CFD Analysis for H_2 Flame Propagation during Spray Operation in the THAI Facility

Hyung Seok Kang [a*], Seong-Wan Hong [a], Sanjeev Gupta [b]
[a]*Korea Atomic Energy Research Institute, 989-111, Daedeok-daero, Yuseong, Daejeon, 305-353, Republic of Korea*
[b]*Becker Technologies GmbH, Koelner Strasses 6, 65760 Eschborn, Germany, gupta@becker-technologies.com*
[*]*Corresponding author: hskang3@kaeri.re.kr*

1. Introduction

The operation of a spray system may reduce a possible local high hydrogen concentration and induce a flame quenching effect in case of a hydrogen deflagration in the containment of nuclear power reactor. Unfavorable effects of the spray operation might be steam condensation which increases the volumetric concentration of the hydrogen with the threat of a more severe combustion in case of an ignition, and enhanced gas turbulence generated by the falling droplets which increases a flame speed. In this paper discussion is focused on the three tests HD-30, HD-31, and HD-32.1 conducted in the THAI test facility to investigate the influence of water spray operation on hydrogen deflagration behavior. Test results have been extensively used by the project partners for further development and validation of computational codes within the frame of the OECD THAI-2 project. In order to quantify the influence of spray operation on hydrogen deflagration behavior, test results are compared with the reference tests conducted with same initial thermal-hydraulic conditions but without spray in the frame of OECD-THAI project [1].

2. Experimental Research [2]

2.1 Test Facility

Main component of the facility is a cylindrical stainless steel vessel of 9.2 m height and 3.2 m diameter with a total volume of 60 m³ (Fig. 1). The vessel outer wall is completely enveloped by a 120 mm rockwool thermal insulation. A full cone whirl spray nozzle was used for the tests. The spray nozzle outlet was positioned vertically downward at elevation H = 7.4 m in the geometric center of the vessel. The spray nozzle location inside the vessel gives a ratio of nozzle injection height to the total vessel height of 0.8, which is a ratio similar to that in a real PWR containment. A spray angle of 30^{o} was selected to exclude any change in spray patterns due to interactions with the vessel walls. An air-driven axial fan is installed in the lower plenum of the vessel to allow homogenization of the vessel gas atmosphere (air-steam-H_2 mixture) prior to the ignition in tests HD-30 and HD-31. A start of the ignition is done about 10 – 15 min after ending the mixing fan operation. In test HD-32.1, homogenization of the vessel atmosphere was achieved by means of a convective flow generated by heating the sump compartment walls to about 3 ^{o}C higher than the other vessel walls.

A remotely controlled arc igniter is installed in the sump compartment at an elevation of 0.5 m. The ignition energy delivered by the igniter in the tests may vary between 0.6 – 1.5 mJ. The local hydrogen concentration in the vessel is measured by a continuous sampling system at 15 locations prior to and after the hydrogen deflagration test. To monitor the flame front propagation and flame temperature during hydrogen combustion, 43 fast sheathed thermocouples with outer diameter 0.5 mm are installed at 13 different elevations in the vessel. The combustion pressure transient is measured with one slow and two fast pressure transducers. The measurement uncertainty of gas concentration, temperature, and pressure is shown in Table 1.

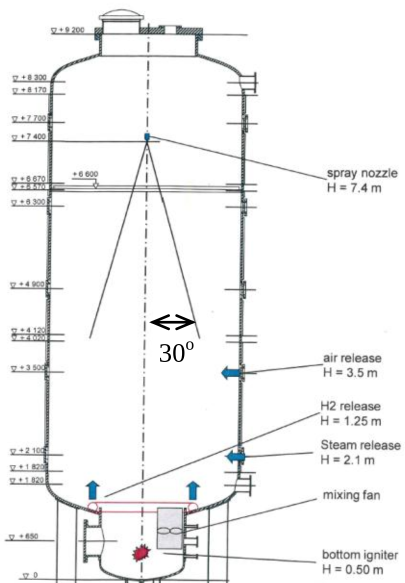


Fig. 1. THAI facility for Tests HD-30 to HD-32.1

Table 1: Uncertainty of Measuring Devices

Gas concentration	Thermocouple	Pressure
±0.5 vol%	±2.5 ^{o}C up to 333 ^{o}C ±0.75% above 333 ^{o}C	±4 mbar

