CFD Simulation of Flame Propagation Speed for Premixed Hydrogen Combustion using Flamelet model in OpenFOAM

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1. Introduction

In the case of a nuclear power plant (NPP) severe accident, the explosion of hydrogen generated inside the containment building must be prevented, but it is very important to predict the extent of the explosion in case of emergency.

Very large amount of experiments and simulations of hydrogen flame are still ongoing, among which the THAI-HD series experiments was also carried out at OECD-NEA. Among the THAI–HD (Thermal-hydraulics, Hydrogen, Aerosols and Iodine – Hydrogen Deflagration) tests, HD-15 measured the behavior of 10% concentration (equivalent ratio φ = 0.26) of hydrogen-air flame in cylindrical vessel, with a height of 9.2 m, and a diameter of the main part of 3.2m. The ignition was in the center at the 0.5 m height from the vessel bottom. Detailed experimental condition can be found in Table 1. [1]

Table 1. Experimental condition

Reactant	Hydrogen + air (H_2 10%, Air 90%)
Equivalent ratio	0.26
Pressure	1.46 bar
Gas temperature	90℃

The laminar speed of 10 % hydrogen-air mixture flame in the reference condition (Su_0) measured in the experiment is 0.2 m/s. [2]

As the flame propagates, the temperature and pressure of the surrounding environment increase, and the speed of the flame also changes as the temperature and pressure change rate. This can be expressed as following equation. [3]

$$Su = Su_0\,(T_u/T_0)^{\alpha}\,(p/p_0)^{\beta} \tag{1}$$

Where, T_u – unburnt gas temperature, T_0 – reference temperature (300 K), p – pressure, p_0 – reference pressure (1 bar),

$$\alpha = 2.18 - 0.8(\varphi - 1) \tag{2}$$

$$\beta = - 0.16 + 0.22(\varphi - 1) \tag{3}$$

This simulation study benchmarked the HD-15 experiment by applying the above equation (1) to the XiFoam solver in OpenFOAM. [4]

2. Methods

In XiFoam, the propagation of the flame surface, temperature and pressure are calculated by using flamelet combustion model.

2.1. Governing equation

In the flamelet model, the flame front is determined according to the regress variable b. The regress variable can be obtained by solving the follow equation (4).

$$\frac{\partial}{\partial t}(\rho b) + \nabla\cdot(\rho\vec{u}b) - \nabla\cdot\left(\frac{\mu_t}{Sc_t}\nabla b\right) = -\rho S_c \tag{4}$$

Where, b - combustion regress variable, Sc_t - turbulent Schmidt number, S_c - reaction regress source term. And source term can be written as equation (5).

$$-\rho S_c = \rho_u S_u \xi |\nabla b| \tag{5}$$

Where, S_u – laminar flame speed (eq. 1), ρ_u – density of unburnt mixture, and ξ – flame wrinkling. The laminar flame speed multiplied by flame wrinkling is the turbulent flame speed transitioned as the flame surface propagates.

The flame wrinkling can be calculated by solving the transport equation (6).

$$\frac{\partial\xi}{\partial t} + U\cdot\nabla\xi = G\xi - R(\xi - 1) + (\sigma_s - \sigma_t)\xi \tag{6}$$

Where, U is the average velocity at the flame surface, σ_s is the strain rate, the subscript s means the surface. G and R are given by :

$$\mathrm{G} = \mathrm{R}\,\frac{\xi_{eq}-1}{\xi_{eq}} \tag{7}$$

$$R = \frac{0.28}{\tau}\frac{\partial\xi_{eq}}{\xi_{eq}^{*}-1} \tag{8}$$

and,

$$\xi_{eq}^{*} = 1 + 0.62\sqrt{\frac{u'}{S_u}}R_{\eta} \tag{9}$$

$$\xi_{eq} = 1 + 2(1-\mathrm{b})(\xi_{eq}^{*} - 1) \tag{10}$$

where :

u' is the turbulence intensity, R_η is the Kolmogorov Reynolds number, τ is the Kolmogorov time scale.

2.2 Simulation set-up

Using snappyHexMesh, a utility of OpenFOAM, the mesh of the same geometry as the HD-15 experimental vessel was generated. The simulation domain consists of 1.17 million cells with 78% of hexahedral elements. (Fig. 1)

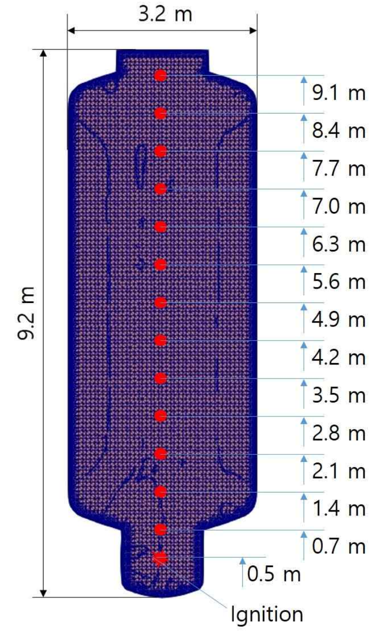

Fig. 1. Cross section of geometry, location of measuring points and mesh generation

The simulation was carried out by selecting k-omega SST model as the turbulence model, and additionally, buoyant k-omega SST model considering the effects of gravity and buoyancy was used. Specifically, in the buoyant k-omega SST model, the buoyancy term is added to the turbulence kinetic energy term in the k-omega SST model as shown in the following equations.

