14th International Conference on
Shock & Impact Loads on Structures
30-31 March 2023, Singapore

HYDROGEN DETONATION SIMULATION BASED ON CESE IBM FSI SOLVER WITH SKELETAL H_2-AIR REACTION MECHANISM

Di Chen, Chengqing Wu and Jun Li

*University of Technology Sydney
Sydney, NSW, 2007, Australia
e-mail: <Chengqing.wu@uts.edu.au>;
webpage: https://profiles.uts.edu.au/Chengqing.Wu

Keywords: Hydrogen detonation, Fluid-structure interaction, skeletal reaction mechanism

Abstract. *A numerical fluid-structure interaction model of H_2-air detonation is presented and validated. The compressible fluid solver, Conservation Element/Solution Element (CESE) solver, coupling with the FEM solver were employed to solve the FSI problem via Immersed Boundary Method (IBM). A skeletal H_2-air reaction mechanism containing 9 species and 22-step reactions was utilized to solve the chemical reaction which fully coupled with the CESE solver. The numerical model was verified against existing experimental data, and the numerical results agreed well with the experimental ones. The findings provided an approach to the modelling of structural responses subjected to H_2-air detonation.*

1 INTRODUCTION

Hydrogen is a central pillar of the energy transformation as the world is limiting global warming to two degrees Celsius by 2050, which requires 60% of energy-related CO_2 to be reduced[1]. The Hydrogen Council predicted that 18% of the final energy demand will be provided by hydrogen in 2050[1]. The importance of hydrogen energy development has risen to strategically high which would support a nation's energy, climate, economy, technology, and security. Therefore, many countries or organizations, such as the Netherlands, Norway, Portugal, Japan, South Korea, Australia, New Zealand, and Germany, the US, the European Union, have issued their hydrogen energy strategies and development roadmap for 2050. Australia's National Hydrogen Strategy released in 2019 states that Australia aims to become a "major player" in global hydrogen production and trade by 2030[2]. China also published its national hydrogen strategy in 2019 and predicts that more than 10% of China's energy system will be accounted for by hydrogen in 2050[3].

Hydrogen is highly flammable gases, whose oxidization process can develop into explosion accidents, then cause severe personnel injuries and fatalities, economic loss and immeasurable social disruption. Blast mitigation wall is widely used as a protection method to withstand the explosion load so the equipment, personnel and any other objects behind the wall could be protected. Reliable blast resistance design requires a comprehensive knowledge of blast loading characteristics and dynamic response predictions of the blast mitigation wall. Experimental study is the most direct way to obtain this information, but it is not always feasible due to the high cost, long preparing time and safety issues[4]. With advances in computational mechanics, it is possible to model the responses of blast mitigation wall subject to hydrogen explosion loads.

Detonation is the strongest form of explosion for gas explosion and has the potential to cause severest consequences. In this study, the newly developed CESE IBM FSI solver with skeletal H_2-air reaction mechanism in LS-DYNA is used to model the blast wall response subjected to H_2-air detonation. The accuracy of this model was validated against the experimental data in literature.

2 PHYSICAL AND NUMERICAL MODEL

2.1 The physical model

In this study, data from the H_2-air detonation experiment carried out by Nozu et al. [5] was compared with the numerical results. As shown in Figure 1, the explosion source is a 5.27 m^3 H_2-air mixture which contains 30% H_2 and 70% air. A reinforced concrete wall, with dimensions of 2 m tall, 10 m long and 0.15 m thick, and a compressive strength of 48 MPa, stands 4 m away from the explosion source. A 10 g of C-4 high explosive was placed at the bottom centre of the explosion source to trigger a direct detonation.

