

Simulation of Wet Hydrogen Combustion using Flamelet model in OpenFOAM

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1. Introduction

As seen in Fukushima nuclear power plant (NPP) accident the most dangerous situation in the severe NPP accident is the hydrogen explosion. For this reason, it is very important to have an accurate understanding of hydrogen combustion behavior in the reactor containment. However, in actual accidents, in addition to hydrogen, a large amount of water vapor is generated inside the reactor containment. Therefore, the effect of the water vapor to the combustion behavior cannot be ignored.

In the OECD-NEA, a project called THAI (Thermal-hydraulics, hydrogen, aerosols and iodine) project was designed to fill knowledge gaps by delivering data for the evaluation and simulation of the hydrogen and fission product interactions, thereby supporting the validation of accident simulation codes and models. Among them, in the experiment called HD (hydrogen deflagration)-series, a combustion experiment in a mixture of hydrogen and water vapor was performed. [1]

Currently, the development of new generation code (ContainmentFOAM [2]) based on CFD technology for NPP containment safety analysis is in progress, and it is continuously pursuing to increase the prediction accuracy of the effects of wet hydrogen flame. ContainmentFOAM is developing based on open-source CFD library OpenFOAM. [3]

As an alternative combustion model for NPP containment, the XiFoam solver with flamelet model [4] was used in this study. In XiFoam, as in any flamelet model, the propagation of the flame surface, temperature and pressure are calculated using the regress variable without solving chemical(reaction) kinetics. The solver calculates the flame velocity, temperature and pressure according to the concentration of the fuel(hydrogen), and is only valid within the flammable limit(in case of hydrogen, 4 ~ 75% by volume of air).

2. Method

2.1. Governing equation

The regress variable can be obtained by solving the transport equation (1).

$$\frac{\partial}{\partial t}(\rho b) + \nabla \cdot (\rho \vec{u} b) - \nabla \cdot \left(\frac{\mu_t}{Sc_t} \nabla b \right) = -\rho S_c \quad (1)$$

Where, b - mean reaction regress variable, Sc_t - turbulent Schmidt number, S_c - reaction regress source term. And source term can be written in equation (2). The

turbulent Schmidt number can be defined as ratio of kinematic viscosity and mass diffusivity.

$$-\rho S_c = \rho_u S_u \xi |\nabla b| \quad (2)$$

Where, S_u - laminar flame speed, ρ_u - density of unburnt mixture, and ξ means the rate ratio of turbulent flame speed and laminar flame speed, and is called flame wrinkling. [5]

Rewriting the transport equations (1) and (2) to obtain the value b is as follows.

$$\frac{\partial}{\partial t}(\rho b) + \nabla \cdot (\rho \vec{u} b) - \nabla \cdot \left(\frac{\mu_t}{Sc_t} \nabla b \right) = \rho_u S_u \xi |\nabla b| \quad (3)$$

The algebraic equation for obtaining the ξ value is as follows.

$$\xi_{eq}^* = 1 + 0.62 \sqrt{\frac{u'}{S_u}} R_\eta \quad (4)$$

$$\xi_{eq} = 1 + 2(1 - b)(\xi_{eq}^* - 1) \quad (5)$$

The laminar flame rate S_u in XiFoam can be obtained by calculating the Gulderson formulation (6). In the equation below, Φ is the equivalence ratio, and W , η , α , and β are given as unique coefficients depending on the fuel type.

$$S_u = W \Phi^\eta \exp[-\xi(\Phi - 1.075)^2] \left(\frac{T}{T_0} \right)^\alpha \left(\frac{P}{P_0} \right)^\beta \quad (6)$$

2.2. Absolute enthalpy

The method of calculating absolute enthalpy in the XiFoam solver is obtained by polynomial approximation of molecular mass and C_p values of each species in the mixture according to the JANAF tables. The method of calculation is divided into homogeneous and inhomogeneous, depending on the type of mixture. The following equation is a schematic reaction equation of wet hydrogen.



