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Résumé

Recent events have emphasized explosion simulations in industrial risk studies. Two main information are looked for : the pressure time history signal of an air blast ; and the structural analysis to determine the damages undergone by the structural integrity. Most of the software available for explosion studies deal only with the first issue. Moreover a lot of cells are usually needed in the detonation wave to constitute the front after combustion. The usual method consists in developping an 1D spherical wave. Once the wave is formed, it is remapped on the 3D mesh of the real domain. We present here a 3D methodology capable of modeling the combustion of the explosive with only a few cells while getting the theoretical Chapman Jouguet parameters of pressure, density and detonation velocity. The approach was validated against some experimental cases used in the defense domain. Then, this methodology has been applied to an actual industrial risk study. *fluidyn*-FSI has been chosen for the implementation of this method because of its capabilities in fluid-structure interactions. This software allows for a strong coupling between finite volume analysis for fluids and finite elements methodology for structures, which is extremely useful for subsequent structural integrity calculations.

1. INTRODUCTION

Recent events (in particular the explosion of the AZF factory in downtown Toulouse, France) have prompted an increasing interest in explosion simulation for risk studies of industrial units. This kind of explosion studies have been performed so far essentially for military and defense purposes. However, over the years, a lot of potentially hazardous industries have found themselves in densely populated areas, due to population increase and expansion of the cities. Thus an explosion (due to a process accident or to intentional evildoers) can have dramatic effects, not only for the working people on the site but also for people living in nearby residential areas. Two effects have to be taken into account : the physiological impact of the shock wave itself (140 mbar and 50 mbar being the exposure limit for a person) and the impact of the shock on the structural integrity of the buildings.

The knowledge of the pressure time history signal of an air blast is essential to perform a structural analysis and determine the damages undergone by the structural integrity. However, the numerical simulation of an air blast raises a few questions regarding its modeling. In high-energy explosions, there may be more than one explosion zone with a different ignition delay-time for each one of them. Moreover, the shock is extremely thin and requires a great number of elements to be correctly captured by numerical simulations. Therefore the combination of these two aspects implies a prohibitive number of computational elements for an accurate description of the pressure wave propagation due to a detonation.

Most of the software available for explosion studies have to insert 20 to 40 cells in the detonation wave to constitute the detonation front after completion of the explosive combustion. The usual way to overcome this difficulty consists in performing a 1D spherical wave, (assuming a spherical-shaped explosive). Once the detonation wave is formed, it is remapped on the 3D mesh of the real domain. This methodology of course is heavy and prone to difficulties. The explosive charge has to be spherical and cannot take into account random geometry. It also cannot deal with several detonations occurring at various locations and different times, as could happened in a domino-like series of catastrophic events.

In this paper, we present a 3D methodology capable of modeling the combustion of the explosive with only a few cells while getting the theoretical Chapman Jouguet parameters of P, Ro and detonation velocity. The approach was validated against some experimental cases. Two of them are presented here before applying this methodology to an actual industrial risk study. Moreover the numerical code used in this paper, *fluidyn*-FSI, allows for explosion simulation as well as structural integrity calculations.

2. METHODOLOGY

In this paper, we present a simple and efficient solution procedure to propagate the shock following a detonation without the computing costs or difficulty usually associated with these simulations. *fluidyn*-FSI offers several highly conservative TVD schemes which can resolve very sharp pressure gradients. These schemes are used for the simulation of shock propagation directly in the 3D domain, without preliminary calculations in 1D.

The explosive region is meshed as well and is represented by the Jones-Wilkins-Lee equation of state for explosives. This formulation replaces the chemical reaction of combustion. It essentially works on the formation of detonation wave as defined by the Chapman-Jouguet formulation. Thus the wave inside the explosive should verify $P=P_{cj}$, Density=D_{cj} (the subscript cj standing for Chapman-Jouguet) and velocity = detonation velocity as measured in experiments.

The pressure on the walls is then used to perform a structural analysis using fluidyn-FSI, which combines the best methodology for fluids (finite volumes) with the best methodology for structure (finite elements) inside the same solver and with a strong coupling and automatic remeshing.

