Large Eddy Simulation of Hydrogen Deflagration in Open Space and Vented Enclosure

T. Nozu, K. Hibi, T. Nishiie

***Abstract*—**This paper discusses the applicability of the numerical model for a damage prediction method of the accidental hydrogen explosion occurring in a hydrogen facility.

The numerical model was based on an unstructured finite volume method (FVM) code "NuFD/FrontFlowRed". For simulating unsteady turbulent combustion of leaked hydrogen gas, a combination of Large Eddy Simulation (LES) and a combustion model were used. The combustion model was based on a two scalar flamelet approach, where a G-equation model and a conserved scalar model expressed a propagation of premixed flame surface and a diffusion combustion process, respectively. For validation of this numerical model, we have simulated the previous two types of hydrogen explosion tests. One is open-space explosion test, and the source was a prismatic 5.27 m^3 volume with 30% of hydrogen-air mixture. A reinforced concrete wall was set 4 m away from the front surface of the source. The source was ignited at the bottom center by a spark. The other is vented enclosure explosion test, and the chamber was 4.6 m × 4.6 m × 3.0 m with a vent opening on one side. Vent area of 5.4 m^2 was used. Test was performed with ignition at the center of the wall opposite the vent. Hydrogen-air mixtures with hydrogen concentrations close to 18% vol. were used in the tests.

The results from the numerical simulations are compared with the previous experimental data for the accuracy of the numerical model, and we have verified that the simulated overpressures and flame time-of-arrival data were in good agreement with the results of the previous two explosion tests.

***Keywords*—**Deflagration, Large Eddy Simulation, Turbulent combustion, Vented enclosure.

I. Introduction

HYDROGEN energy has recently attracted a great deal of attention as an eco-friendly energy and CO2 free energy. Therefore, some projects are starting aimed at realizing a hydrogen energy-based society in Japan. Especially, the Tokyo metropolitan government has decided that the Athletes' Village for the 2020 Tokyo Olympic and Paralympic Games will be made into a "hydrogen town" where electricity and hot water are supplied through hydrogen energy. For this reason, hydrogen equipment or a hydrogen facility (e.g. H2 gas storage tank, H2 pipelines etc.) may be installed or used inside rooms or near buildings in a town in the future. However, since hydrogen gas can burn in mixtures with air ranging from very lean to quite rich, hydrogen gas has a risk to lead an explosion accident if hydrogen gas leaked from hydrogen equipment stagnates in a closed space, enclosure inside or around buildings. Therefore, many experimental studies on hydrogen explosion have been constructed for safety in use of hydrogen gas and for evaluating the hydrogen explosion force to the structure [1]-[3]. The explosion phenomenon is very complicated and it is difficult to analyze in detail. Besides, the experimental approach usually requires a lot of money and time to carry out experimental studies. On the other hand, the numerical approach is expected to reproduce the explosion phenomenon at low cost and time. In order to use a Computational Fluid Dynamic code for safety computations, first of all the code must be validated versus available experimental data.

In this study, we have applied the LES method for hydrogen deflagration in open-space and vented enclosure, and we have confirmed the applicability of the numerical model for a prediction method of the accidental hydrogen explosion occurring in a hydrogen facility.

II. Numerical Formulation

A. Governing Equations

In this study, Large Eddy Simulations were carried out in order to predict unsteady flame propagation and pressure development in the hydrogen explosion. The filtered governing equations consist of the Navier-Stokes equation, and the continuity equation and the momentum equation are written as:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \overline{\rho} \widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_i \widetilde{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i}\right) - \tau_{ij}^{SGS}\right] \tag{2}$$

where t, ρ, u_i, p, μ and τ_{ij}^{SGS} stand for time, density, velocity, pressure, viscosity and sub-grid scale (SGS) turbulent stress, respectively.

