Preliminary study on reactingFoam for the prediction of hydrogen flame propagation

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1. Introduction

Hydrogen can be generated by the interactions of the core melt with containment structures and water during severe accident in a nuclear reactor. In case of releasing into the reactor containment, it can induce the hydrogen combustion. It may result in detonation in a nuclear power plant and can threaten the containment integrity.

Various mitigation measures such as PAR(passive mitigation system) were prepared to prevent the hydrogen combustion in containment. Although the related safety measures were prepared, Hydrogen combustion is still one of the key issues in nuclear power plant.

Many researches on Hydrogen combustion in nuclear power plant have been performed. The large scale experiments on the effect of obstacles and transverse venting on flame acceleration and transition to detonation have been conducted by SNL[1]. Experimental research on hydrogen and fission product behaviour in containments have been done in THAI test facility[2]. Kim et al.[3] have performed numerical analysis of hydrogen flame acceleration in a containment.

Combustion is a complex phenomenon accompanying not only heat and mass transfer but also chemical reactions so that the related numerical analysis needs lots of computational resources. Recently various open-source tools such as Cantera[4] and OpenFOAM[5] are available that can handle the problems involving chemical kinetics, thermodynamics and transport process.

In this study parametric analysis has been conducted using an open source solver[5] as a preliminary research for the analysis of hydrogen combustion phenomena in a reactor. The numerical model for the analysis was introduced and parameter's effect was evaluated. The preliminary application on hydrogen flame propagation in a channel has been conducted.

2. Method

In this evaluation, the reactingFoam solver in OpenFOAM(version 2006) is employed. OpenFOAM is composed of various solvers which are designed to solve a specific problem in fluid (or continuum) mechanics.

(1) Geometry

The FLAME(Flame Acceleration Measurements and Experiments) facility was selected as a base geometry. It is a large rectangular channel having a size of 1.83m (W) x 2.44 m (H) x 30.48 m (L). Fig. 1 shows the schematics of the facility.

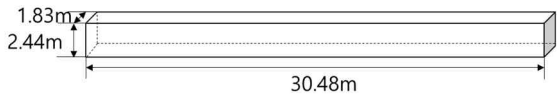

Fig. 1 Schematics of FLAME facility

In the experiment, the vertically installed thermocouple along the mid plane of the channel was used to measure the flame time of arrival[1]. The similar time of arrival concept was employed during post-process procedures.

(2) Numerical model

Standard k-ε model was employed as turbulence model. For chemical reaction simulation, simple one-step irreversible reaction mechanism[6] was employed. A simple grid resolution of 100 (L) x 24 (H) x 18 (W) was selected for parametric study. PaSR(Partially Stirred Reactor) model was adopted as combustion model. In PaSR model, a computational cell is split into two different zones, one is reacting zone, in which all reactions occur, and another is non-reacting zone, in which mixing occur without any reactions as shown in Fig. 2[7].

In the figure, Y_i^0 and $\widetilde{Y}_i$ describes the initial and final mass fraction of ith species in reaction zone, κ is the fraction of the reactive zone.

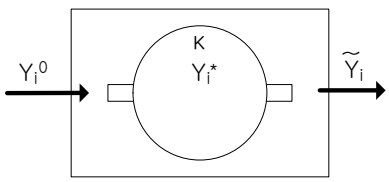

Fig. 2 Concepts of PaSR

The reacting part can be expressed as eq. (1)

$$\kappa = \frac{\tau_0}{\tau_0 + \tau_{m\,ik}} \quad (1)$$

where τ_0 and $\tau_{m\,ik}$ are characteristic chemical and mixing time scales in each cell. $\tau_{m\,ik}$ can be obtained from k-ε equation as eq. (2),

$$\tau_{m\,ik} = C_{m\,ik}\frac{k}{\varepsilon} \quad (2)$$

where $C_{m\,ik}$, k and ε are coefficient for evaluating characteristic mixing time scale, turbulent kinetic energy and turbulent dissipation rate, respectively.

Calculations were performed at atmospheric pressure condition. The initial chamber was assumed to be filled

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with premixed Hydrogen-air mixture and the concentration of Hydrogen was set to be 12.3% based on mole fraction.

3. Results

In PaSR model, τ_{mix} accounts for the exchange process between the fresh, unreacting mixture, and the reaction products. In order to estimate the effect of Cmix on flame propagation, flame time of arrival[1] was plotted with respect to various Cmix. As shown in Fig. 3 the time of arrival was reduced by decreasing Cmix. In this calculation Cmix was selected to be 0.05.

In turbulent condition typical value of Cmix was reported to be varied between 0.001-0.3[8]. The Cmix is approaching 0 as flow condition becomes fully turbulent. Based on this, the selected value was found to be within a reasonable range.

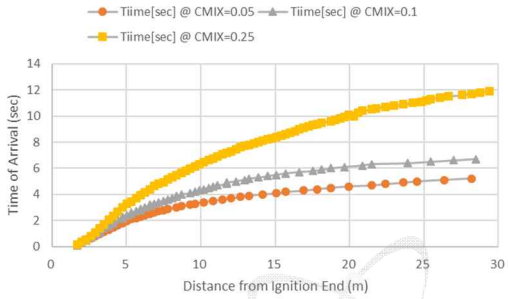

Fig. 3 Effects of Cmix on Time of Arrival

Fig. 4 shows the flame movement with respect to time variation. Temperature profiles were plotted in every one seconds except for the last one. As shown in figure, the flame traveling distance per one second (ie. flame propagating speed) is increased as combustion proceeds.

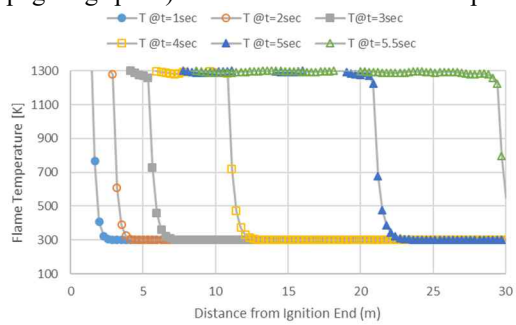

Fig. 4 Temperature profiles with respect to time variation

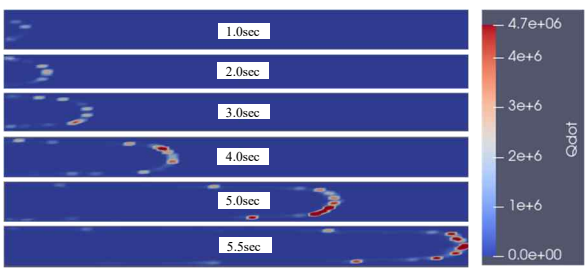

Fig. 5 Variation of heat release rate with respect to time variation

In order to see the variation of heat release rate behavior within flame surface, the heat release rate with respect to time was plotted in Fig. 5. As shown in Fig. 5 heat release rate was relatively small at initial stage(1sec). However, it increased as it propagated to the end of channel.

4. Conclusions

The parametric study of PaSR combustion model in reactingFOAM has been done. Based on the selected parameter value, the capability of reactingFoam was evaluated as a preliminary steps for flame propagation prediction. Cmix parameter was found to affect the prediction of flame speed so that it should be decided by considering flow condition. ReactingFoam solver found to be able to simulate the variation of propagating speed and intensity of flame in a channel.

In order to increase the capability of flame propagation prediction, the further studies on reaction mechanisms, combustion models, other available solvers need to be conducted.

5. Acknowledgement

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