3. VALIDATION

3.1. Gaseous detonation of a H_2/O_2 mix

The first of the validation cases presented here deals with the gaseous detonation of a H_2/O_2 mix in a hemisphere. The hemispherical mix has a radius of 0.07 m. The composition of the H_2/O_2 mix is stoechiometric and the initial conditions are 1 atm for pressure and 20°C for temperature. The energy released is 6.59 MJ/m^3. The chamber is 0.5 x 0.4 x 0.3 m^3. Due to the symmetry conditions of the domain, only half of the domain has been modeled and meshed with 74 400 cells (figure 1).

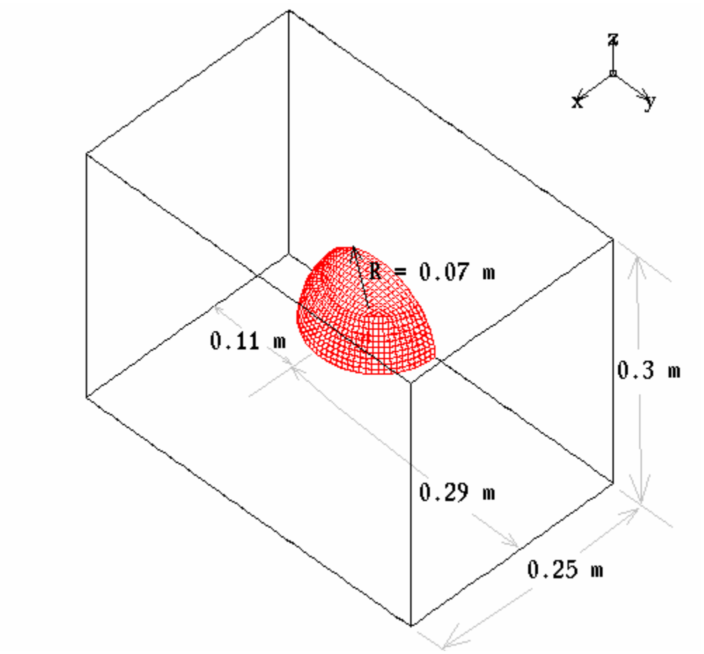

Figure 1 : Geometry and mesh on the explosive

Although it has been developed for solid combustion, the JWL equation of state has been used here. Previous simulations have shown that hydrogen/oxygen detonation behaves a lot like solid combustion and tests using the actual kinetics of the reaction have shown little difference in the results. Therefore, the JWL equation of state has been modified in order to accommodate this almost instantaneous reaction.

Table 1 below presents the numerical results and compares them with the experimental pressures. With respect to the small number of cells used and therefore the small computational cost of the simulation, the numerical results compare very well with the experimental results. The error is about 20% on the time which means less than 0.1 ms except on G1, the first monitor point, which is the closest to the explosion point. Results on G1 can be misleading. This point is so close that even a very small delay in time or pressure will seem significant whereas when the shock develops, the results are quite satisfying. With a finer mesh, even better results can be expected.

Table 1 : Comparison of numerical and experimental results

	First peak			
	Time (ms)		**Pressure (bar)**	
	CFD	***Exp***	***CFD***	***Exp***
G1	0.076	0.113	4.58	3.46
G2	0.39	0.48	2.18	2.4
G3	0.39	0.48	1.62	1.25
G4	0.48	0.585	1.24	1.19

3.2. TNT explosion in a tunnel

An explosion of 18.5 g of TNT occurs at the entrance of a T-shaped tunnel of cylindrical cross section. The tunnel diameter is 168 mm and the parent branch has a length of 1.28 m. The branching takes place at 836 mm and the second branch is 1.5 m long (figure 1). G1, G2, G3 and G4 are monitor points.

