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Detonation of a Reactive Gas Mixture in an Enclosure including the Fluid-Structure Interaction

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Abstract

A numerical model for the reactive fluid flow analysis coupled with the structural dynamics, and fluid-structure mechanical/thermal interaction, Fluidyn-EXPLODE, has been developed. In this model the reactive fluid flow is modeled by solving the 3D conservation equations for the momentum, energy, and species using finite volume method and the nonlinear transient stress calculations are performed by finite element method. The algorithm used for the structural response is large displacement, high strain rate, and explicit resolution to account for the changing material properties of the concrete. In the coupled analysis for the fluid-structure interaction, boundary condition data is exchanged between the fluid and the structure continuously. Pressure is applied to the structure as a force boundary condition, while the deforming structure influences the fluid flow as a moving boundary. To obtain the accurate transmission of a continuously changing pressure loading and to explore the conditions where the structural damage may lead to changed pressure loading, the fluid flow and structural equations are solved simultaneously instead of calculating pressures first and applying them on the structures. Using this model, a typical problem of detonation of a reactive mixture in an enclosure with deforming obstructing structures is simulated. The evolution of the pressure in the domain, the hydrostatic pressure in and the deformation of the structure are presented.

Introduction

Analysis of major hazards in the Industry shows that vapor cloud explosions are mainly linked to deflagration process, leading to subsonic flame propagation. However, in some confined environmental conditions, detonation can be generated, according to the DDT process. In these cases, pressure front reflections from walls may converge in high overpressures in corners and other structurally critical areas. Thus stability loss of a structure such as a vessel or a chemical reactor may lead to an eventual collapse and release of a large volume of toxic/ flammable agent.

The general industry standard for designing a structure such as a vessel or chemical reactor is to accept the detonation pressure as the worst possible loading. Still we have seen many structures collapsing even when the formation of a large stochiometric mixture inside the structure was considered highly unlikely. One plausible explanation is that a small explosion has led to a loss of stability of structure and subsequent release of a much larger cloud. A very frequent hearing of a small explosion, reported before a large explosion, may have its origin in such a scenario. AZF factory explosion in Toulouse is such cases in point.

Unfortunately, contrary to deflagration front, which is relatively weak and may dampen quickly while propagating in an inert medium, a detonation front can be carried to large distances and meet other detonation fronts reflected from walls and other obstacles. Thus the cumulative pressure built-up locally may reach as much as 4 times the detonation pressure. Now as is the general practice, we design the structure such as it can withstand the maximum pressure everywhere the cost will be prohibitive. Thus the general consensus had been to load the fatality factor and accept such consequences. However recent years have seen a considerable increase in size and operational conditions such as pressures and temperatures of vessels and reactors, which increases the cost of such design compromises. A Bhopal, where fatal leak of toxic materials was caused by the failure of a storage tank, is no more acceptable to public awareness today even in a third world country like India.

The objective of this work is to develop a numerical model, which will allow us to identify those parts of the structure, which may have to withstand higher pressures and may need more strengthening. In this attempt, we propose to prepare a model, which will do detailed structural response analysis to an internal explosion. The important aspect of the analysis is the transient coupling of the shock propagation in the structures and the pressure wave inside. The time history of loading and unloading may change the rupture limit leading to early spalling of concrete. This is done by simulating the fluid-structure interaction in a wide range of environments and identifying critical parameters and structural features, which may require a revisit for localized strengthening. Further a test problem is solved to demonstrate its ability to calculate the propagation of a pressure wave generated by chemical reaction of a reactive mixture in a confined volume with obstacles in the form of columns, and to determine the interactions with the structures in the area. Next section describes the computational model used. After this, the physical problem selected to demonstrate the capability of the model is explained. The following section gives the geometric model, boundary and initial conditions and the properties used in the calculation. Finally some of the results are presented.

