Preliminary study on reactingFoam for the prediction of hydrogen flame propagation

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Objective

- Analysis of model's parameter effects on flame propagation prediction
- Evaluation of capability of reactingFoam

Related researches

- SNL(Sandia National Laboratory) : the large scale experiments on the effect of obstacles and transverse venting on flame acceleration and transition to detonation
- Becker Technology GmbH: Experimental research on hydrogen and fission product behavior in containments have been done in THAI test facility
- KAERI : Numerical analysis of hydrogen flame acceleration in APR1400 containment
- Numerical analysis of flame propagation during spray operation in THAI facility

Geometry & Condition

- 12.3% H_2 by mole fraction in air
- STP(Standard Temperature and Pressure) without flow
- X : Y : Z = 30.48 : 2.44 : 1.83

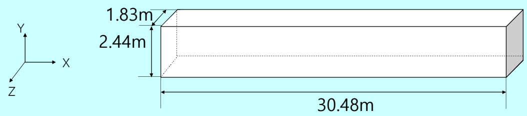

Fig. Schematics of experiment facility

Numerical model

- ReactingFoam : open source CFD platform for flame analysis
- Standard k-ε turbulence model
- One step irreversible reaction mechanism
- PaSR(Partially Stirred Reactor) combustion model

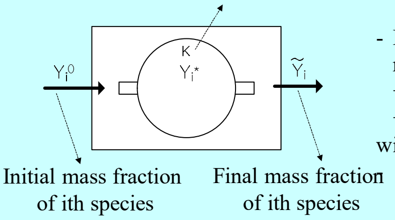

Fig. Concepts of PaSR

Table. Reaction mechanism candidate

	Reaction	A [mol/ cm^3s]	T [K]
(1) Hasemi RM	$2H_2+O_2 \rightarrow 2H_2O$	1.8E+13	1.7614E+4
(2) Marinov RM	$H_2+ ½ O_2 \rightarrow H_2O$	9.9E+20	1.515E+4

<u>Concept of PaSR</u>

- Every computational cell is split into reacting zone and non-reacting zone.
  + Reacting zone : all reaction occur
  + Non-reacting zone : mixing occur without any reaction

Reactive zone can be expressed as followings

$$\kappa = \frac{\tau_0}{\tau_0+\tau_{mix}}$$

- where τ_0 and τ_{mix} are characteristic chemical and mixing time scales in each cell. τ_{mix} can be obtained from k-ε equation as following eq.

$$\tau_{mix} = C_{mix}\frac{k}{\varepsilon}$$

- where Cmix , k and ε are coefficient for evaluating characteristic mixing time scale, turbulent kinetic energy and turbulent dissipation rate, respectively.

Sensitivity analysis

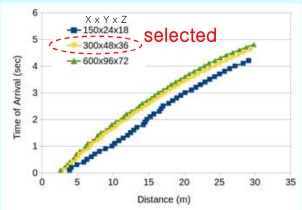

Fig. Computational grid sensitivity

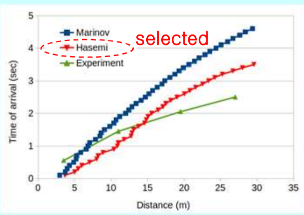

Fig. Reaction mechanism comparison

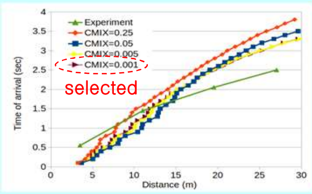

Fig. Cmix effects on flame propagation

Flame propagation prediction

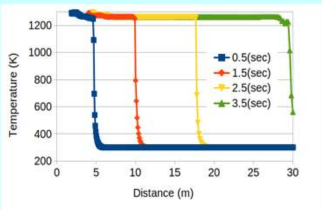

Fig. Temperature profiles with respect to time variation

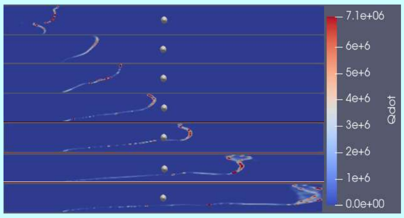

Fig. Variation of heat release rate from 0.5 sec to 3.5 sec

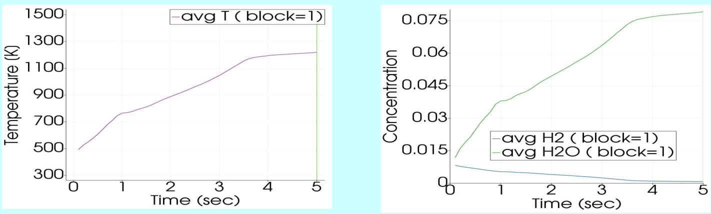

Fig. Variation of averaged temperature and concentration within facility

Conclusion and Future work

- The capability of reactingFoam was evaluated as a preliminary steps for flame propagation prediction.
- Sensitiviy analysis on Cmix parameter and reaction mechanism as well as no. of grid should be evaluated before they were applied to prediction.
- ReactingFoam solver was able to simulate the variation of propagating speed and intensity of flame in a channel.
- However, the further studies on reaction mechanisms, combustion models, other available solvers need to be conducted in the future.

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