The combustion model is based on a two-scalar flamelet approach coupling the two concepts of diffusion flame and premixed flame [4], [5]. In this approach, equations of combustion field are composed of a transport equation of the mixture fraction and a G-equation. The scalar transport equation is expressed as:

$$\frac{\partial \overline{\rho} \widetilde{Z}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_j \widetilde{Z}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu}{Sc}\frac{\partial \widetilde{Z}}{\partial x_j}\right) + \frac{\partial q_{zi}}{\partial x_i} \tag{3}$$

where, Z, Sc and q_{zi} stand for mixture fraction, the Schmidt number and gradient-diffusion assumption for the effect of

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SGS fluctuation, respectively. On the other hand, the G-equation is given as:

$$\frac{\partial \bar{\rho}\widetilde{G}}{\partial t}+\frac{\partial \bar{\rho}\widetilde{u}_j\widetilde{G}}{\partial x_j}=\bar{\rho}S_T\left|\frac{\partial \widetilde{G}}{\partial x_j}\right|, \quad (4)$$

where, G and S_T stand for the levelset function and the turbulent flame speed. The above equation actually describes propagation of flame front moving at the turbulent flame speed. The level-set function G distinguishes between the unburned ($G = 0$) and fully burnt ($G = 1$) states in the partially premixed flame, and the flame front locates at $G = 0.5$.

Turbulent flame speed is strongly related to the degrees of local turbulence and flame front wrinkling, and laminar flame speed. The correlation between turbulent and laminar flame speeds needs to be properly modeled in order to predict the hydrogen explosion. In this study, we used Bauwens' formulation [6] as a turbulent flame speed model which is given by

$$\frac{S_T}{S_L}=\Xi_I\Xi_T, \quad (5)$$

where, S_L, Ξ_I and Ξ_T stand for a laminar flame speed, hydrodynamic instability and sub-grid wrinkling due to turbulence, respectively.

The local laminar flame speed, the local density, the local mass fraction and the local temperature at burnt state are determined by reference to "flamelet database", which was generated by the chemical reaction analysis using CHEMKIN with the elemental chemical reaction GRI-MECH 3.0.

B. Benchmark Experiments for Validation

For validation of this numerical model, we have simulated the previous two types of hydrogen explosion tests. One is open-space explosion test [7], and the source was a prismatic 5.27 m^3 volume that contained homogeneous hydrogen-air mixture (30% hydrogen and 70% air). A reinforced concrete wall, 2 m tall by 10m wide and 0.15 m thick, was set 4 m away from the front surface of the source (see Fig. 1). The source was ignited at the bottom center by a spark. Overpressure data were obtained on the both a front and back surface of the wall and on the ground surface.

The other is vented enclosure explosion test which was carried out by [6]. Although they conducted a series of experiments regarding hydrogen-air deflagration venting, we selected one case of these experiments for validation. The chamber was 4.6 m × 4.6 m × 3.0 m with a square vent opening on one side of the wall. Vent areas of 5.4 m^2 were used. Test was performed with ignition at the center of the wall opposite the vent. Homogeneous hydrogen-air mixtures with hydrogen concentrations close to 18% vol. were used in the test. Pressure data and flame time-of-arrival data were obtained both inside and outside the chamber near the vent.

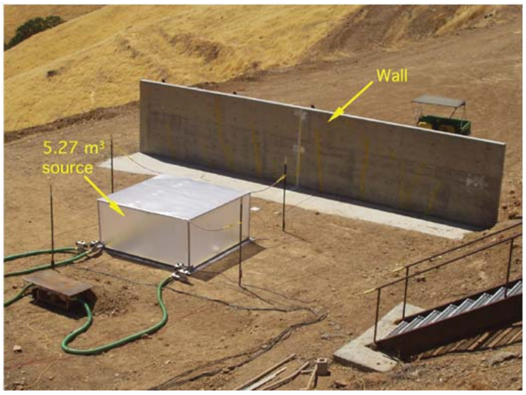
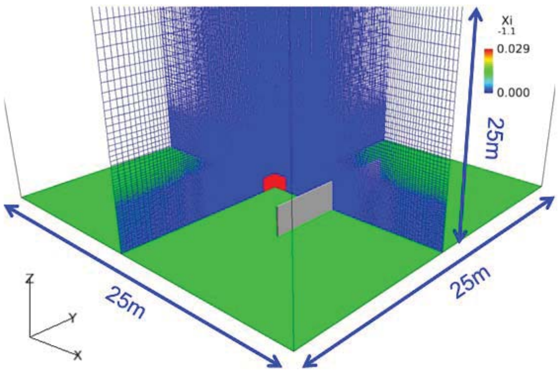


