FSI with Detailed Chemistry and their Applications in LS-DYNA® CESE Compressible Solver

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Abstract

Recently, we have developed a new module of the modeling fluid structure interaction with the finite-rate chemistry in compressible CESE solver, which is based on the immersed bounday FSI method, and fully coupled with the LS-DYNA® structual FEM solver. In the CESE fluid structure interaction solver, we have two principal treatment methods, i.e., the immersed boundary method with a direct-forcing strategy and the moving mesh method. Although the moving mesh method is more accurate than the immersed boundary method, the latter is most efficient and robust when the problem involves large deformation such as a structure demolition by explosion. In the present report, we have demonstrated most practical fluid structure interaction problems by using the immersed boundary method with chemistry: i) shock-induced combustion in front of a spherical projectile moving at supersonic speed, ii) the blast refief wall simulation in methane and air mixture (CH_4/Air), and iii) the fracture of the shell and solid structures by high explosive spots in an H_2/O_2 premixed environment. The results are validated with existing experimental data and descriptions of the keyword setup are provided in details for users.

1 Introduction

The fluid structure interaction (FSI) problems at which either an internal or external fluid flow interacts with one or more solid stuructures play prominent roles in many scientific and engineering fields. However, a comprehensive study of such problems remains a challenge due to the strong nonlinearity and multidisciplinary nature [1-3]. Furthermore, analytical solutions for most FSI involved problems are not possible to obtain, whereas experiments in laboratory are limited in their scope. Thus, the numerical simulation models are greatly necessiated to investigate the fundamental physics involved in such complex interaction between fluids and solids.

LS-DYNA® is a well-known general-purpose highly nonlinear, transient dynamics finite element mechanical software capable of simulating complex real world problems, and is widely used in automobile, aerospace, construction, manufacturing, and bioengineering industries. By coupling with the LS-DYNA® FEM structural solver, we developed a CESE-FSI solver with detailed chemistry for solving the safety and explosion problems. Currently, we provide two FSI technics: a moving mesh method (MMM) and an immersed boundary method (IBM). In the MMM, the fluid mesh follows the structural interface motion and the interfaces between the fluid and the structure are treated as moving solid walls. The MMM is a natural extension of the CESE framework and thus it can be applied to solve more accurate problems such as a fluid boundary layer calculation. However, it takes more time to solve a problem since it requires additional calculation time for the mesh motions. Therefore, it is most suitable for small deformation problems. In the IBM, the fluid mesh is fixed and the structure moves through the CESE mesh. FSI interfaces are detected by the CESE solver and treated using a direct-forcing pulsing ghost-fluid approach. So, it is very robust and can handle large deformation problems such as explosions. To demonstrate the IBM FSI with the chemistry solver, the present report slected three practical applications: i) shock-induced combustion (SIC), ii) the blast relief wall (BRW), and iii) the fracture of the shell and solid structure problems.

One of proper problems using IBM FSI is the shock-induced combustion (SIC) in front of a spherical projectile which is moving supersonic speed. The SIC is the self ignited combustion phenomena of premixed gas induced by the flight of supersonic projectile in a combustible gas mixture. Thus, the SIC flow field is characterized by the hypersonic flight and finite rate exothermic chemistry behind the shock wave. Among the various features of SIC, periodically unstable regime around a blunt body would be a most interesting case due to ist naturally oscillating phenomena [4].

The flammable gas could be released due to internal structure ruptures in a off-shore plant and then, such gases will entrain air to form an explosive gas mixture. An accidental gas explosion may occur when the gas mixture meets a suitable ignition condition in a local position. In such a scenario, the BRWs or explosion relief panels reduce consierable damages in structures which may have the potential for explosion in an industrial plant located either on-shore or off-shore [5].

The fractures of the shell and solid structures by high explosive spots can possibly occur in nuclear reactors where the flammable hydrogen-air mixture (H_2/O_2 premixed environment) can be formed easily around the coolants.