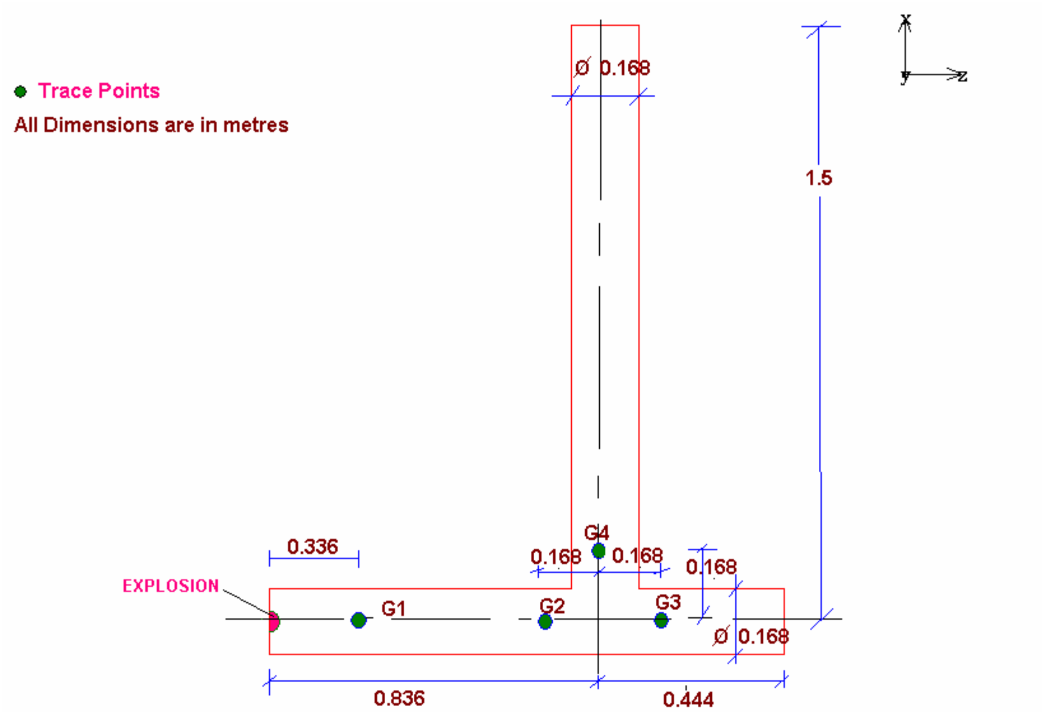

Figure 2 : Tunnel geometry

Due to symmetry in Y-direction (⊥ to plane of tunnel), only half of the tunnel is simulated (figures 1 and 2). The mesh is structured and the domain has been extended outside the tunnel to handle properly the boundary condition at that point (figure 2).

The results concerning the first peak (before reflection on the tunnel ends) are presented in table 2. Once again, the first monitor point is so close that a slight delay in time looks significant although it becomes quite negligeable later on. The experimental results are correctly reproduced at a small computational cost.

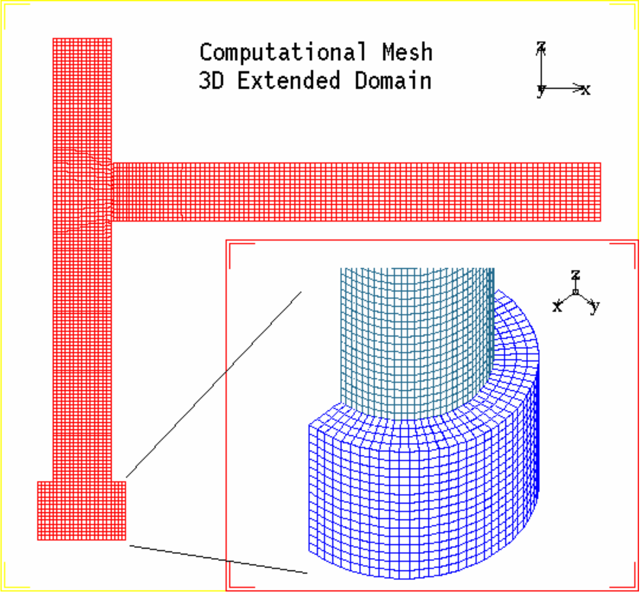

Figure 3 : Mesh of the half tunnel and zoom on the extended domain where TNT is located

Table 2 : Numerical results compared to experiments

	Time		Pressure	
	CFD	*Exp*	*CFD*	*Exp*
	0.151	0.099	30.65	31
G2	0.353	0.47	21.66	18.36
G3	0.589	0.492	13.61	16
G4	0.559	0.505	3.64	4.5

4. APPLICATION TO INDUSTRIAL CASES

Once this approach has been validated against cases used in defence domain, it was applied for risk studies in industrial units. The scenarii described below are typical scenarii for any kind of industry dealing with a boiler. The first case concerns an overpressure in the boiler above the structural limits of the boiler due to some kind of malfunctioning. The second case deals with the leakage of natural gas on a pipe leading to the furnace of the boiler, but will not be presented here.