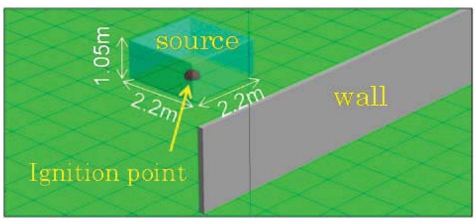
Fig. 1 Wall and explosive source in open-space explosion test [1]

C. Mesh Geometry and Numerical Condition

The calculation domain for the open-space explosion test was created matching the significant features of the experimental setup. The domain size was 25 m × 25 m × 25 m in the X-, Y-, and Z-directions. The mesh grid size inside the prismatic source (2.2 m × 2.2 m × 1.05 m) was 0.05m. The total grid number of the calculation domain was about 9,000,000. Fig. 2 shows the calculation domain and the computational mesh. On the other hand, the calculation domain for the vented enclosure explosion test was 25 m × 16 m × 20 m in the X-, Y-, and Z-directions. The mesh grid size of 0.05m was used in the region inside the chamber and the area immediately outside the chamber to resolve the external explosion. The total grid number of the calculation domain was about 4,000,000. Fig. 3 shows the calculation domain and the computational mesh.

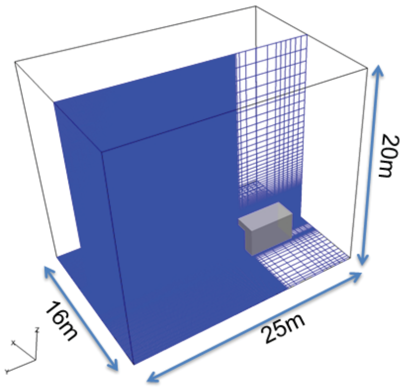


(a)



(b)

Fig. 2 Computational domain and computational mesh in open-space explosion case. (a) calculation domain, (b) source and wall



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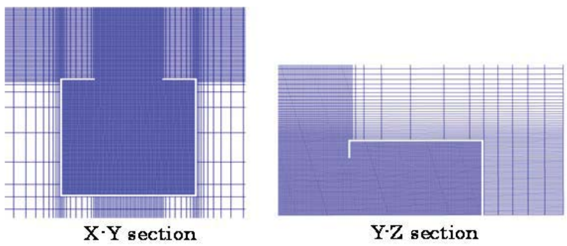


(b)

Fig. 3 Computational domain and computational mesh in vented enclosure explosion case. (a) calculation domain, (b) plane section

The present simulations are calculated with an unstructured fully compressible pressure-based FVM solver "NuFD/FrontFlowRed" which is extended by Numerical Flow Designing CO., LTD. from "FrontFlow/Red" originally developed by University of Tokyo under the project of Revolutionary Simulation Software [8]. For advection term of the governing equations, the MUSCL scheme is applied. However, momentum equations of velocity field are blended by first-order upwind scheme of 5% to suppress numerical oscillation. The time integration method is used the Euler implicit scheme. Time steps of these calculations are 2.0×10^{-4} s and 5.0×10^{-4} s, respectively.