2.2 Test Specification and Test Procedure

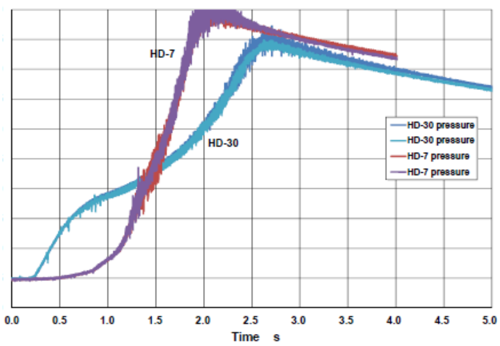
Table 2 summarizes the specified initial test condition for tests HD-30, HD-31, and HD-32.1. The spray water was operated at 2 s before the start of the ignition, and lasted 13 s (HD-30) and 28 s (HD-31 and HD-32.1) after the hydrogen combustion took place from the bottom region in the THAI facility. The preconditioning process was performed to meet the specified initial condition before the start of the spray operation.

Table 2: Initial Test Conditions as Specified

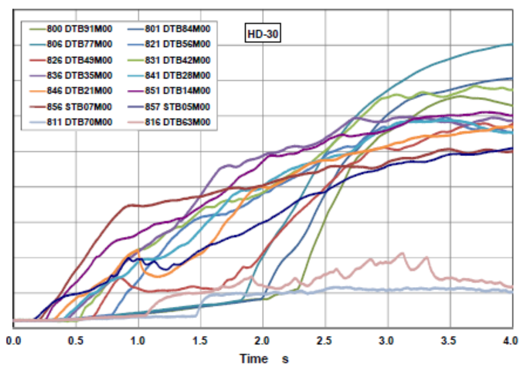
	HD-30	HD-31	HD-32.1
Vessel pressure	1.5 bar	1.5 bar	1.5 bar
Gas temperature	20 °C	90 °C	90 °C
H_2 concentration	10 vol%	10 vol%	10 vol%
Steam content	None	25 vol%	25 vol%
Spray water - Temperature - Mass flow rate - Droplet size(d_{32})	- 20 °C - 1 kg/s - 600 μm	- 20 °C - 1 kg/s - 600 μm	- 90 °C - 1 kg/s - 600 μm

2.3 Discussion on Test Results

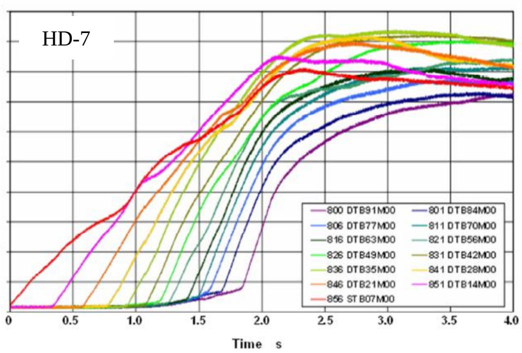
Fig. 2(a) shows the pressure transients for the test HD-30 and for comparison with that of the test HD-7. There are slight differences in the pressure increase time to reach the peak pressure plateau, the pressure increase behavior, and the peak pressure. The longer pressure increase time and the lower peak pressure of HD-30 give an indication of a suppressing effect of the spray. Fig. 2(b) and (c) show the temperature transients along the vessel centerline of the tests HD-30 and HD-7. Time to reach the peak temperature plateau is almost the same for both test, however, the peak temperatures are clearly lower for test HD-30 than for the test HD-7. Temperatures show a continuous increase for the test HD-7, whereas for the test HD-30 temperature shows a temporary decrease in the lower part of the vessel, sensors 826, 846 and 857. The sensor 811 at H = 7.0 m and sensor 816 at H = 6.3 m in Fig. 2(b) exhibit very low temperatures. In this part of the vessel close to the centerline combustion is efficiently suppressed.