Computational Model

This section gives a brief description of the computational model used. ***fluidyn*-MP,** a general purpose code for the fluid flow analysis, structural dynamics, and fluid-structure mechanical/thermal interaction, has been in use for several years for defense and nuclear applications. A derived model **Fluidyn-Explode** for chemical, petrochemical industry has been used in the present study. The overpressures in the gaseous media, due to deflagration and/or detonation, are calculated by solving the conservation equations for the mass, momentum, energy, and species in a 3-dimensional framework using the finite volume method. The computational model incorporates a wide range of deflagration, detonation and/or turbulence models and can handle multiple-species, multi-step chemical reaction schemes[1-4]. The response of the structures, which surrounds and interacts with the gaseous media and thus subjected to the transient overpressures, is obtained through a nonlinear transient stress analysis using the finite element method. The algorithm used is large displacement, high strain rate, explicit resolution to account for the changing material properties of the concrete[5,6]. The above models for the reactive fluid flow and structural response have been validated by comparing the results obtained with previous numerical results and experimental measurements. In the strongly coupled analysis for the fluid-structure interaction, boundary condition data is exchanged between the fluid and structure continuously. Pressure is applied to the structure as a force boundary condition, while the deforming structure influences the fluid flow as a moving boundary. Following any structural displacement the fluid domain is re-meshed to account for the change in the shape and size of the domain.

Instead of calculating pressures first and applying them on the structures, we have solved them simultaneously. Not only this solves the problem of accurate transmission of a continuously changing pressure loading but also it helps explore the conditions where the structural damage, such as a total loss of a wall, may lead to changed pressure loading.

Physical Problem

Figure 1 shows the problem domain. It is a rectangular enclosure with square concrete columns inside. The cross-sectional area of each beam is 0.65 m $\times$ 0.65 m and the height is 9.25 m. Initially the whole enclosure is filled with a stoichiometric mixture of ethylene and air at standard atmospheric pressure and 20^{o}C. The ignition point location is at (24.98, 4.1, 0.6) m from the left bottom corner as shown in Figure 1.

In the present calculation the reactive mixture was ignited using a very high ignition energy causing the deflagration wave to accelerate to a detonation wave. Chemical reaction in the mixture is assumed to take place through a single-step global reaction of the form

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O + \Delta Q,$$

where, ΔQ is the heat released due to the reaction. The Arrhenius type of equation was used to calculate the rate of change of mass of different species. (The developed CFD model is general and can incorporate many reactions and the species. It also includes different models for turbulence and eddy break up model for turbulent combustion).

In the present study we have done two computations: (a) with the non-deforming columns, and (b) including the deformation of the columns.

Geometric Model, Boundary and Initial Conditions, and Properties

The entire domain is discretized using 31680 non-uniform Cartesian cells of which 912 are structural elements and the remaining are fluid control volumes. No-slip conditions for velocity with zero flux for scalars are used at the walls. Also, the walls are assumed to be adiabatic. The fluid boundary faces at the fluid-structure interface (surrounding the vertical columns) follow the structural displacement. All the columns are assumed to be fixed at the bottom.

Initially the whole domain is at a pressure of 1.01325×10^5 Pa and a temperature of 300 K. The initial mass fractions of the species, namely C_2H_4, N_2, and O_2, throughout the domain are 0.064, 0.716, and 0.22 respectively. The concrete columns are assumed to be at rest initially.

The fluid properties used are: kinematic viscosity of the mixture = 1.89×10^{-5} m^2/s, Prandtl number of the mixture = 0.72, and mass diffusivity = 2.63×10^{-5} m^2/s. Specific heats for all the species are calculated from the enthalpy values given in JANNAF tables. The structure properties used are: Density = 2400 kg/m^3, Poisson's ratio = 0.3, and Elastic modulus = 14 GPa.

Results

This section presents some of the results of the detonation wave propagation including the fluid-structure interaction. Immediately after ignition the reaction front accelerated to a detonation wave with very high pressure and supersonic speeds. Figure 2 shows the evolution of pressure in a horizontal section at a height of 1m from the bottom. The pressure behind the detonation wave in the unobstructed regions is about 14 bar and the average propagation speed is 2000 m/s.

However, when the pressure wave is obstructed by a structure, either a column or the enclosing walls, the reflections and the combinations of the waves increase the local pressure significantly. Hence, from a structural design or analysis point of view knowledge of the detonation pressure of reactive mixture is not sufficient.