2.1.1 Homogeneous

In the case of a homogeneous mixture, it is assumed that the species in the computational domain are well mixed and thus have a single property. Only reactant and combustion products exist in the computation cell (control volume), and their ratio is calculated by the following equation by the regress variable 'b'. Reactant

has physical properties of $H_2 + O_2 + N_2 + H_2O$, and product has physical properties of $H_2O + N_2$.

```

if (b > 0.999)
{
    return reactants_;
}
else if (b < 0.001)
{
    return products_;
}
else
{
    mixture_ = b*reactants_;
    mixture_ += (1 - b)*products_;

    return mixture_;
}
    
```

2.1.2. Inhomogeneous

In the case of an inhomogeneous mixture, a mass fraction of fuel and other species can be used respectively, and the ratio of these inside the cell as combustion proceeds is solved by the calculation formula for 'b'. The equation of the inhomogeneous mixture for the combustion of wet hydrogen in XiFoam code is as follows.

```

{
    fu = b*ft;
    ox = 1 - ft - N2 - H2O - (ft - fu)*stoicRatio().value();
    pr = 1 - fu - ox;

    mixture_ = fu*fuel_;
    mixture_ += ox*oxidant_;
    mixture_ += pr*products_;

    return mixture_;
}
    
```

ft is the initial fuel mass fraction, and **fu** is the fuel mass fraction remaining in the cell after combustion proceeds by 'b'. **ox** is the amount of oxidant remaining after combustion, in this case oxygen. **stoicRatio ()**, **value ()** means stoichiometry air-fuel mass ratio. The amount of N_2 and H_2O that does not participate in combustion is subtracted from the total mass fraction. In this case, since the product has the same physical properties as H_2O , the initial H_2O amount is included in the product amount after combustion.

3. Results

The accuracy of the simulation results was evaluated in comparison with an experiment in one of the OECD-NEA THAI projects. It is an experiment that measures the propagation speed, temperature and pressure of a wet hydrogen flame by igniting in a state in which flow in the container is formed by a blower installed inside the container.

3.1. Mesh and geometry

The schematic geometry of the experiment is shown in Figure 1 below. Airflow from the top of the PAD to the bottom is formed by the blower installed inside the PAD, and the ignition is at the bottom of the TTV.

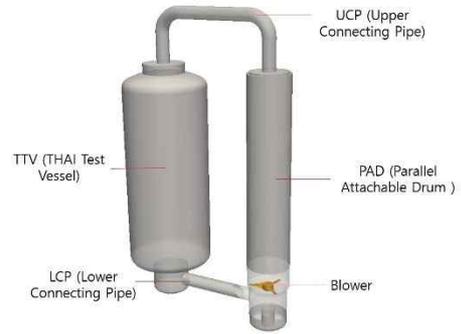


Fig. 1. Schematic geometry of the experiment

Figure 2 shows the mesh of the THAI HD experimental geometry using the OpenFOAM's internal utility SnappyHexMesh. [6] Number of cell is approximately 0.9 million cells with 76% of hexahedral elements. The internal flow generated by the rotation of the blower before ignition can be seen in Figure 3.

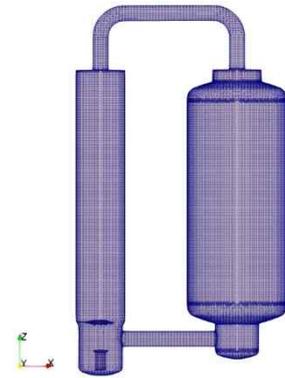


Fig. 2. 3-D mesh generation

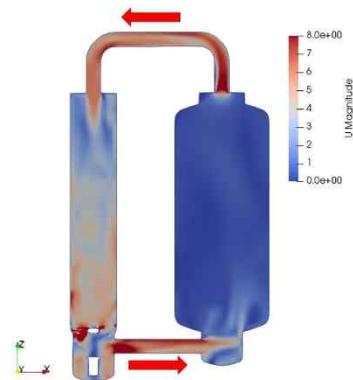


Fig. 3. Fluid flow in test apparatus

Table 1 shown the condition of test and simulation.

