CFD Analysis for SRI's H_2 Explosion Test at the Stoichiometry Condition in an Open Space

Hyung Seok Kang [a], Sang Baik Kim [a], Min-Hwan Kim [a], Hee Cheon NO [b]

[a] *KAERI, P. O. Box 105,Yuseong,Taejon, Republic of Korea, 305-600, hskang3@kaeri.re.kr*
[b] *KAIST, 373-1, Guseong, Yuseong, Taejon, Republic of Korea, 305-701*

1. Introduction

A safety distance between a Very High Temperature Gas-Cooled Reactor (VHTR) and a H_2 production facility is usually determined by basing it on the peak overpressure under the assumption of a hypothetical H_2 explosion accident [1]. A computational fluid dynamics (CFD) code with the one step chemical reaction model was introduced as a useful tool to simulate an overpressure buildup phenomenon due to H_2 flame acceleration. A H_2 explosion test result performed by the SRI [2] was used to validate a CFD analysis method because the CFD results may be easily varied according to a selected numerical model. In this study, the CFD analysis against the H_2 explosion test at the stoichiometry condition was first performed.

2. SRI H_2 Explosion Test

The SRI performed the H_2 explosion test in the open space by varying the H_2 concentration, the H_2-Air mixture volume, the ignition energy and the existence of an obstacle [2]. The SRI measured the overpressure (P1~P5) and the flame front TOA (Ion1~Ion7) inside the tent where the flammable gas was located (Fig. 1) [2] after an ignition by an electric spark device. Also, th e overpressure at 11m, 21m and 41m from the tent was measured. As for the first comparison with the CFD resu lt, the selected test case is a 5.6 m^3 volume mixture of H_2-Air (30 vol. %) with an obstacle under a spark igniti on of 40J. This test was repeated twice at the same conditions except the ambient temperature (Table 1).

Table 1: H_2 Explosion Test Conditions [2]

Test No	H_2 Concentration	Ambient Temperature
2	29.9 %	283.75K
2-01	30.0 %	298.75K

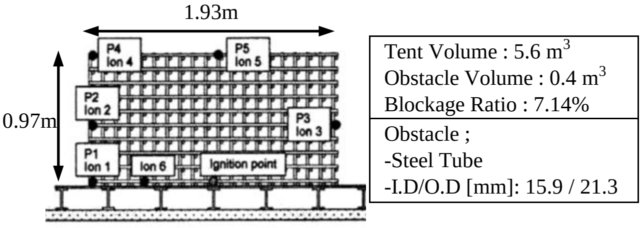

Fig. 1. H_2 Explosion Test Facility [2]

Figs. 2 and 3 show the measured flame front TOA and overpressure values. Twice repeated test data with the different ambient temperature show a weak reproducibility. The difference of the flame front TOA values at Ion 6 between Test 2 and Test 2-01 is about 34%. The flame front TOA difference from Ion 6 to Ion 4 at Test 2 and Test 2-1 are 1.564 ms and 1.356 ms. This means that the flame of Test 2-1 passes the obstacles faster than that of Test 2. This fast propagation of Test 2-1 may cause a 2.6 times higher overpressure buildup at P4 location (Fig. 2).

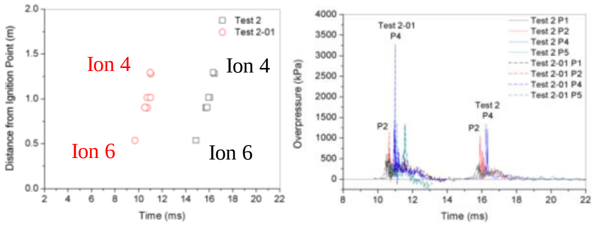

Fig. 2. H_2 Explosion Test Results [2]

3. CFD Analysis

3.1 Grid Model, Initial and Boundary Conditions

A 3-dimensional and quarter symmetric grid model (Fig. 3) for simulating the tent and its environment was generated on the basis of the SRI test facility [2]. A total of 14,832,100 hexahedral mesh cells were produced, and a dense mesh cell distribution with a 1cm cell length was located around the tent region (2.11 m x 2.11 m x 2.13 m) to resolve the rapid flame splitting and propagation due to the obstacle structure. A coarse mesh cell distribution with a 4 cm cell length from the tent region boundary to the far distance of 7 m was generated only to assure the pressure wave propagation. The stoichiometry gas distribution of H_2, O_2 and N_2 was given to the tent region as an initial condition. An activated spherical region simulating the spark ignition energy of 40J was also given to the ignition point as the initial condition. According to the spark ignition model and previous results, the selected radius, temperature and pressure of the activated region for the CFD calculation are 6 cm, 105.79 kPa, and 1000 K [3]. The initial temperature and pressure at the outer region of the spark ignition boundary is 293 K and 1 atm. An opening condition (Fig. 3) [4] was applied to all the surrounding surfaces except for the bottom surface and the quarter cut surface. A symmetric condition was applied on the cut surface.

