEA/CSNI/R(2010)3, 2010
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[3] Weller, H. G. "The development of a new flame area combustion model using conditional averaging." Thermo-fluids section report TF 9307 (1993).
[4] S. Kim and J. Kim, “Simulation of Wet Hydrogen Combustion using Flamelet model in OpenFOAM.” KNS Spring Meeting (2020).
[5] S. Kim and J. Kim, “CFD Simulation of Flame Propagation Speed for Premixed Hydrogen Combustion using Flamelet model in OpenFOAM.” KNS Autumn Meeting (2020).