(a) Pressure transient (HD-30 vs. HD-7)

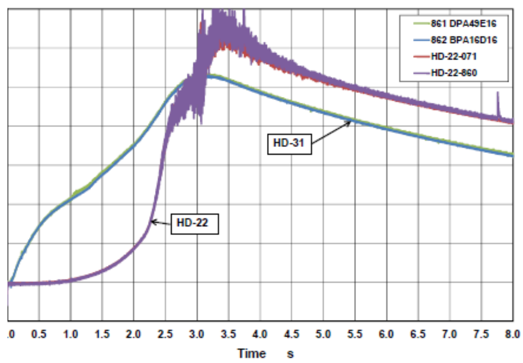


(b) Temperature transient (HD-30)

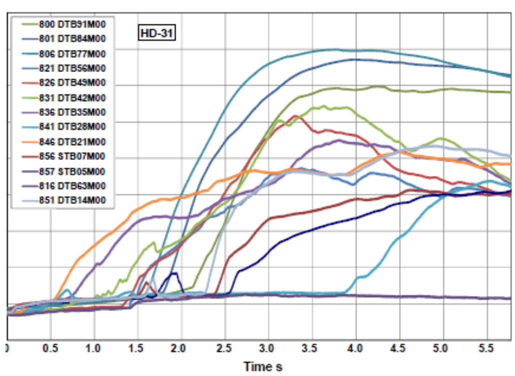


(c) Temperature transient (HD-7)

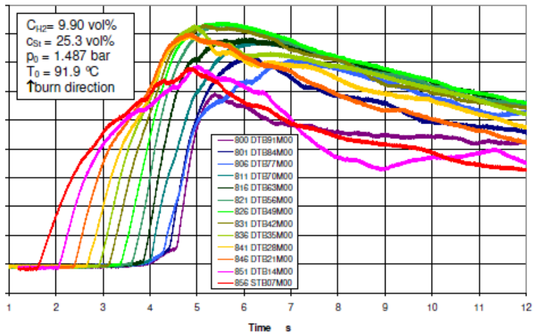
Fig. 2. Test results of HD-30



(a) Pressure transient (HD-31 vs. HD-22)

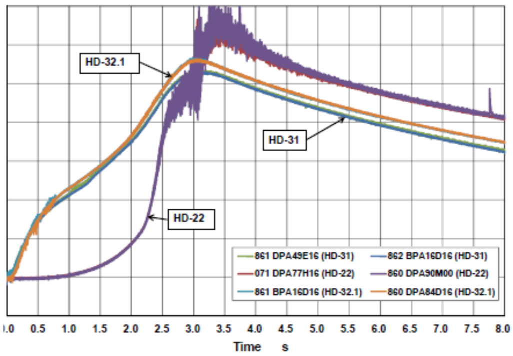


(b) Temperature transient (HD-31)

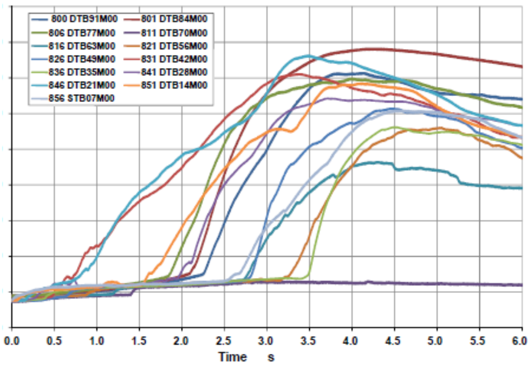


(c) Temperature transient (HD-22)

Fig. 3. Test results of HD-32



(a) Pressure transient (HD-22, HD-31, HD-32.1)



(b) Temperature transient (HD-32.1)

Fig. 4. Test results of HD-32.1

Fig. 3(a) shows the pressure transients for the test HD-31 and for comparison with that of the test HD-22. There is a slight difference in the pressure increase time to reach the peak pressure plateau. More marked is the difference in pressure increase gradient for HD-31, gradual increase at the beginning, then steep increase at a relatively constant increase gradient for HD-22. The peak pressure difference between HD-31 and HD-22 is in the same range as for HD-30 and HD-7, but the peak pressures are significantly lower for the tests with 25 vol% steam content, compared to HD-30 and HD-7 without steam. Fig. 3(b) and (c) show the temperature transients along the vessel centerline of the tests HD-31 and HD-22. Time to reach the peak temperature plateau is almost the same for both tests. However, the peak temperatures are clearly lower for HD-31 than for HD-22. Flame front propagation in the vessel centerline is steady for HD-22, but extremely unsteady for HD-31 with very low temperatures in the lower part of the vessel during the first 0.6 s of the combustion (sensors 846, 851, 856, and 857). The three other sensors outside of the vessel centerline at elevation H = 2.1 m and H = 2.8 m do not show this effect. Combustion in this region of the vessel is strongly suppressed by the spray, and the flame travels upwards outside of the vessel centerline.

