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

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Introduction

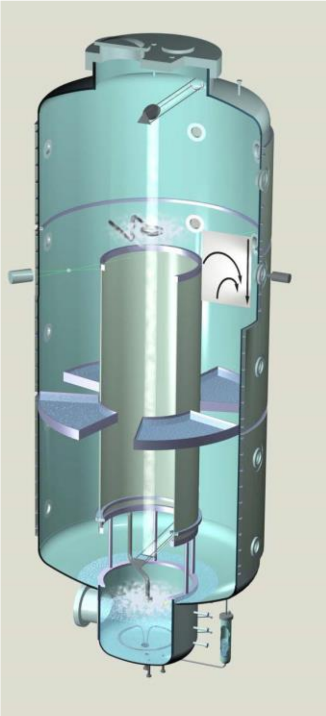
In the case of a nuclear power plant (NPP) severe accident, the explosion of hydrogen generated inside the containment building must be prevented, but it is very important to predict the extent of the explosion in case of emergency.

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.

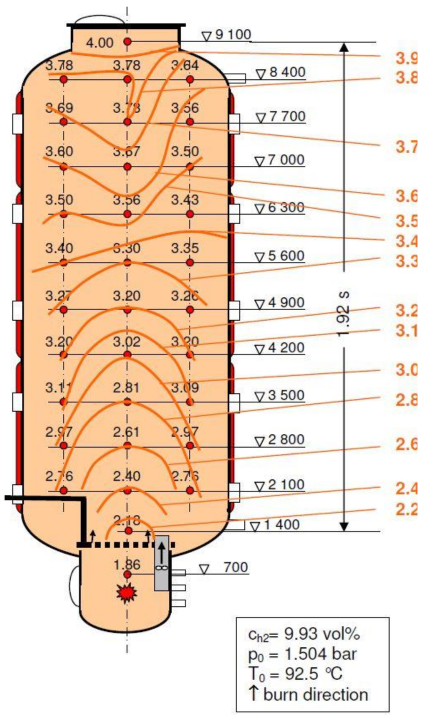
Table 1. Experimental condition

Reactant	hydrogen + air (H_2 10%, Air 90%)
Pressure	1.504 bar
Gas Temperature	92.5℃
Equivalent ratio	0.26

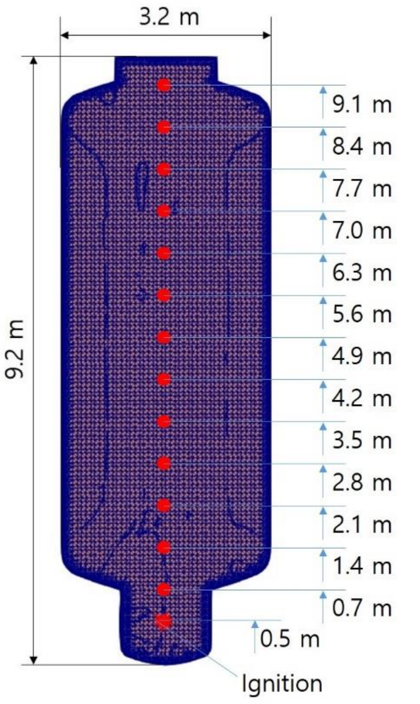
THAI HD-15 TEST



- THAI test vessel (inner cylinder and condensate trays removed for HD-tests).



- Flame front propagation as isochrones



- Cross section of geometry, location of measuring points and mesh generation

CFD Method and Results

XiFoam

- OpenFOAM solver for compressible premixed/partially-premixed combustion
- Using flamelet combustion model (without solving chemical(reaction) kinetics)
- The propagation of the flame surface, temperature and pressure are calculated using the regress variable 'b'.