Figure 3 shows the temporal variation of pressure at three monitor points. In the present case the difference between the temporal variation fluid pressure obtained with a rigid structure and a deforming structure was very small. However, under certain circumstances the structural deformation may affect the pressure wave propagation inside a confined volume significantly as seen in a companion study[7].

When the pressure wave hits the columns the structure is subjected to very high hydrostatic pressures. Figure 4 shows the development of hydrostatic pressures in the columns. The hydrostatic pressure is calculated as the average of the normal stress on a structural element. In the present model hydrostatic pressure is positive if the element is subjected to tensile forces and is negative when the element is under compression. It can be seen from Figures 2 and 4 that the evolution of hydrostatic pressure corresponds to that of the evolution of pressure in the fluid. It can also be seen from Figure 4 that loading of the columns subjected to the reflected waves is significantly higher than that is subjected only to the detonation waves.

Figure 5 shows the deformation of the columns due to the pressure waves. It also shows the displacement of the structural elements in the x-direction (see Figure 1). In this model at each time step the mesh in the fluid region is rearranged according to the structural deformation.

Conclusion

The initiation of the detonation of a reactive gas mixture and the consecutive propagation of the pressure wave is modeled. Some representative results show the pressure in the fluid and the corresponding stress in the concrete columns. It is observed that the reflections of the pressure wave from the columns increase the pressure in the fluid near the fluid-structure boundary significantly.

The study demonstrates the capability of Fluidyn-Explode in simulating the fluid-structure interaction. Though a simplified model for the reinforced concrete is used in the study, the steel reinforcements may be modeled separately using beam elements with elasto-plastic material properties. A more accurate formulation using the smeared crack approach to model initiation and propagation of crack in reinforced concrete is under implementation in the code.

References

1. Rosten H.I., Worrell J.K., "Generalised wall functions for turbulent flows", PHOENICS Journal of CFD, Vol 1, No. 1, p. 81, January 1988.
2. Magnussen B. F. and Hjertager B. H., "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion", *16th Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh (1977).
3. Chen Y.S. and Kim S.W., "Computation of turbulent flows using an extended k-ε turbulence closure model", NASA CR-179204, (1987).
4. E.L.Lee, H.C. Hornig and J.W. Kury, "Adiabatic Expansion of High Explosive Detonation Products", May 1968, UCRL-50422, Lawrence Livermore Laboratory,Livermore,California.

5. Belytschko,T and Hsieh,B (1973), International Journal of Numerical Methods in Engineering. Vol. 7, pp 255-271.

6. Kennedy,J.M., Belytschko,T and Lin,J.I. (1986), Journal of Nuclear Engineering And Design, Vol. 97, pp 1-24.

7. K. R. Anil Kumar[1], T. C. Arun Murthy, K. Suresh, P. Pillai, and A. Tripathi, “Modeling of Deflagration and Explosion coupled with the Structural Response” submitted for presentation at the International Colloquium on the Application of Detonation for Propulsion, St. Petersburg, July 6-9, 2004.