Fig. 4(a) shows the pressure transients of the test HD-32.1, HD-31, and HD-22. As for the other tests with spray, pressure increase is almost instantaneous and steep, thereafter the pressure increase gradient becomes smaller. Compared to the test HD-22 and HD-31, the peak pressure of HD-32.1 is clearly lower than for the test without spray, but slightly higher than for HD-31. The cooling effect of the heated spray water is less pronounced, and the slightly higher combustion temperature produces a slightly higher peak pressure. Fig. 4(b) shows the temperature transients of the test HD-32.1. Time to reach the peak temperature plateau is almost the same for HD-31 and HD-32.1. However, the peak temperatures at elevations below H = 7.7 m are somewhat lower for HD-31 than HD-32.1, and flame front propagation in the vessel centerline is steady for HD-32.1, but unsteady for HD-31. The first significant temperature increase in the vessel centerline for HD-32.1 occurs at elevation H = 2.1 m, sensor 846, and H = 4.2 m, sensor 831, is similar to those of HD-31at elevation H = 2.1 m and H = 3.5 m. The temperature transient of HD-32.1 also indicated the reduced cooling of the hot spray water.

3. CFD Analysis

3.1 Grid Model and Flow Field Models

A 3-dimensional grid model including a spray nozzle with a half symmetric condition was used to represent the THAI facility (Fig. 5). The spray nozzle was modeled such as a semispherical shape to assure the spray angle 30°. A total of about 1,562,000 hexahedral cells with a cell length of 2 mm - 30 mm were generated in the grid model. A wall condition with a constant temperature of about 298 K was applied on the outer surface of the grid model.

$$\frac{\partial\left(\bar{\rho}\tilde{c}\right)}{\partial t}+\frac{\partial\left(\bar{\rho}\tilde{U}_j\tilde{c}\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_c}\frac{\partial\tilde{c}}{\partial x_j}\right)+\rho_u S_T\left|\nabla\tilde{c}\right| \qquad (1)$$

$$S_T = AGu'^{0.75} S_L^{0.5}\lambda_u^{-0.25} l_t^{0.25} \qquad (2)$$

$$A=1.6\times step(T-750)+0.000016\times(750-T) \qquad (3)$$

ANSYS CFX-13 [4] with a burning velocity model (BVM, Eqs. (1) to (3)) was used to simulate the hydrogen deflagration during spray operation in the test results of HD-30, 31, and 32.1 because the BVM can accurately predict the hydrogen flame propagation in a large space without an obstacle using the correlation of turbulent flame speed (Eq. (2)). The laminar flame speeds (ι_t) according to the hydrogen concentrations [5] were given as the input data of the BVM [4]. The model constant of A in the turbulent flame speed correlation of the BVM was proposed as a temperature-dependent function (Eq. (3)) to account for the ignition temperature of about 750 K for hydrogen combustion. The proposed constant A was validated through a CFD analysis against the hydrogen deflagration test HD-7 without a spray operation (Fig. 6). A particle model of Lagrange method in ANSYS CFX-13 (Table 3) was chosen for simulating the vaporization of liquid droplets owing to a heat transfer from the hydrogen combustion energy in the test. The particle model was also checked through a CFD analysis against the spray test in the THAI facility. A radiative heat transfer model was not included for the hydrogen combustion calculation for HD-30 to HD-32.1 because the effect of the radiative heat transfer in the CFD results of HD-7 was negligible (Fig. 6(b)). A turbulent flow was modeled by the shear stress transport (SST) turbulent model [4]. The time step size in these transient calculations was 0.25 ms - 0.5 ms for obtaining converged solutions.