The present paper will give the results of the explosion tests using CESE FSI solver with detailed chemistry models such as H_2/O_2 and CH_4/Air reactions.

2 FSI Model

Based upon the treatment of meshes, the numerical procedures to solve these FSI problems can be classified into two approaches: the conforming mesh methods and non-conforming mesh methods. The method with a conforming mesh considers the interface conditions as physical boundary conditions, and it is required that their meshes conform to the interface. Owing to the movement and/or deformation of the solid structure, mesh updating (even re-meshing) is needed as the solution is advanced. So, this method is extremly time consuming and thus not good choice to the explosion problems.

In the non-conforming mesh methods, the fluid-structure interface conditions are treated as constraints on the model equations so that a non-conforming mesh can be employed. As a result, the fluid and solid structural equations can be conveniently solved independently from each other with their respective grids. Moreover, re-meshing is not necessary. LS-DYNA® IBM is a representative method in this category. Here, a force-equivalent term is added to the fluid equations to represent the fluid-structure interaction and to avoid mesh update in the numerical procedure.

Such a IBM was originally developed by Peskin [6] for studying blood flow through a beating heart, and has since been extensively studied and applied to a wide variety of FSI problems. One of its variants is the direct forcing method [7]. By simply imposing the no-slip condition on the fluid momentum equations at the interface, this method directly evaluates the FSI force from the fluid equations with the incorporation of the known structural interfacial velocity through interpolation. One advantage of this method is that it avoids the numerical stiffness usually encountered in various penalty forcing techniques, also it can be used for compressible flows.

In CESE IBM FSI solver, the fluid equations are solved using the CESE method and the solid structural equations are solved by the LS-DYNA® FEM program, while for the elements near the fluid-structure interface it is treated with the direct forcing immersed boundary method, plus the ghost fluid method (GFM) [8]. The fluid solver gets the displacements and velocity of the interfaces from the structural solver and feeds back the fluid pressures to the structural solver as external boundary conditions as shown in Fig. 1.

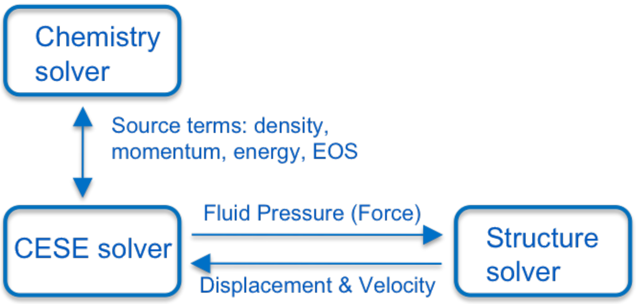

Figure 1 Interface data transfer

The followings are the main steps in the procedure:

1. Generate meshes for the fluid and the structure; those meshes are independent of each other. Then, initialize the flow field and structural state variables.
2. Calculate the shortest distance from the structure boundary to an individual solution element (SE) point. Using the distance, the SE points can be separated as the inner fluid one (A in Fig. 2), nearby fluid point (B in Fig.2), ghost fluid point (C in Fig. 2), or potential fluid point (D in Fig. 2).
3. Solve the solid structural equations using the LS-DYNA® FEM solver based on the structure loading and the fluid-structure interface boundary conditions obtained from the fluid solver.
4. Get the updated fluid-structure interface location and interface velocity from the structural solver.

5. Update the shortest distances (only for the near interface SE points) to get a new inner fluid point, nearby fluid point, ghost fluid point classification.
6. Update the fluid solution for inner fluid points using the CESE scheme.
7. Update the fluid solution for nearby fluid points using direct-forcing IBM, or the regular CESE scheme.
8. Use the ghost fluid method to treat the ghost fluid points since some of them may be needed in the next time step inner fluid point solution calculations.
9. Feedback the fluid pressure to the structural solver as external force acting on the fluid-structure interface as a boundary condition.
10. Go back to step 2 if the termination time has not been reached.