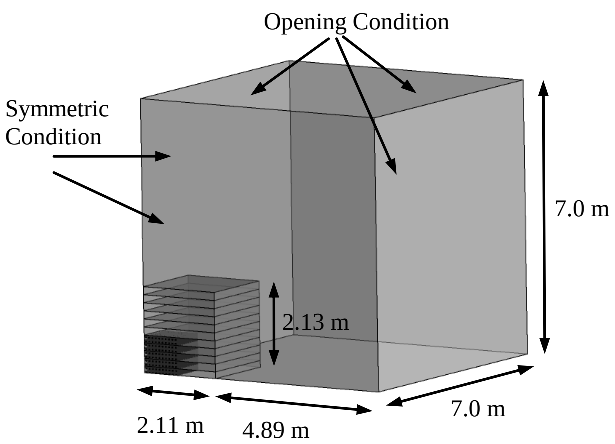

Fig. 3. Grid Model and Boundary Conditions

3.2 Flow Field Models and Combustion Model

The governing equations used in this study are the Navier-Stokes, the energy and the species transport equations with a coupled solver algorithm [4]. Turbulent flow was modeled by the standard k-ε turbulent model, and the buoyancy flow was modeled by the full buoyancy model [4]. The discrete transfer model [4] was used for the simulation of the radiative heat transfer. The eddy dissipation model (EDM) [4] was used for the one step combustion reaction of the H_2-Air mixture. In the EDM, the following model was used for the global reaction rate by using the model constant B=0.8 because the product reaction rate can simulate a better stable flame propagation:

$$R_p = AB\rho\frac{\varepsilon}{k}\left(\frac{Y_p}{1+r_f}\right) \quad (1)$$

To start the combustion using the EDM with the product reaction rate model, 10% of the H_2 product mass was given in the spark ignition region. As for a transient calculation, a time step size of $5.0\mathrm{x}10^{-5}$ s, $1.0\mathrm{x}10^{-5}$ s and $5.0\mathrm{x}10^{-6}$ s was separately applied to evaluate the effect of the time step size on the pressure wave behavior because the pressure wave may affect the density value.

Table 2: CFD Sensitivity Calculation Conditions

	EDM Constant A, B	Time Step Size	CFL Number
Case-1	A=10, B=0.8	0.05 ms	< 6.7
Case-2	A=10, B=0.8	0.01 ms	< 1.4
Case-3	A=10, B=0.8	0.005 ms	< 0.6

* Ambient temperature of Case-1, Case-2, and Case-3 is 293K.

3.3 Discussion on the CFD Analysis Results

The flame front TOAs of Case-2 and Case-3 locate in the measured data between Test 2 and Test 2-01 (Fig. 4). Case-2 calculated the flame front TOA from Ion 6 to Ion 4 with an error range of 27% when compared the test data, and Case-3 calculated with an error range of 37%. The flame front TOAs of Case-1 is faster than the test results. This may be explained by the fact that the time step size of 0.05 ms overpredicted the pressure wave propagation. Case-2 predicted the peak overpressure at P4 with an error range of about 53% compared to the test data, whereas Case-3 predicted with an error range of about 62%.

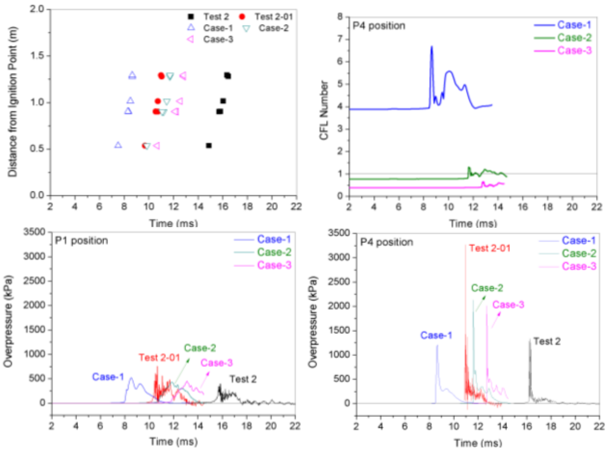

Fig. 4. CFD Results (flame front TOA, CFL at P4 position, overpressure at P1 and P4 positions)

4. Conclusions

The CFD analysis for the H_2 explosion test at a stoichiometric condition was performed to establish the CFD analysis method. The CFD sensitivity study showed that the CFD analysis with the following input reasonably predicted the measured overpressure buildup and flame front TOA: the EDM constant of A=10 and B=0.8, the time step size of 0.001 ms (CFL < 1.4), the cell length of 1 cm around the obstacle. Therefore, it is known that the CFD analysis may be used as an evaluation tool to provide the 3-dimesnional information of the flame front TOA and overpressure buildup phenomenon if proper conditions for the CFD analysis method are chosen.

ACKNOWLEDGEMENTS

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