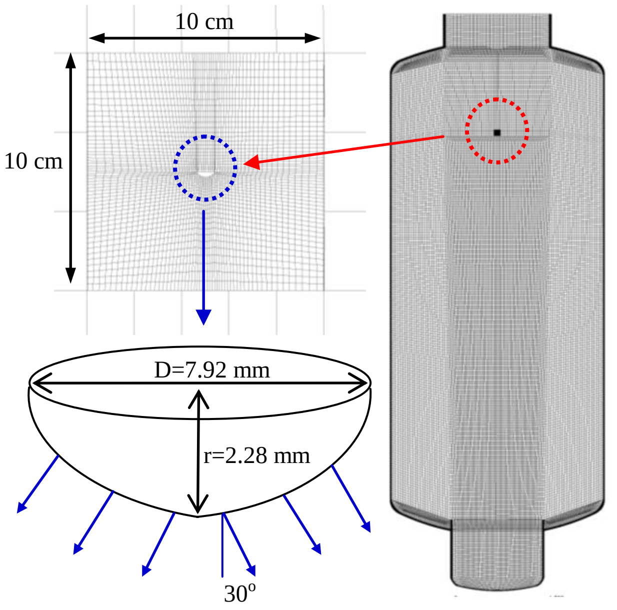
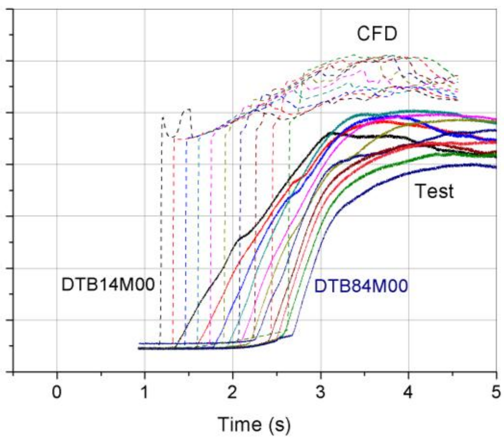


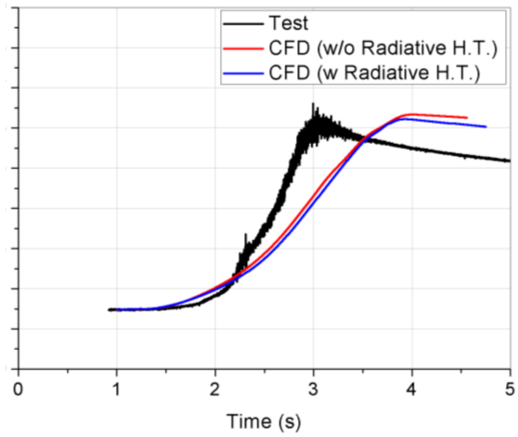
Fig. 5. Grid model for HD-30, HD-31, and HD-32.1

Table 3: Spray Water Model

Spray Model (Lagrange method)
- Diameter (d_{32}) = 0.6 mm - Mass flow rate = 1 kg/s (U = 19.89 m/s) - Nozzle diameter = 7.92 mm - Ejected particle number = 29498 [1/s]
Phase Change Model (Liquid droplet)
- $T_{particle} > T_{boil}$: Phase change - $T_{particle} > T_{boil}$: Diffusion or Convection



(a) Temperatures along vessel centerline



(b) Pressure behaviors at 4.9 m

Fig. 6. Comparison of temperature and pressure between the test and CFD results for HD-7

