Multi-dimensional Simulation of Hydrogen Detonations

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Introduction

Since the Three Mile Island accident in 1979, in which the loss of coolant in the reactor core led to hydrogen generation and subsequent burning, studies have been made to assess the risk of hydrogen detonation in Pressurized Water Reactors. When considering complex geometries such as those of a reactor containment with its many compartments and equipments, multi-dimensional effects are important and CFD codes represent a valuable tool for the safety engineer.

From a numerical point of view, the simulation of a detonation induced by obstacles is a very challenging problem, characterized by many shock and wall interactions that can cause quenching and re-initiation. An example of a complex geometric structure in which Deflagration to Detonation Transition (DDT) may occur due to multiple shock focusing is shown in figure 1. This geometry resembles that of the canyon of the RUT facility [1] (Kurchatov Institute, Moscow), where a number of hydrogen combustion experiments have been performed over the past years.

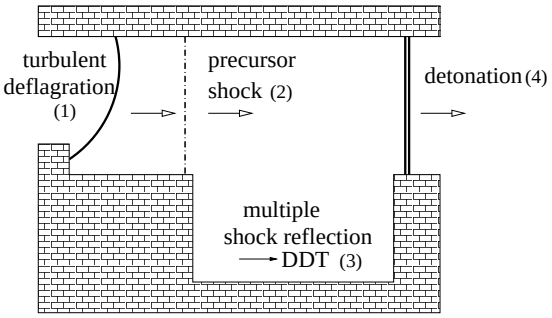

Figure 1: Typical problem geometry

In some of these experiments, the DDT phenomenon is thought to have occurred in four stages: acceleration of a turbulent flame (1) in the 35m long, obstacle-filled channel, generation of a precursor shock (2), onset of a detonation by a yet unclear mechanism involving turbulence and multiple shock reflections (3), detonation propagation (4) down the remaining length of the channel. There have been many investigations concerning DDT in tubes by the use of wall obstacles. The mechanism of onset of the detonation was attributed to the generation of turbulence around the obstacles but more recent studies have also pointed out the importance of the multiple reflections of pressure waves [2, 3].

The work presented here is mainly concerned with the development of a robust and accurate 3D unstructured grid solver for simulating the propagation of detonation waves in complex geometries, and studying the effect of multiple shock reflections on the detonability of the gas mixtures.

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Physical and numerical models

The equations governing inviscid detonation wave propagation are the reactive Euler equations. For the hydrogen case, we have considered considered only four species, hydrogen (H_2), oxygen (O_2), water vapor (H_2O), and nitrogen (N_2). Thermally perfect Joule gas mixtures have also been assumed for which the heat capacities are polynomial functions of temperature [4]. The chemical reaction between hydrogen and oxygen is modelled by a one-step global reaction mechanism, $2H_2 + O_2 \xrightarrow{\dot{\omega}} 2H_2O$ where the reaction rate is given by a general Arrhenius law of the form, $\dot{\omega} = A\rho^3 {Y_{H_2}}^2 Y_{O_2} T^{-b} \exp(-T_a/T)\mathcal{H}(T - T_s)$ (in mol m^{-3} s^{-1}) with $A = 1.1725 \times 10^{14}$ (for S.I units), $T_a = 8310^o$ K, $b = 0.91$, $\mathcal{H}$ is the Heavyside function and T_s a threshold temperature.

The equations are discretized using a 3D unstructured finite volume formulation, where convective fluxes are based on upwind differencing. Higher-order space and time accuracy are obtained by a predictor-corrector scheme and Hancock and linearly exact reconstruction on arbitrary meshes.

Extensive comparisons of numerical fluxes (Godunov, Roe's Flux Difference Splitting, van Leer's Flux Vector Splitting, HUS, AUSM$^+$ and CUSP) have been performed on test-cases involving high speed compressible flows with multiple wave interactions [5, 6]. Their robustness, accuracy, computational cost and sensibility to well-known deficiencies characterizing upwind solvers [7] have been assessed. The following computations are made with the Flux Vector Splitting scheme of van Leer which we have found to be adequate for our simulations.

1D simulation of propagating detonation wave

An unsupported detonation propagating in a 20m long tube filled with a nearly stoichiometric mixture of hydrogen and air at nearly atmospheric conditions ($p = 0.997$ bars and $T = 285$ K) is computed. Experimental data [8] is available for comparison. In figure 2 we have shown the pressure as a function of time at different stations, as well as the diagram $(1/\rho, p)$. Omitting the chemical induction time in the combustion model, a reactive leading shock is computed. The numerical flame speed is found to be about 2100 m/s, in close agreement with ZND theory (2090 m/s). The pressure and density pikes lie between the Chapman-Jouguet and von Neumann states.