III. Results and Discussion

A. Open-Space Explosion Test

Fig. 4 shows instantaneous pressure contours and flame front (G=0.5) at various time steps in the open-space explosion test. In the first stage of the explosion, the blast wave propagation was formed a hemisphere, and when the blast wave pressure encountered the barrier wall it was reflected at t = 0.06 s, and a diffraction of the blast wave occurred at the corner of the wall. The flame did not propagate far from the original source area.

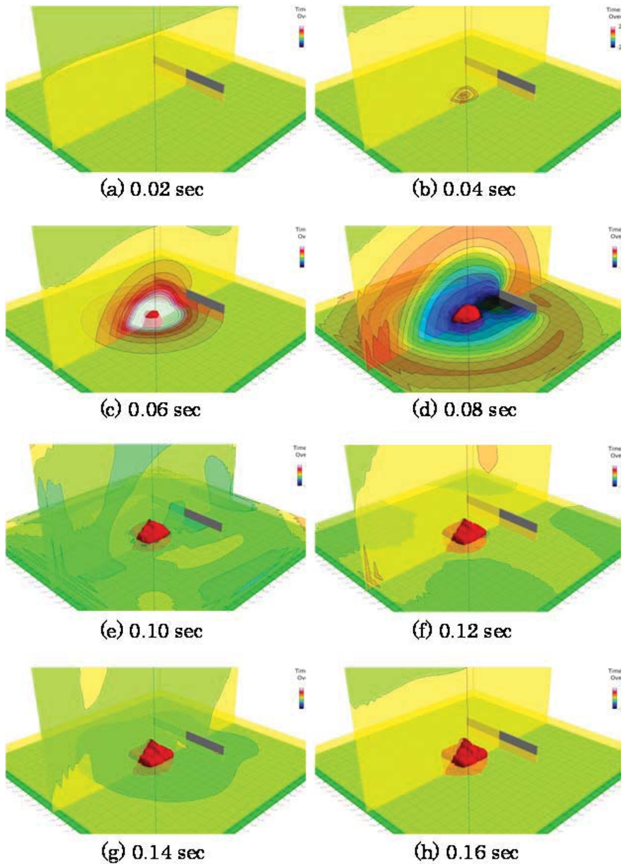
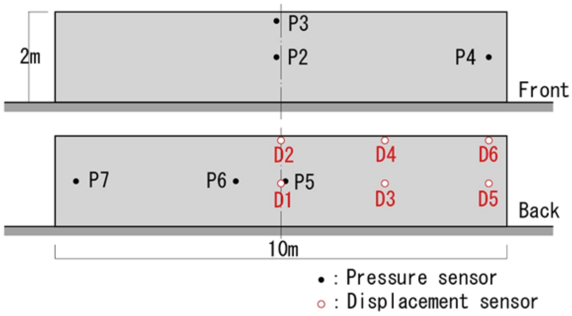


Fig. 4 Instantaneous pressure contours and flame front at various time steps

Fig. 5 shows the comparison of blast wave pressure time histories on the both a front and back surfaces of the barrier wall between the previous experiment and the numerical simulation. Some experimental pressures on the front surface of the wall show a small time negative drift due to the thermal load from the explosion. In the experimental results, we can confirm that pressures on the back surface of the barrier wall reduce almost by half compared to those on the front surface of the wall. Numerical simulation can reproduce a similar behavior to the experimental results.



(a)

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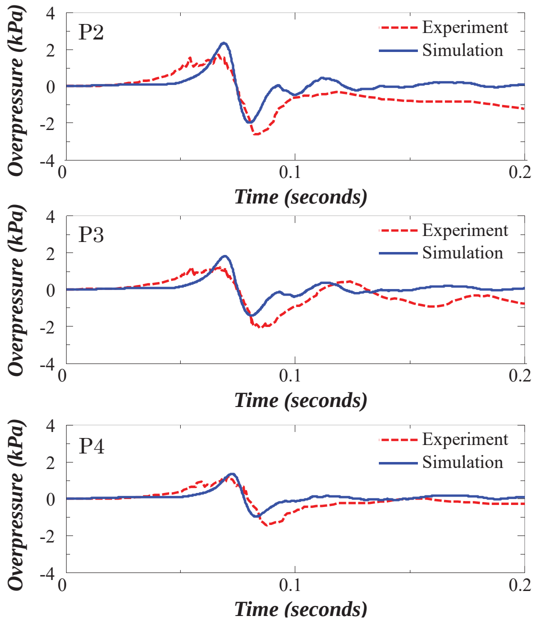