4.1. Overpressure in a boiler

Figure 5 shows an isometric view of the boiler room inside this typical industrial unit. In green, red and blue colors are represented the doors leading to other rooms and to outside. The windows are represented in yellow. The boiler (not represnted) is located at the center of the room.

The operating point of the boiler is 10 bar. However its breaking point is at 21 bar. Therefore, the value of 21 bar of pressure has been used for the risk study. The TNT equivalent charge has been calculated and located at the boiler location (center of the room). Monitor points are located on the walls and openings.

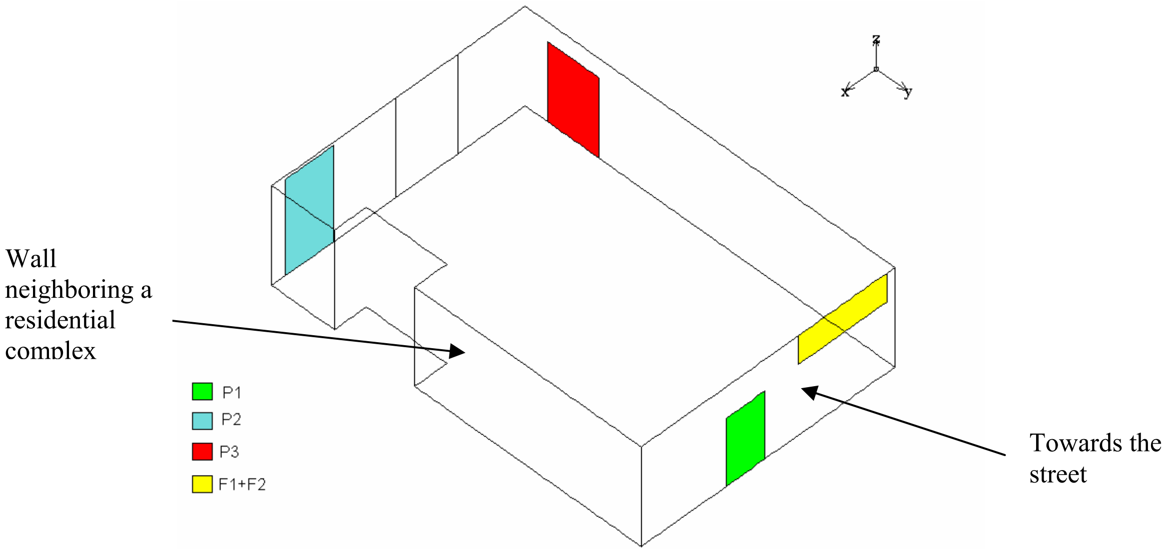

Figure 5 Diagram of the boiler room

The results are shown below. The targets are essentially outside the boiler room (the green door and the yellow windows are opening towards the streets) as well as the wall neighboring a residential complex (figure 5). Figure 6 shows pressure history for the openings (doors and windows : monitor points 1 and 2), figure 7 for the wall next to the residential building(monitor points 8, 9 and 10). The maximum pressure is about 6 bar on figure 6. This value is above the authorized limits. However, the next residential building being across the street at 3.5 meters from there, the wave is expected to decrease to 0.48 bar, which is within allowable values. The maximum pressure exerted on the walls is about 10 bar.

fluidyn-FSI, by strongly coupling the finite volume method to the finite element resolution, makes it possible to infer the structural deformations and rupture from the pressure loads exerted on the walls. Then the structural study performed by *fluidyn*-FSI shows that the wall design on this side of the room enables the structure to keep its integrity, thereby effectively shielding the inhabitants from harmful effects of the boiler blow-up.