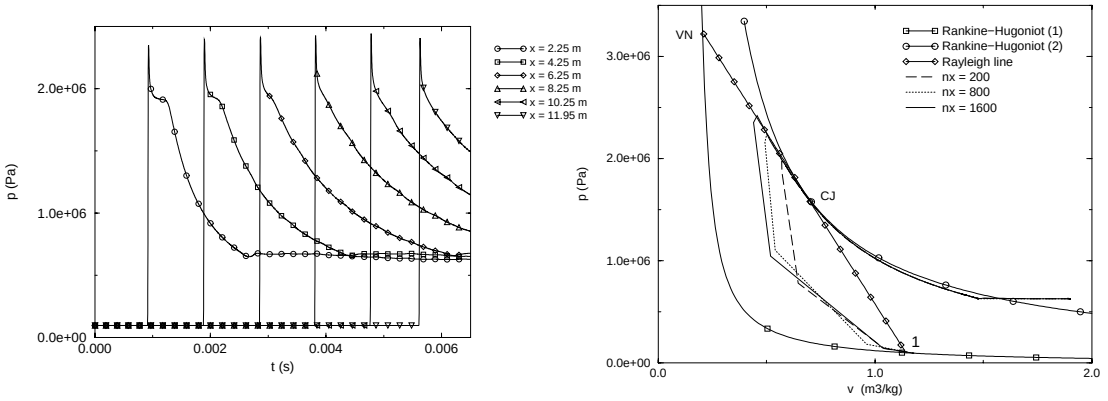

Figure 2: 1D propagating detonation waves; flame propagation and numerical computations in the $(1/\rho, p)$-diagram

2D simulation of detonation wave diffraction around corner

This test case concerns the modelling of the experiment smt4 carried out in the RUT facility. The large-scale containment is filled with a nearly stoichiometric mixture of hydrogen and air at

atmospheric conditions. In this test, a detonation wave, travelling from the inlet channel, diffracts over the corner into the canyon.

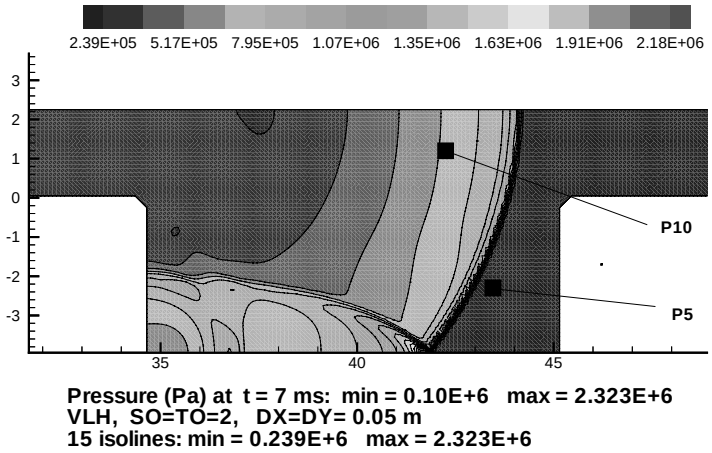

Figure 3: Pressure isolines at $t = 7$ms

In our numerical computation, we have not observed the quenching of the detonation after the diffraction. The reactive shock reflects onto the bottom wall first as a regular reflection, then as a Mach reflection as shown in figure 3. Finally complex multiple shock structures arise when the detonation reaches the right wall of the canyon. In Figure 4 which shows time evolutions of pressure at two stations, relatively good agreement between numerical and experimental results is observed.

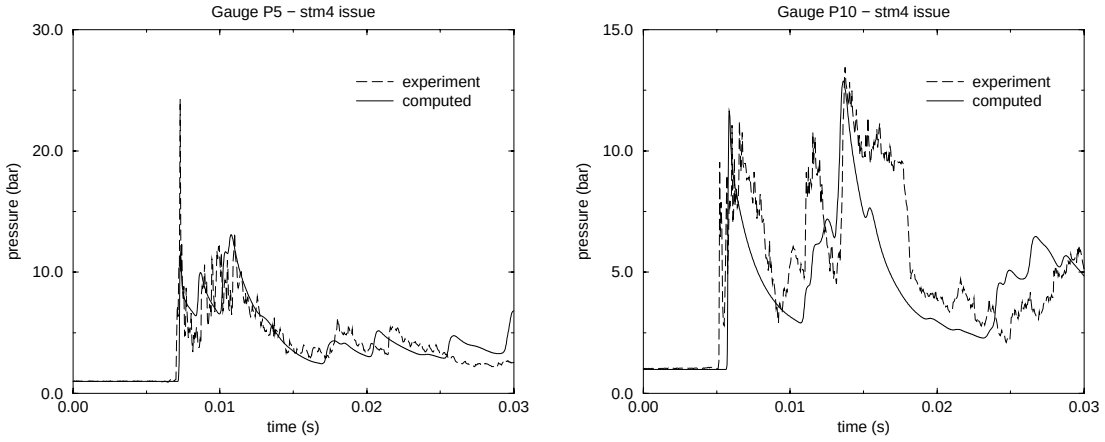

Figure 4: Comparison between experimental and numerical results.