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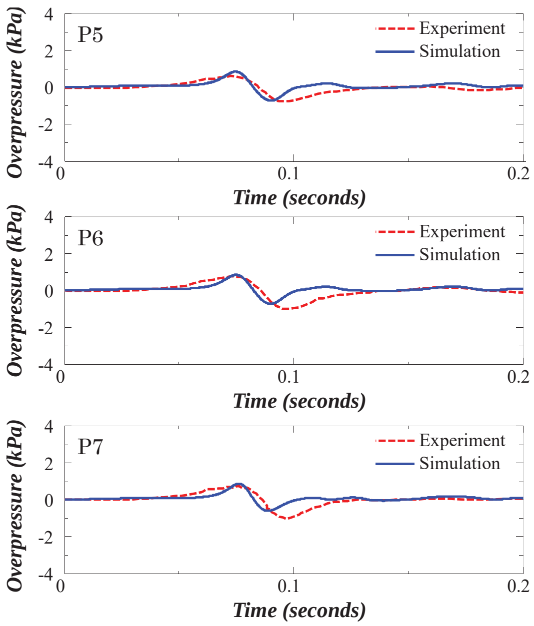

(c)

Fig. 5 Comparison of blast wave pressure time histories on the surface of the wall. (a) pressure sensor locations (b) front sides (c) back sides