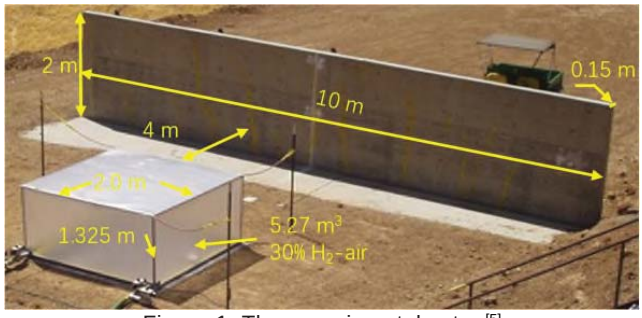
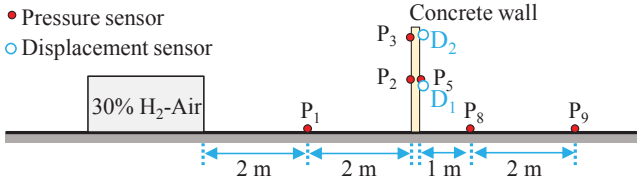
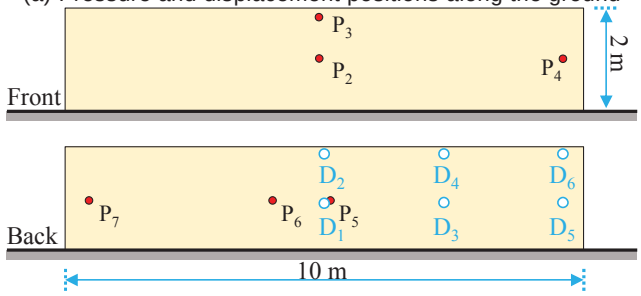


Figure 1: The experimental setup[5]

Figure 2 presents the locations of pressure and displacement sensors. Three pressure sensors (P_1, P_8, P_9) were located along the ground surface in front of and behind the concrete wall, and six pressure sensors were installed on the surface of the wall (P_2, P_3 and P_4 at front, and P_5, P_6 and P_7 at rear). Six displacement sensors were installed at the back of the wall of which three of them (D_1, D_3 and D_5) were at the middle height of the wall and another three (D_2, D_4 and D_6) at the top of the wall.



(a) Pressure and displacement positions along the ground



(b) Pressure and displacement positions on the concrete surface

Figure 2: The distribution of sensors[5]

2.2 The numerical model

A chemically reacting flow coupled with strong fluid-structure interaction (FSI) was involved in the abovementioned experiment. The commercial code, LS-DYNA R 11.2.2, was utilized to perform the numerical simulation. The recently developed module, CESE IBM FSI solver, which is specialized for modelling FSI was used to solve the flow field and structural response in this study. The chemistry solver which based on the finite-rate chemistry theory was coupled with the CESE solver to solve the chemistry reaction involved in the detonation process[6]. Specifically, The CESE

solver is a compressive CFD solver based on the space-time conservation element and solution element (CESE) method[7]. This solver has many obvious advantages, such as high accuracy, unified space-time treatment, and simple shock capturing strategy[8]. It can be fully coupled with the LS-DYNA FEM structural solver. Hence, it is naturally suitable for solving blast and shock wave interactions. The immersed boundary method (IBM) is used to treat the interface between fluid and structure. The method allows the fluid and structure meshed independent from each other. The fluid mesh is fixed while the structure mech can move inside the fluid mesh. The CESE solver detects the displacement and velocity of interface from the FEM solver, and feedback pressure to the FEM solver[6]. IBM method is very robust and can handle large deformation problems such as explosions. Meanwhile, the Chemistry solver contained in the LS-DYNA package can compute chemical kinetics models and couple with the CESE solver. Therefore, the chemically reacting flows can be solved by the coupling of Chemistry and CESE solver. The data flow among the three solvers is presented in Figure 3.