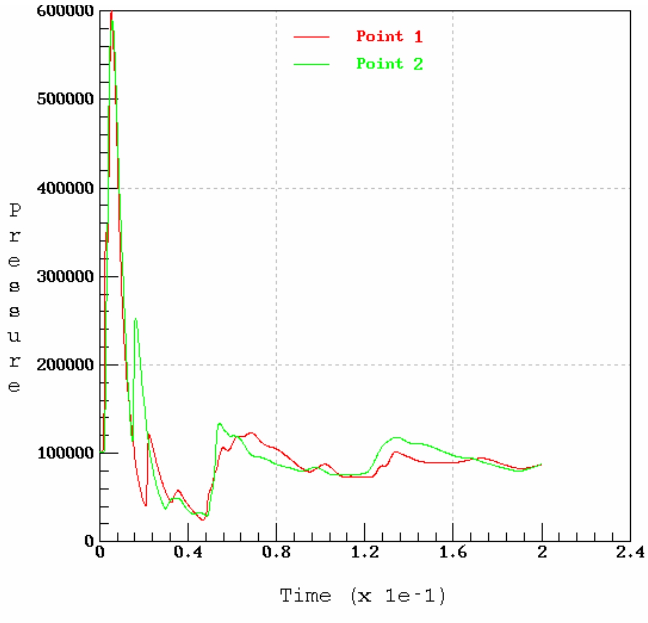

Figure 6 :Pressure trace plots at point 1,2

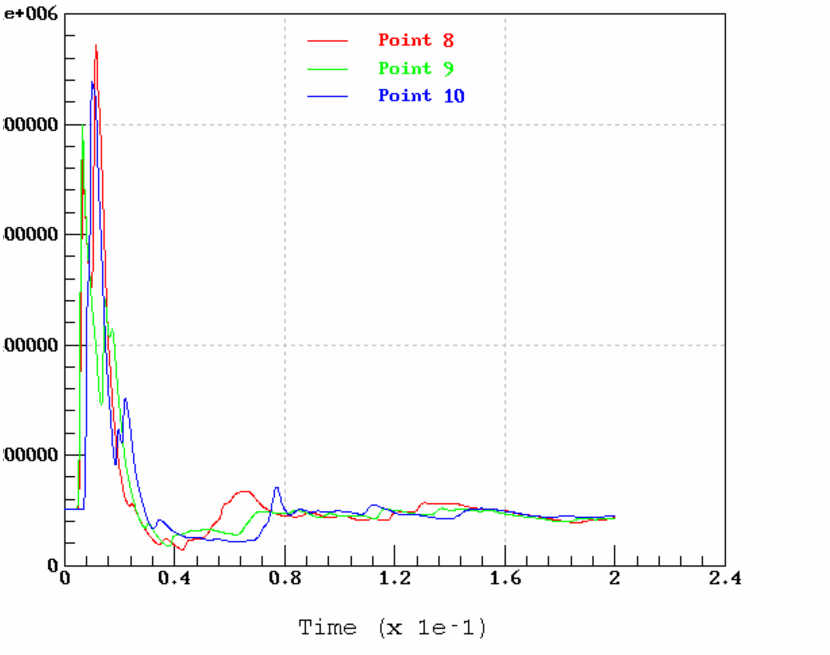

Figure 7:Pressure trace plots at monitor points on wall towards building

5. CONCLUSION

A new methodology has been presented here for simulating explosion in industrial contexts. Based on a non-diffusive scheme, this approach, implemented into fluidyn-NS, allows to model the shock wave by only 4 to 5 cells in the front. This approach has been validated against traditional defense validation cases and applied to industrial scenarii to determine the domains of consequences and structural damages.

REFERENCES

1. Lee E.L., Hornig H.C. and Kury J.W. UCRL-50422 (Lawrence Livermore Laboratory, Livermore, California)
2. Liou M.S., van Leer B. and Shuen J.S. J. of Comp. Phys., **87**, 1-24 (1990).
3. van Leer, B., J. of Comp. Phys., **23**, 276 (1977).
4. Roe P.L., J. of Comp. Phys, **43**, 357-372 (1981).
5. Batten P., Leschziner M.A., Goldberg U.C. J. of Comp. Phys, **137**, 38-78, (1997).