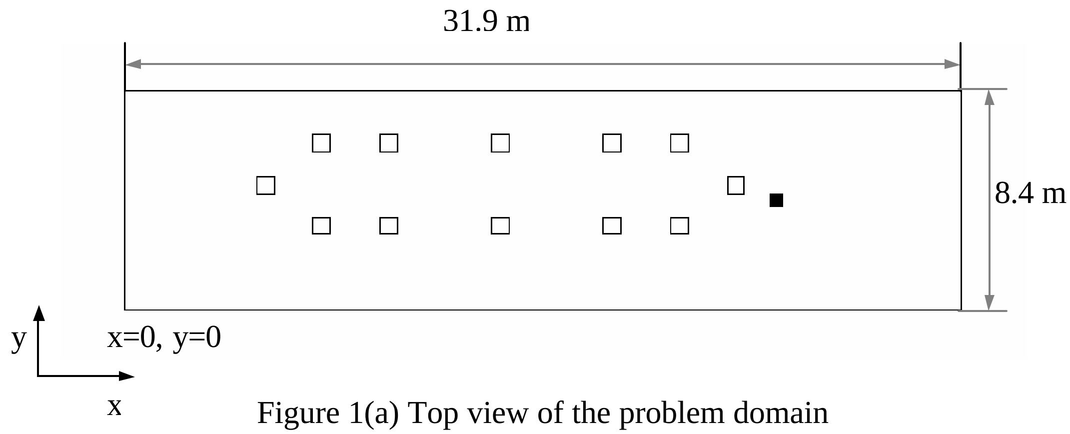


Figure 1(a) Top view of the problem domain

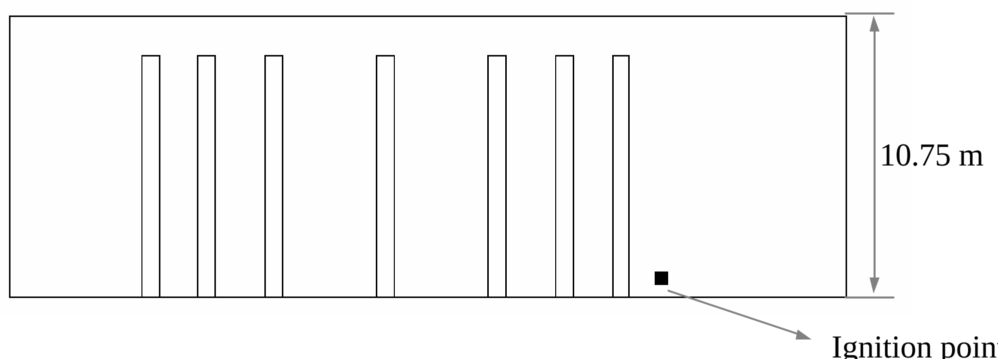


Figure 1(b) Front view of the problem domain

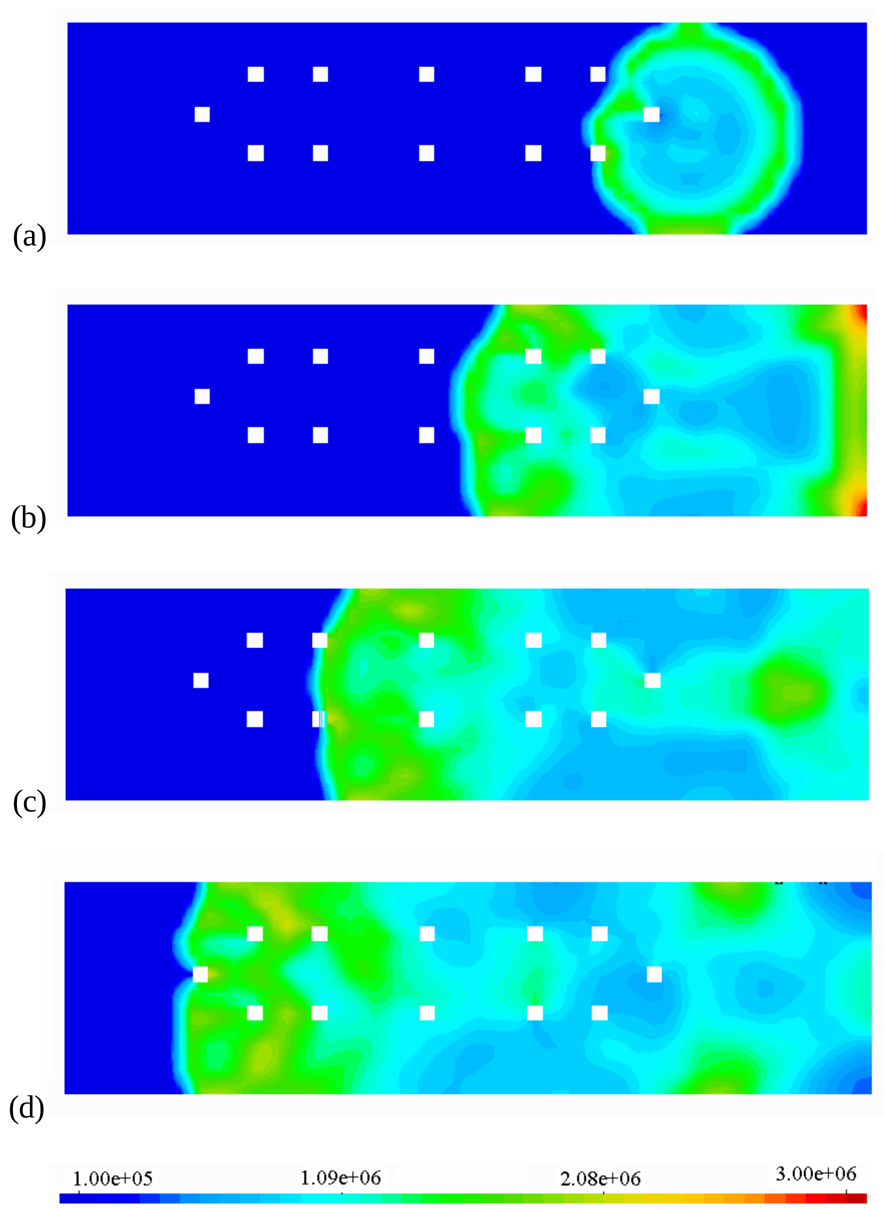


Figure 2: Evolution of pressure, Pa, at a height of 1m:
(a) 0.0025 s, (b) 0.005 s, (c) 0.0075 s, and (d) 0.01 s.

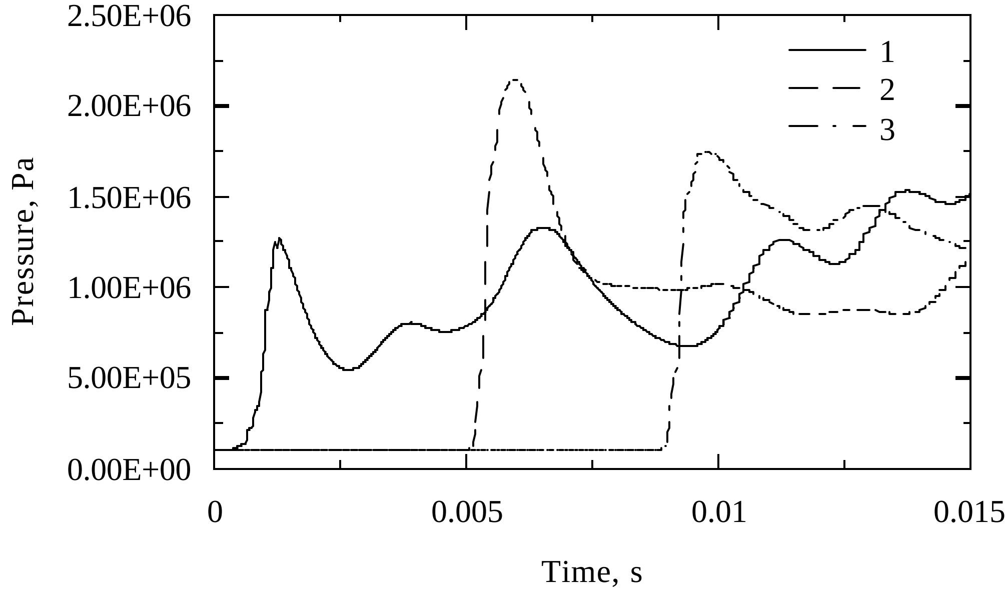


Figure 4: Temporal evolution of pressure at three monitor points with coordinates (in m)

1- (23.9, 4.6,1), 2- (14.9, 3.06,1), and 3-(5.9, 4.6, 1)