3D simulation of a hemispherical detonation

In this test case, we model a small-scale experiment performed at Laboratoire Energétique Explosions Structures [9] and sketched in figure 5: a soap bubble is filled with a mixture of O_2+2.5 H_2 and the detonation, induced by the vaporization of a copper wire, generates a hemispherical shock wave, which reflects onto the walls of the containment, thereby generating complex wave interactions. Figure 6 represents the pressure signal captured by two transducers: again, simulation results show good agreement with experimental measurements.

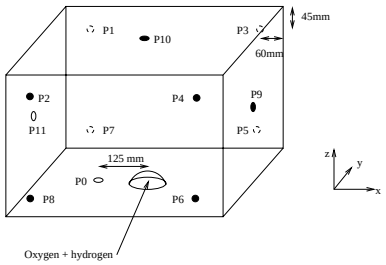

Figure 5: Experimental set-up

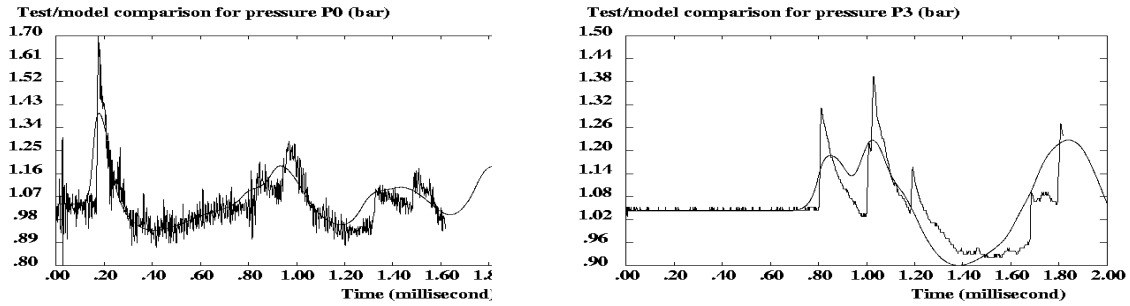

Figure 6: Hemispherical shock wave propagation: experimental and numerical results.

Conclusions

An unstructured solver for computing hydrogen detonation propagation has been briefly described, and three different simulations have been described showing good agreement with experimental data. Future work will focus on the simulation of the onset of a detonation caused by multiple shock reflections.

Acknowledgments

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References

[1] S.B. Dorofeev, V.P. Sidorov, E. Dvoinishnikov, and W. Breitung. Deflagration to Detonation Transition in Large Confined Voluume of Lean Hydrogen-Air Mixtures. *Combust. Flame*, 104:95–110, 1996.

[2] A. Teodorczyk, H. S. Lee, and R. Knystautas. Propagation Mechanism of Quasi-Detonations, 1988. in *Twenty-Second Symposium on Combustion/The Combustion Institute.*

[3] M. Fischer, T. Kratzel, and E. Pantow. Turbulent Flame Acceleration and Detonation Quenching and Reinitiation - Modelling and Validation. pages 401–412, 1996. Proc. of the OECD/NEA/CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques, Winnipeg, May 13-15, 1996.

[4] A. Beccantini and H. Paillère. Modelling of hydrogen detonation for application to reactor safety, 1998. Proc. 6th Int. Conf. on Nuclear Engineering, May 10-15, 1998, San Diego, USA.

[5] A. Beccantini and H. Paillère. Upwind Flux Splitting Schemes for the 1D Euler Equations: Application to Shock Tube and Blast Wave Model Problems. Technical report, CEA DMT, 1997.

[6] A. Beccantini and H. Paillère. A Two-Dimensional High Order Unstructured Grid Solver for Unsteady Shock Propagation Problems. Technical report, CEA DMT, 1998.

[7] J.J. Quirk. Godunov-type Schemes applied to Detonation Flows. In J. Buckmaster, T.L. Jackson, and A. Kumar, editors, *Combustion in High-Speed Flows*, pages 575–596. Kluwer Academic Publishers, Dordrecht, 1994.

[8] W. Breitung, H. Massier, M. Möschke, R. Redlinger, A. Veser, P. Galon, and M. Lepareux. Hydrogen-air detonation experiments in complex geometry and their analysis with different codes. FISA-95 Symposium 'EU Research on Severe Accidents', Luxembourg, 20-22 November, 1995.

[9] I. Sochet J. Renard, A. Trimoulet and C. Desrosier. Etude Expérimentale des Interactions Onde de Choc et Structures Lors d'une Explosion en Espace Confiné. Technical report, LEES, Bourges, 1997.