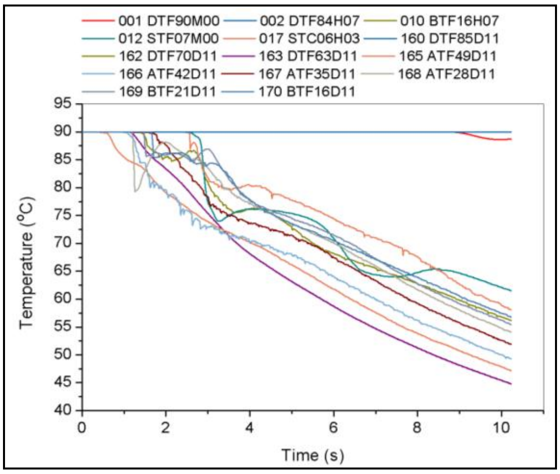
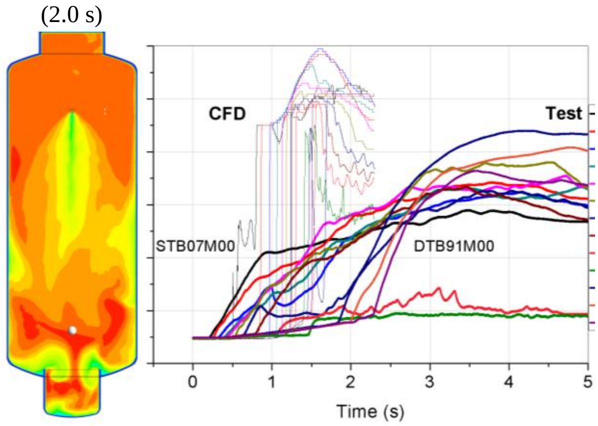


Fig. 7. CFD results for the spray model
(Initial conditions: T = 90 ^{o}C, P = 1.5 bar)

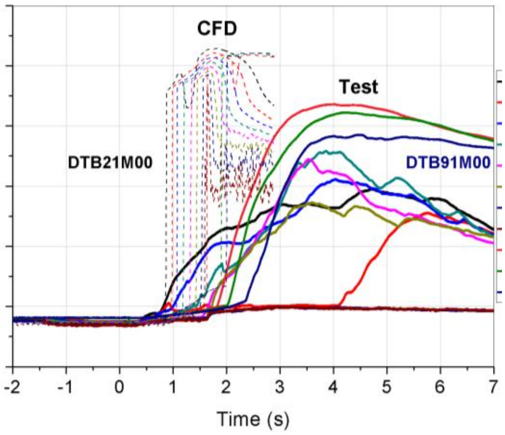
3.2 Discussion on the CFD Results

The CFD analyses for the test of HD-30, 31, and 32.1 were performed using ANSYS CFX-13 with a validated combustion model and spray water model. The CFD results for HD-30 (Fig. 8) show that the simulated spray water reduces the maximum gas temperature of about 140 K when compared to the CFD results for the test data without the spray operation (HD-7). However, the CFD results can not accurately simulate the disturbance of the chemical reaction of H_2-Air mixture owing to the spray water. This may be explained by the fact that the laminar flame speed given according to the hydrogen concentration in the BVM (Eq. (2)) sustained the hydrogen flame propagation. In addition, turbulence generated by spray droplets increased the hydrogen flame speed because the magnitude of the turbulence flame speed in this correlation is proportional to the calculated turbulent intensity (Eq. (2)). Thus, the high turbulent intensity (Fig. 9), which results from the spray droplets induce faster flame propagation compared to the simulation results for the test data without the spray operation (HD-7). Therefore, we found that the correlation of the turbulent flame speed implemented in the BVM should be modified for simulating the hydrogen deflagration during the spray operation.

However, the CFD results can accurately simulate the peak pressure at 4.9 m in the tests HD-30 and HD-31 with an error range of about 5% (Fig. 10). This may be explained by the fact that the overestimated gas temperature during the H_2-Air combustion was quickly cooled down by the spray water. The CFD results can accurately predict the peak pressure difference between HD-30 and HD-31. This difference may be resulted from that the steam content 25 vol% in the test HD-31 reduced the heat capacity of the mixture gas when compared to that of HD-30. In addition, the CFD results can accurately simulate the peak pressure difference due to the spray water temperature difference (Table 2).