Note that in some cases, the sub-iterations between the fluid and structure solution may be needed in order to make the FSI solver more stable. Also, the conjugate heat transfer solver can be added in the above procedure, in such case, the step 4 need to get one more structural variable i.e., temperature, from the structure solver and also in step 9 the heat flux of the fluid should feedback at the FSI interface.

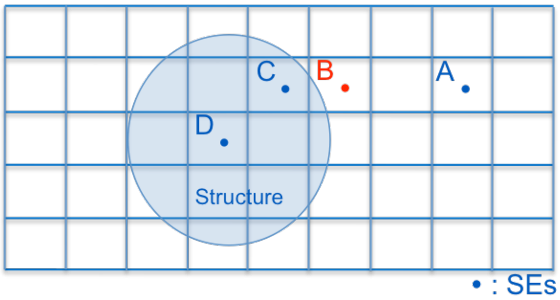

Figure 2 Different SE points in computational domain

The above FSI treatment takes advantage of both the LS-DYNA® FEM structural solver and the CESE method. It is very efficient and robust, and can be suitable for large deformation problems.

3 Results and Discussion

3.1 Shock-Induced Combustion

Figure 3 shows the schematic of the simulation domain of the SIC driving by supersonic bullet and its corresponding shadow image from Lehr's research [4]. Initially, the domain is filled with a stoichiometric hydrogen-air mixture at a pressure of 42663 Pa. The projectile body has a 15 mm diameter hemispherical projectile and cylindrical afterbody. The projectile is flying over the detonation velocity of the gas mixture and the reaction starts near the centerine of the body showing a shock-deflagration system.

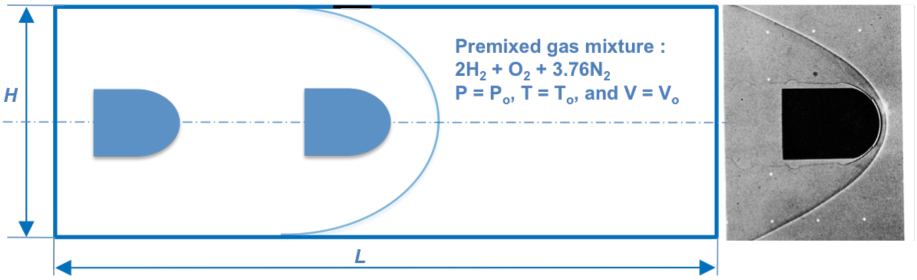

Figure 3 Schematic computational domain of the shock-induced combustion by superonic bullet.

3.2 Blast Relief Wall

The purpose of the blast reflief wall is to vent the combustion gases and pressures resulting from a deflagration within an enclosure so that structural and mechanical damage is minimized. Figure 4 shows a blast chamber with a hinged door presented flammable gas mixed with air. The selected gas mixed with air is methane(CH_4) since it is widely tested in offshore plants and also highly explosives. The combustible limits of the metane in terms of the mixture volume range 5~15 %. Test chamber was desigened as following the NFPA regulation [9]: a cube has the volume of 4 m^3 and the area of a blast relief wall having a material property of SUS 316 or Aluminum is 0.399 m^2. An electric ignitor of 100 J is set at a thrid of the position along the centerline of the chamber shown in Fig. 4.