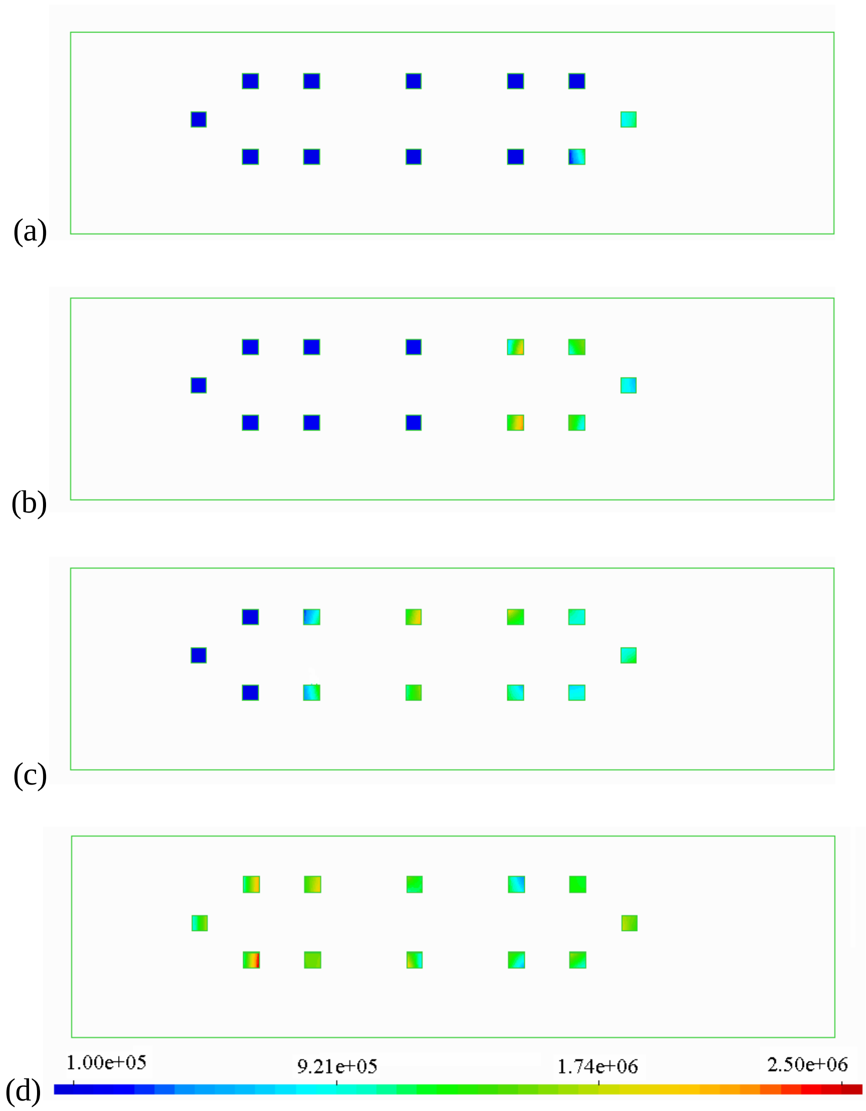
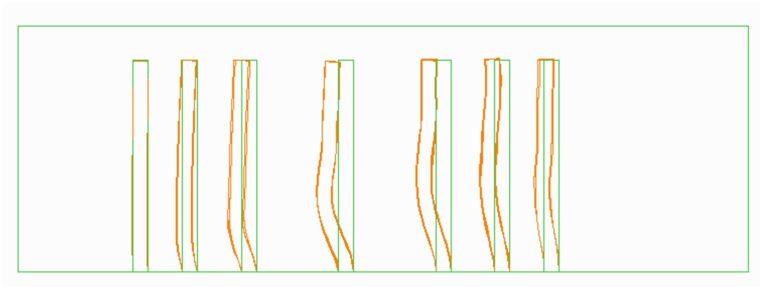
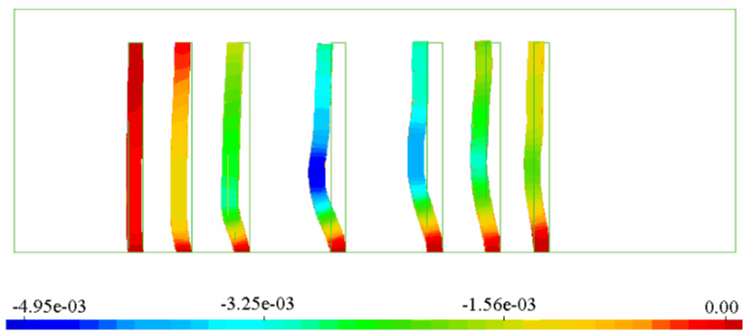


Figure 4: Evolution of the hydrostatic pressure in the structural columns: (a) 0.0025 s, (b) 0.005 s, (c) 0.0075 s, and (d) 0.01 s.



(a)



(b)

Figure 5: (a) Deformation of the columns (magnified by 200 times), and (b) Displacement in the x direction in m after 0.01 s