The turbulence kinetic energy term of the k-omega SST :

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\rho(v + \sigma_k v_t)\frac{\partial k}{\partial x_j}\right] = \rho p_k - \rho\beta^* \omega k \quad (11)$$

The turbulence kinetic energy term of the buoyant k-omega SST :

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\rho(v + \sigma_k v_t)\frac{\partial k}{\partial x_j}\right] = \rho p_k - \rho\beta^* \omega k + G_b \quad (12)$$

The buoyancy term

$$G_b = -\frac{v_t}{\sigma_t}\frac{\partial \rho}{\partial x_j} g_j \quad (13)$$

In which σ_t = 0.85. More details can be found in reference [5].

As in the experiment, the temperature was measured at a total of 13 measurement points at 0.7 m intervals along the central axis (0.7 m ~ 9.1 m), and the flame propagation speed was inferred from the flame arrival time.

3. Results

3.1 Flame propagation speed

In the experiment, same as the simulation set-up, 13 thermocouples were installed at 0.7 m intervals along the center of the vessel (0.7 m ~ 9.1 m). The temperature of each thermocouple was measured as the flame passed, and the propagation speed of the flame was compared based on the time when 1000 K was measured in each thermocouple.

In Figure 2, the flame propagation speed in the simulation using the two turbulence models and in the experiment are compared. The gradient of each graph indicates the speed of the flame.

In the simulation using the k-omega turbulence model, the predicted result was that the propagation speed of the flame was faster than that in the experiment. The mesh size used in the simulation was coarse, so the ignition size was relatively large (d = 0.25 m), and accordingly, the initial flame speed was predicted to be faster.

In the buoyant k-omega SST model, the results were close to the experiment by considering the interaction between the buoyancy of the flame and the gravity. However, due to the initial ignition size, the propagation speed of the flame was predicted to be faster until 0.5 s after ignition.

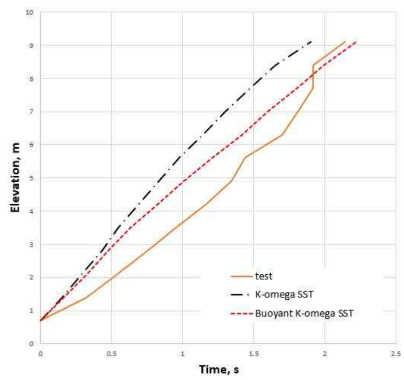

Fig. 2. Flame front propagation

3.2 Pressure

Fig. 3 is a graph showing the pressure change inside the vessel.

As in the result of 3.1, in the simulation, the initial flame propagation speed was fast due to the ignition size, and the pressure rise also tended to be faster than in the experiment.

The maximum pressure measured inside the vessel was predicted to be around 5 bar in both experiment and simulations. However, in the experiment, the maximum pressure was recorded at 2.5 s after ignition, but the buoyant k-omega SST case showed a tendency to bend the pressure rise at 2 s after ignition, and the maximum pressure was recorded at 3 s. The k-omega SST model recorded the highest pressure at 2.7s.

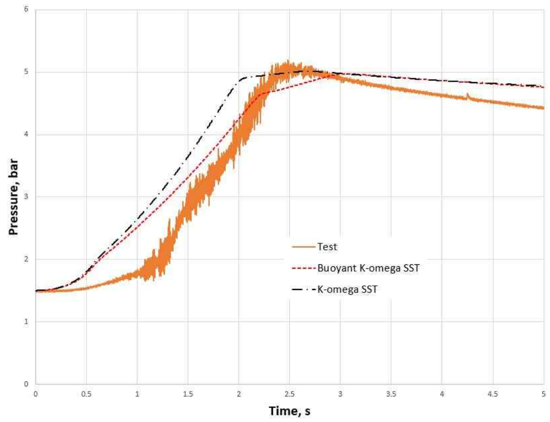

Fig. 3. Pressure rise trend

3.3 Temperature

In Figure 4, the flame temperature was compared with the results recorded at the center of the vessel (h = 4.9 m). In all cases, the highest temperature was recorded at this height. In k-omega SST case, the maximum temperature was recorded 970 ℃ at 3 s after ignition, and in both the experiment and buoyant k-omega SST case, the maximum temperature was 950 ℃ at 3.5 s.

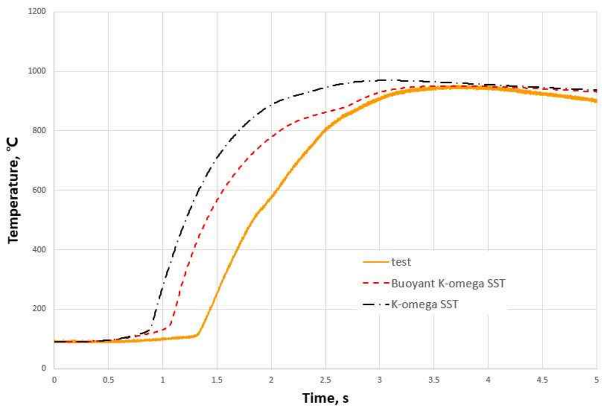

Fig. 4. Temperature change comparison at h = 4.9 m

4. Conclusions

Simulation was performed using an OpenFOAM flamelet combustion model(XiFoam) to predict the hydrogen flame propagation speed. As a result of comparison through the HD-15 test and the case of using the buoyant K-omega SST model that added the effects of gravity and buoyancy was the closest to the test result. However, due to the large ignition size, the initial flame acceleration was overestimated. When simulated using a finer mesh, it will be able to expect better results. Through this study, it will be applicable to prediction of hydrogen flame behavior inside NPP containment in the case of severe accident.

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