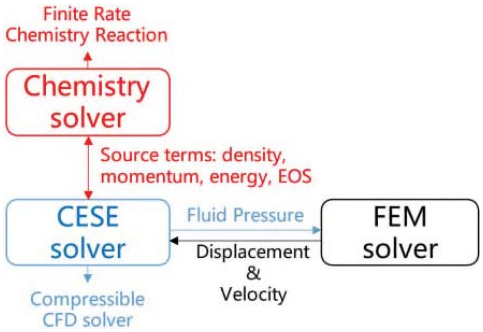


Figure 3: Data flow among the three solvers

It can be noted that the experimental scenario is symmetric, so a half model was numerically established as shown in Figure 4. The computational domain has dimensions of 12 m long, 8 m wide and 5 m high. The fluid mesh size is 2.5 cm between the H_2-air mixture and the location 0.5 m after the back of the blast mitigation wall. Other fluid meshed were stretched with an increment rate of 10% until they reached the boundary. The structure meshes were identical and had the sizes of 3.0 cm. The total number of elements is around 600×10^4. The bottom of the blast mitigation wall was totally constrained, while a symmetric boundary is applied to its symmetric surface. For the fluid boundary, faces ①, ②, ③ and ⑥ were nonreflective boundary, and face ④ is reflective boundary, and the rest one is symmetric boundary. The material model of blast wall is #159 CSCM CONCRETE model with a compressive strength of 48 MPa and a density of 2400 kg/m^3.

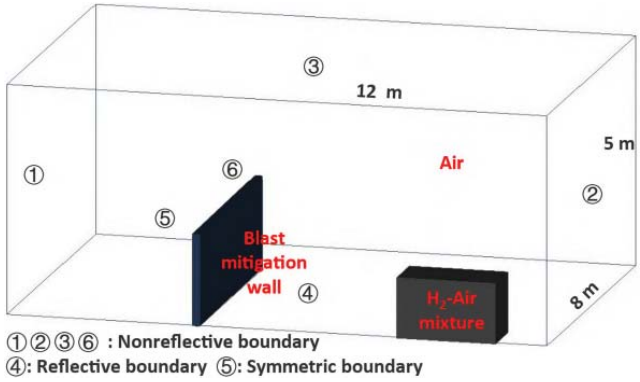


Figure 4: The geometry model and boundary conditions

The Z-22 reaction model for H_2-air combustion process developed by Zettervall in 2018[9] was introduced to simulate the H_2-air chemical reaction in the detonation process. This model contains 9 species and 22-step reactions, and the detailed reactions are listed in Table 1. A cuboid region with dimensions of 0.15×0.15×0.075 m at the bottom of fuel was defined as the initiation location. A temperature of 3000 K and pressure of 5 bar were set in the initiation location.

#	Reaction	A	n	E
1	H2 + O2 => H + HO2	7.40E+05	2.43	53500
2	H2 + M => H + H + M	4.57E+19	-1.4	105100
3	HO2 + H2 => H2O2 + H	3.00E+06	2	21000
4	H + O2 => OH + O	2.45E+14	0	16800
5	OH + O => H + O2	1.20E+13	0	690
6	O + H2 => OH + H	1.80E+10	1	8826
7	OH + H => O + H2	8.00E+09	1	6760
8	H2 + OH => H2O + H	1.17E+09	1.3	3626
9	H2O + H => H2 + OH	5.09E+09	1.3	18588
10	OH + OH => O + H2O	6.00E+08	1.3	0
11	O + H2O => OH + OH	5.90E+09	1.3	17029
12	H + O2 + M => HO2 + M	1.80E+18	-0.8	0
13	H + HO2 => OH + OH	1.50E+14	0	1004
14	H + HO2 => H2 + O2	2.50E+13	0	700
15	OH + HO2 => H2O + O2	2.00E+13	0	1000
16	HO2 + HO2 => H2O2 + O2	8.00E+13	0	0
17	H2O2 + M => OH + OH + M	1.30E+17	0	34500
18	OH + OH + M => H2O2 + M	9.86E+14	0	-5070
19	H2O2 + OH => H2O + HO2	1.00E+13	0	1800
20	H2O + HO2 => H2O2 + OH	2.86E+13	0	32790
21	OH + H + M => H2O + M	2.20E+22	-2	0
22	H + H + M => H2 + M	1.80E+18	-1	0

Table 1: Skeletal H2-O2 reaction mechanism, Units are mole-cm-sec-K-cal [9].

3 RESULTS AND DISCUSSIONS

In this section, the numerical results of pressure and impulse were compared with experimental data.

Figure 5 presents the peak pressure comparison at different distances from the ignition point. The peak pressures from numerical simulation were in good agreement with the data obtained from the experimental test. The present of blast mitigation wall helped reduce the pressure magnitude significantly as the peak pressure after the wall dropped dramatically, which was reproduced well by the numerical model.