(a) HD-30



(b) HD-31

Fig. 8. Comparison of temperature along the vessel centerline between the test and CFD results for HD-30 and HD-31

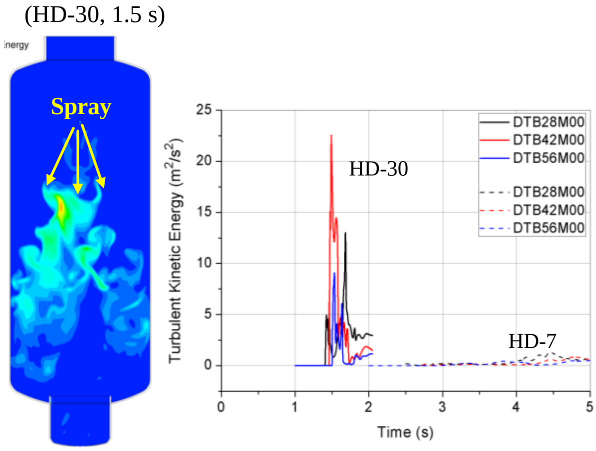


Fig. 9. CFD results of turbulence kinetic energy for HD-30

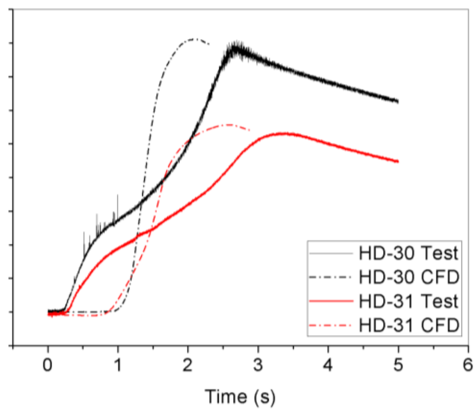


Fig. 10. Comparison of pressures at 4.9 m between the test and CFD results for HD-30 and HD-31

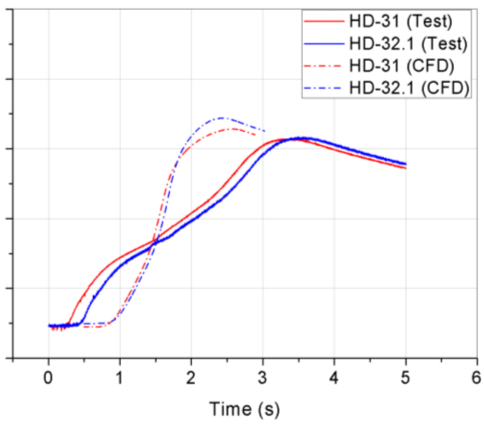


Fig. 11. Comparison of pressures at 1.6 m between the test and CFD results for HD-31 and HD-32.1

4. Conclusions and Further Work

KAERI performed the CFD calculation of the tests HD-30, HD-31, and HD-32.1 conducted in the THAI facility to observe the influence of spray operation on hydrogen combustion for further development and validation of computational codes within the frame of the OECD THAI-2 project. We accurately simulated the measured peak pressure in the tests with an error range of about 5%. However, we cannot accurately simulate the disturbance of the chemical reaction of H_2-Air mixture owing to the spray water. Thus, the calculated gas temperature during the hydrogen combustion was overestimated. In order to reduce this discrepancy between the CFD results and test data, we have to modify the correlation of the turbulent flame speed in the BVM for simulating the hydrogen deflagration during the spray operation.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science, ICT, and Future Planning) (No. 2012M2A8A4025889)

REFERENCES

[1] T. Kanzleiter, S. Gupta, K. Fischer, G. Ahrens, G. Langer, A. Kühnel, G. Poss' G. Langrock, F. Funke: Hydrogen and Fission Product Issues Relevant for Containment Safety Assessment under Severe Accident Conditions. OECD-NEA THAI Project Final Report No. 150 1326–FR 1, Becker Technologies GmbH, Eschborn, Germany, June 2010.

[2] S. Gupta, G. Langer, M. Freitag, M. Colombet, E. Schmidt and B. von Laufenberg, Hydrogen Combustion During Spray Operation: Tests HD-30 to HD-35, Technical Report of OECD-NEA THAI-2 Project, 1501420-TR-HD-30-35, Becker Technologies GmbH, Nov. 2014.

[3] T. Kanzleiter and G. Langer, Hydrogen Deflagration Test HD-22 and HD-23, QLR of OECD-NEA THAI Project, 1501326-HD-QLR6, Sep. 2008.

[4] Ansys Inc., ANSYS CFX-13 Manual, 2011.

[5] A. Kotchourko, A. Lelyakin, J. Yanez, Z. Xu, and K. Ren, COM3D Tutorial Guide Version 4.3, KIT, 2012.