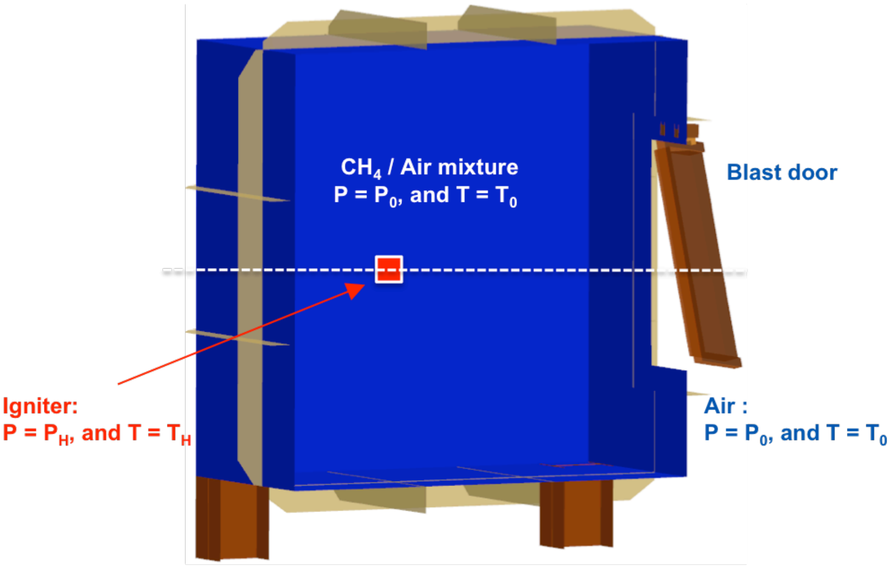

Figure 4 Simulation model of the blast relief wall and blast chamber.

3.3 Fracture of the Shell and Solid Structures

In a containment structure of the nuclear facilities, the hydrogen gas and other volatile radiaactive nuclides were collected and eventually reacted with oxygen, resulting in hydrogen explosion that destroyed the roof and deformed the internal structures. Fracture model of the shell and solid structure is selected here to test our FSI solver with detailed chemistry. Figure 5 shows the heme spherical dome structure constructed inside with bulidings which consist of the solid elements. A stoichiometric high explosive of the H_2/O_2 mixture with a pressure of 30 Mpa and a temperature of 3000K is set at the center position of the domain. The premixed gas mixture (H_2/air) initialized with the lower flammable limmit of the hydrogen gas (4 %) and air is designed outsied of the hemispherical dome.

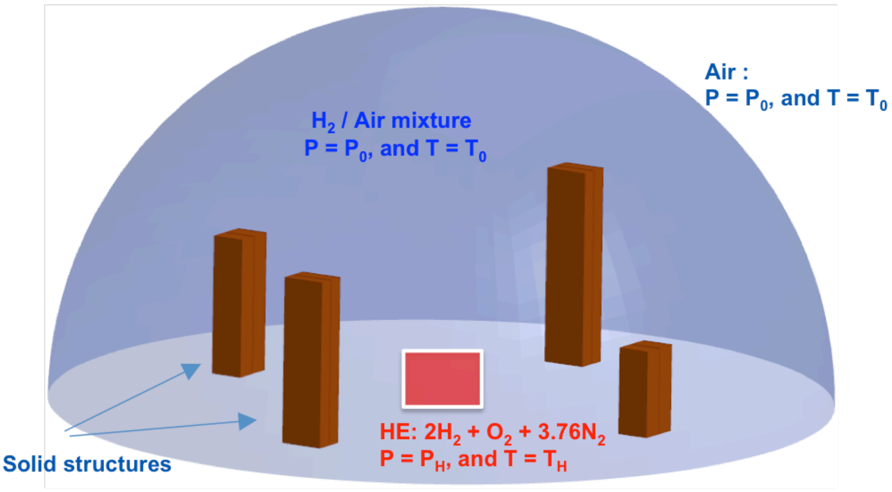

Figure 5 Fracture model of the shell and solid structures by a local high explosive gas.

4 Summary

In the present study, we have demonstrated the performance of the FSI with chemitry for three different practical problems: i) shock-induced combustion in front of a spherical projectile moving supersonic speed, ii) the blast wall simulation in methane and air mixture(CH_4/Air), and iii) fracture of the shell and solid structures by high explosives in H_2/O_2 premixed environment. The results between the numerical simulation and an experimental data set were compared, showing excellent agreement and also the keyword set up for users was illustrated in details. With these developments, we strongly believe that the present solver should provide for users to solve more practical applications in safety and explosion industries.

5 References

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