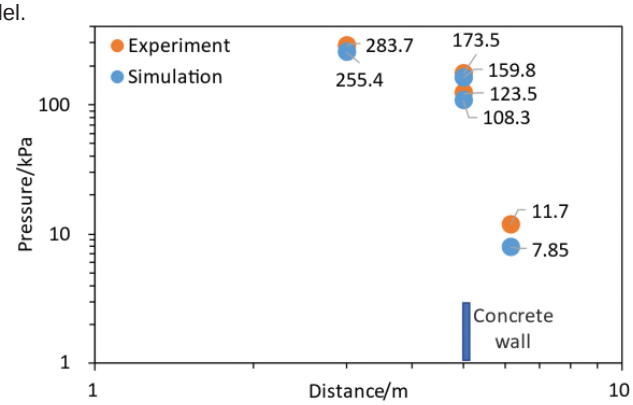
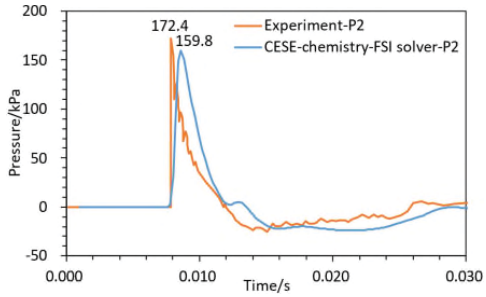
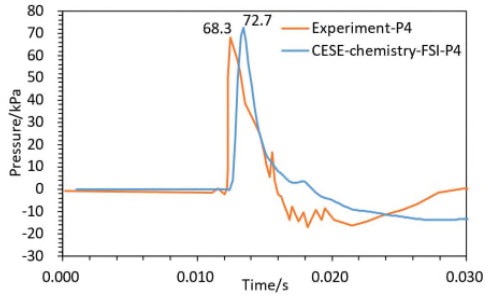


Figure 5: Peak pressure comparison at different distances from the ignition point

Figure 6 illustrates the pressure-time history comparison. It can be noted that the pressure peak and trend at the front side of the blast wall were captured quite well by the numerical model, and the relative differences of peak pressure were less than 10%. The pressure history at the back of the wall was less accurate, but the main trend, such as the dominant pressure peaks and the pressure duration, was reproduced and the peak pressure had a relative error of less than 40%.

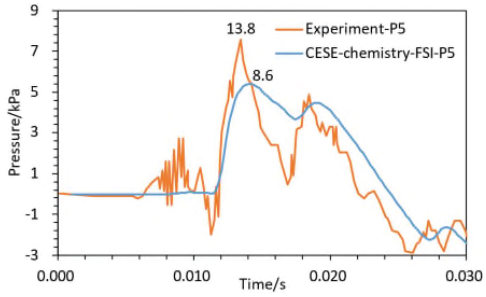


(a) The pressure-time history at the centre of front surface

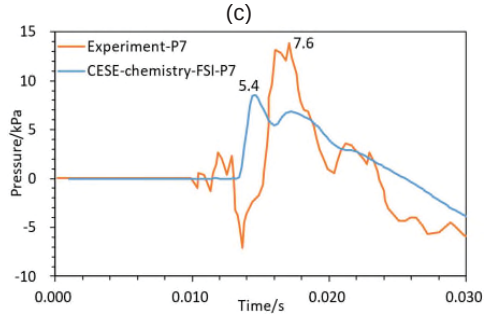


(b) The pressure-time history at the right hand of front surface

(c)



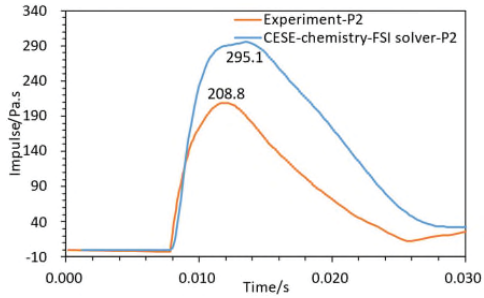
(d) The pressure-time history at the centre of back surface