Govern equation

- Transport Equation for 'b'
- $\frac{\partial}{\partial t}(\rho b) + \nabla \cdot (\rho \vec{u} b) - \nabla \cdot \left(\frac{\mu_t}{Sc_t} \nabla b\right) = \rho_u S_u \xi |\nabla b|$

Laminar flame speed

Simple Power Law

- Su = $Su_0\,(T_u/T_0)^{\alpha}\,(p/p_0)^{\beta}$
- α = 2.18 – 0.8(φ - 1)
- β = – 0.16 + 0.22(φ – 1)

Where,
T_u – unburnt gas temperature,
T_0 – reference temperature,
p – pressure,
p_0 – reference pressure

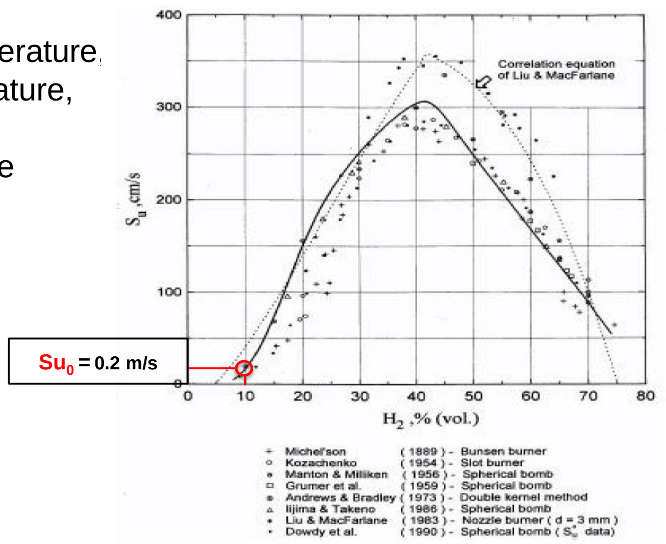


Figure A.1.1. Laminar burning velocity of hydrogen/air mixtures at room temperature and atmospheric pressure measured by various methods. Solid line: computed values for spherical flame propagation; dotted line: correlation equation of Liu and MacFarlane.

Turbulent model

- **The turbulence kinetic energy term**

k-omega SST :

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

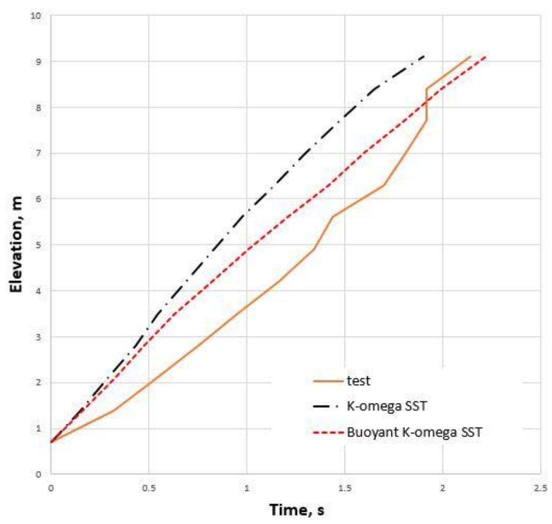
- **buoyant k-omega SST :**

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

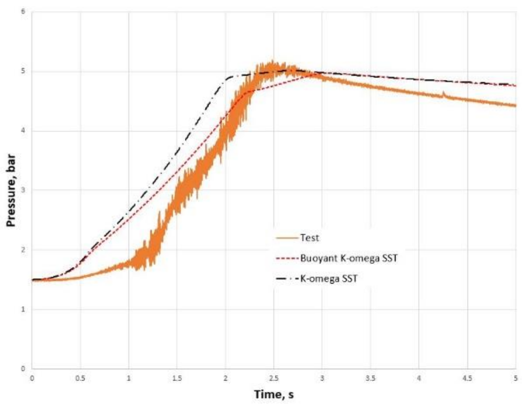
- **The buoyancy term**

$$G_b = -\frac{v_t}{\sigma_t}\frac{\partial \rho}{\partial x_j} g_j$$

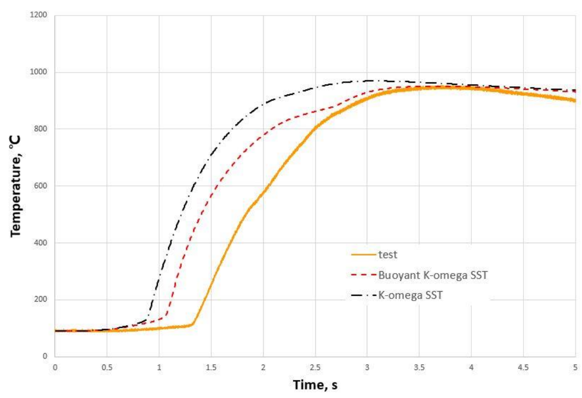
Flame front propagation



Pressure rise trend



Temperature at h = 4.9 m



Conclusion

- 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.