Table 1. Test and simulation condition	
Reactant	Wet hydrogen + air (H_2 10%, H_2O 25%, Air 65%)
Pressure	1.46 bar
Gas temperature	90 °C
Solver	XiFoam
Turbulent model	k-omega SST

Figure 4 shows the maximum measured temperature results in experiment and simulations. The measurement locations are as shown in Figure 5. Both homogeneous and inhomogeneous simulation cases recorded higher temperatures than the experiment, due to the effect of unknown radiation error. One of the reasons for recording the temperature closer to the experimental results in the inhomogeneous was that it was possible to put detailed species components into the analysis input.

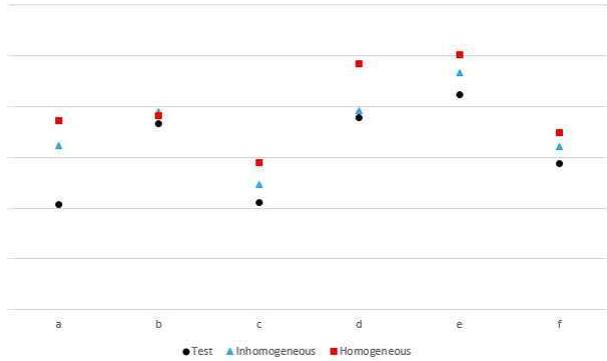


Fig. 4. Maximum temperature at each points

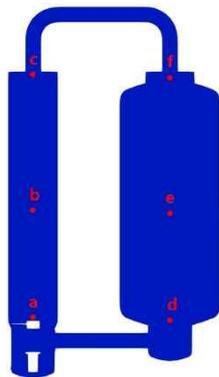


Fig. 5. Temperature measuring points

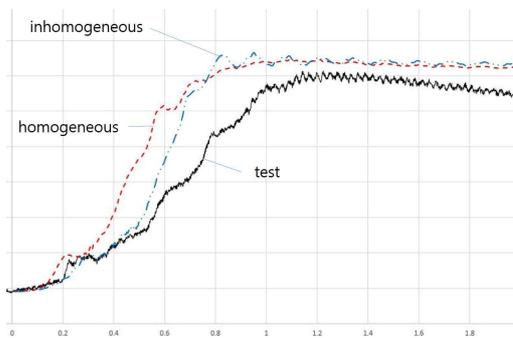


Fig. 6. Pressure comparison

Figure 6 shows the results of internal pressure measurements in experiments and simulations. Up to 0.7 seconds after ignition, the internal pressure increased faster in the case of homogeneous, but the maximum pressure was recorded by the inhomogeneous case. The inhomogeneous case has more similar tendency of pressure rising after ignition than homogeneous case.

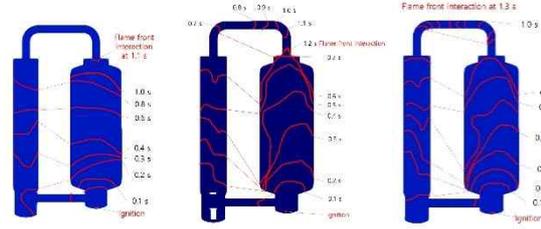


Fig. 6. Flame propagation results (a) – test, (b) – homogeneous, (c) – inhomogeneous

The flame propagation speed was closer to the experimental results in the homogeneous case. Since pressure and flame temperature have a great influence in calculating the flame speed through the Gulderson method (eq. 6), it should be possible to predict the flame propagation more accurately in inhomogeneous, but it can be assumed that there was an error in the input of Gulderson coefficient or turbulence model.

4. Conclusions

For the same wet-hydrogen fuel, combustions were simulated by dividing the conditions of the mixture into homogeneous and inhomogeneous. Overall pressure and flame temperature were recorded higher in the simulation due to unknown radiation error. In the case of the homogeneous mixture, the flame speed was predicted to be closer to the experiment but the inhomogeneous case was closer to the experimental results for temperature and pressure. In order to increase accuracy, it is necessary to consider the radiating effect and use the appropriate Gulderson coefficient and turbulence model.

REFERENCES

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