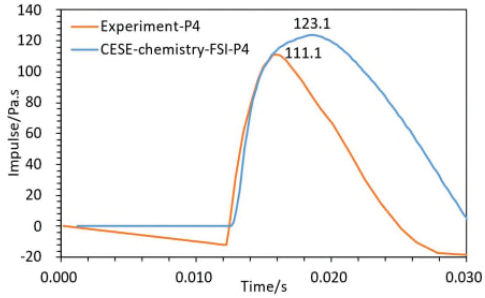
(e) The pressure-time history at the right hand of back surface

Figure 6: The pressure-time history at the front and back of the blast mitigation wall

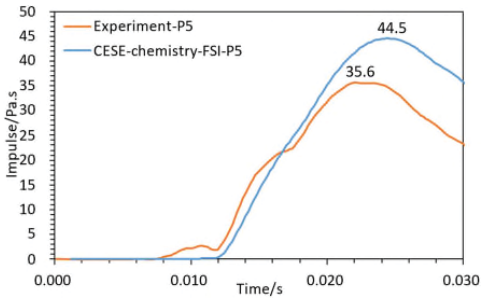
Figure 7 shows the impulse-time comparison oh the front and back of the wall. Again, the trend of impulse was captured well by the numerical model, although the peak impulses from the numerical simulation were slightly higher than the experimental ones, which tends to give conservative prediction for blast mitigation design.



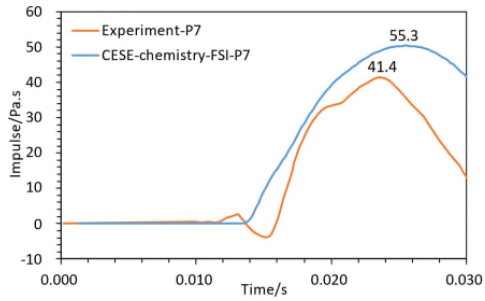
(a) The impulse-time history at the centre of front surface



(b) The impulse-time history at the right hand of front surface



(c) The impulse-time history at the centre of back surface



(d) The impulse-time history at the right hand of back surface

Figure 7: The impulse-time history at the front and back of the blast mitigation wall

4 CONCLUSION

In this study, the numerical model of H_2-air detonation against blast mitigation wall was established based on CESE IBM FSI solver combining with skeletal H_2-air reaction mechanism. Good agreement between the numerical results and experimental data was observed.

ACKNOWLEDGEMENT

This work was supported by the Australia Research Council under ARC Discovery Project DP210101100.

REFERENCES

[1]. Council, H., Hydrogen scaling up: a sustainable pathway for the global energy transition. 2017.

[2]. Australia's National Hydrogen Strategy. 2019, Council of Australian Governments Energy Council: Australia.

[3]. White Paper 2020 on China's Hydrogen Energy and Fuel Cell Industry. 2019, China Hydrogen Alliance: China.

[4]. Chen, D., et al., A numerical study of gas explosion with progressive venting in a utility tunnel. Process Safety and Environmental Protection, 2022. 162: p. 1124-1138.

[5]. Nozu, T., et al., Numerical Simulation of Hydrogen Explosion Tests with a Barrier Wall for Blast Mitigation, in Proceedings of the 1st International Conference on Hydrogen Safety. 2005: Pisa, Italy.

[6]. Zhang, Z., G. Cook and Jr. K. Im, Overview of the CESE Compressible Fluid and FSI Solvers, in 16th International LS-DYNA Users Conference. 2020: Virtual Event.

[7]. Chang, S., The Method of Space-Time Conservation Element and Solution Element—A New Approach for Solving the Navier-Stokes and Euler Equations. Journal of computational physics, 1995. 119(2): p. 295-324.

[8]. Cook, G., Z. Zhang and K. Im, Applications of the CESE method in LS-DYNA, in 21st AIAA Computational Fluid Dynamics Conference. 2013: San Diego, CA.

[9]. Zettervall, N. and C. Fureby, A Computational Study of Ramjet, Scramjet and Dual-mode Ramjet Combustion in Combustor with a Cavity Flameholder, in 2018 AIAA aerospace sciences meeting. 2018: Kissimmee, Florida. p. 1146.