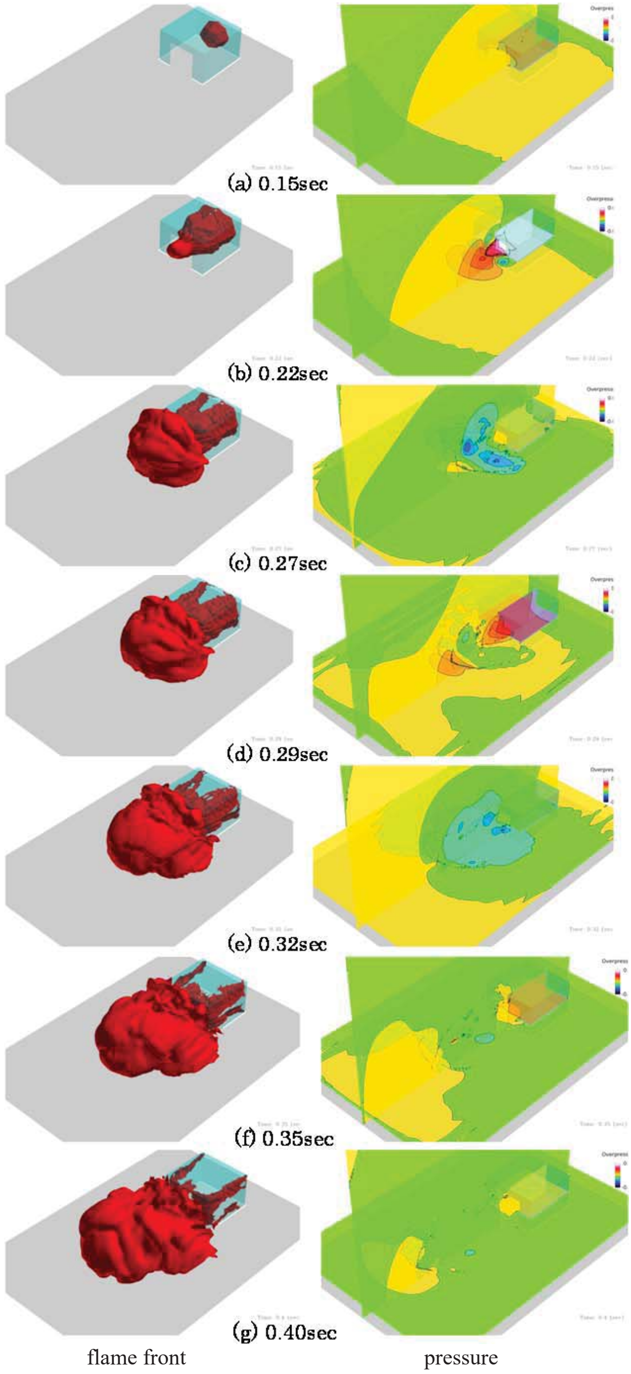

Fig. 6 Instantaneous isosurfaces of flame front and instantaneous pressure contours at various time steps

B. Vented Enclosure Explosion Test

Fig. 6 shows instantaneous isosurfaces of flame front (G =0.5) and instantaneous pressure contours at various time steps in the vented enclosure explosion test. The flame is stretched by a strong outward flow from the vent at t = 0.22 s. And the flame propagated far from the vent at t = 0.32-0.40 s. We can confirm a strong pressure oscillation by Helmholtz oscillation.

Fig. 7 shows flame velocity at the centerline of the combustion chamber with distance from the ignition position including both experimental and simulation results. As the flame front propagates to the vent area inside the chamber, the flame speed is accelerated, and that is slowed down outside the chamber. It can be confirmed that the simulation result is almost perfectly reproduced both inside and outside the chamber.

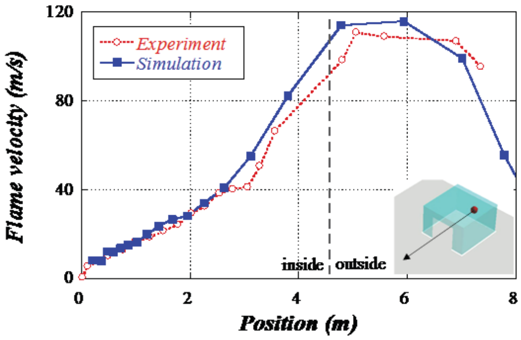

Fig. 7 Flame velocity at the centerline of the combustion chamber with distance from the ignition position

Fig. 8 shows the comparison of the pressure time histories in the chamber between experimental results and numerical results. The simulation result is underestimated the peak pressure comparing with experimental results. However, the numerical simulation can reproduce the pressure fluctuation caused by external explosion followed by a Helmholtz oscillation.

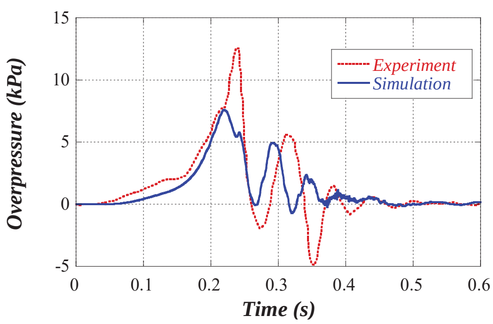

Fig. 8 Comparison of the pressure time histories in the chamber

IV. Conclusion

In this study, we confirmed that the applicability of the numerical model for a prediction method of the accidental hydrogen explosion occurring in a hydrogen facility. The conclusions of this study can be shown as follows:

- Numerical results reproduce basic features observed in experiments, such as overpressures and flame speeds.
- In open-space explosion case, it is confirmed that we can calculate the overpressure on the barrier wall.
- In vented enclosure explosion case, the simulation result is almost perfectly reproduced both inside and outside the chamber. But, CFD result is underestimate the peak pressure in the chamber.
- Further studies are planned to include effects of scale, concentration of hydrogen-air mixture and obstacles in the model validation exercises.

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