

Simulation of Detonation after an Accidental Release in a Hydrogen Reformer

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1 Introduction

This study focuses upon a scenario subsequent to a catastrophic failure in a reformer in which 1 Nm³ of hydrogen at 10 bar (84 g) is released. The dispersion pattern was determined from numerical simulation of the flow during the release. The dispersion cloud is elongated in the direction in which the release takes place. Obstacles constituted by the various equipments installed in the enclosure have not been taken into account. Because reflections will occur and they constrain the flow, they may actually make the situation worse than as simulated. On the other hand, the simulation assumes a two-dimensional geometry, which has the opposite effect. Three cases have been investigated, corresponding to a detonative ignition taking place respectively 1, 1.4 and 2.0 seconds after the start of the release.

2 Physical Model

The flow is inviscid, non-conducting and reactive. Dispersion patterns at ignition time provide initial conditions, and further dispersion as the detonation propagated was neglected. A single step kinetic scheme by Gamezo et al. [1] was used. The enclosure walls were taken to be solid walls, and the equipment inside was ignored. The former simplification only becomes important when shocks reach the boundary; clearly if the enclosure is not fully rigid, moves or breaks, the reflection might not be like it would be for a rigid wall. As to the complex set of equipment inside, its main effect is probably to provide obstacles, thus enhancing the risk of deflagration-to-detonation transition (DDT). To simulate ignition, energy was initially added in a narrow region. Results show that not in all cases detonation occurred as a result, and that a DDT process could take place subsequently at another location.

3 Numerical Solution

The code used is derived from a code originally developed by Xu et al. [2], based upon an ENO scheme, that we have modified extensively and parallelized using the MPI protocol. We have used it extensively [3, 4, 5, 6], primarily to study detonation cells with a number of simplified kinetic schemes. In the results below, accuracy is second order both in space and time.

The grid used corresponded to 2000 cells in the length equal to 2.9 m, and 1400 cells in the height which was 2.1 m.

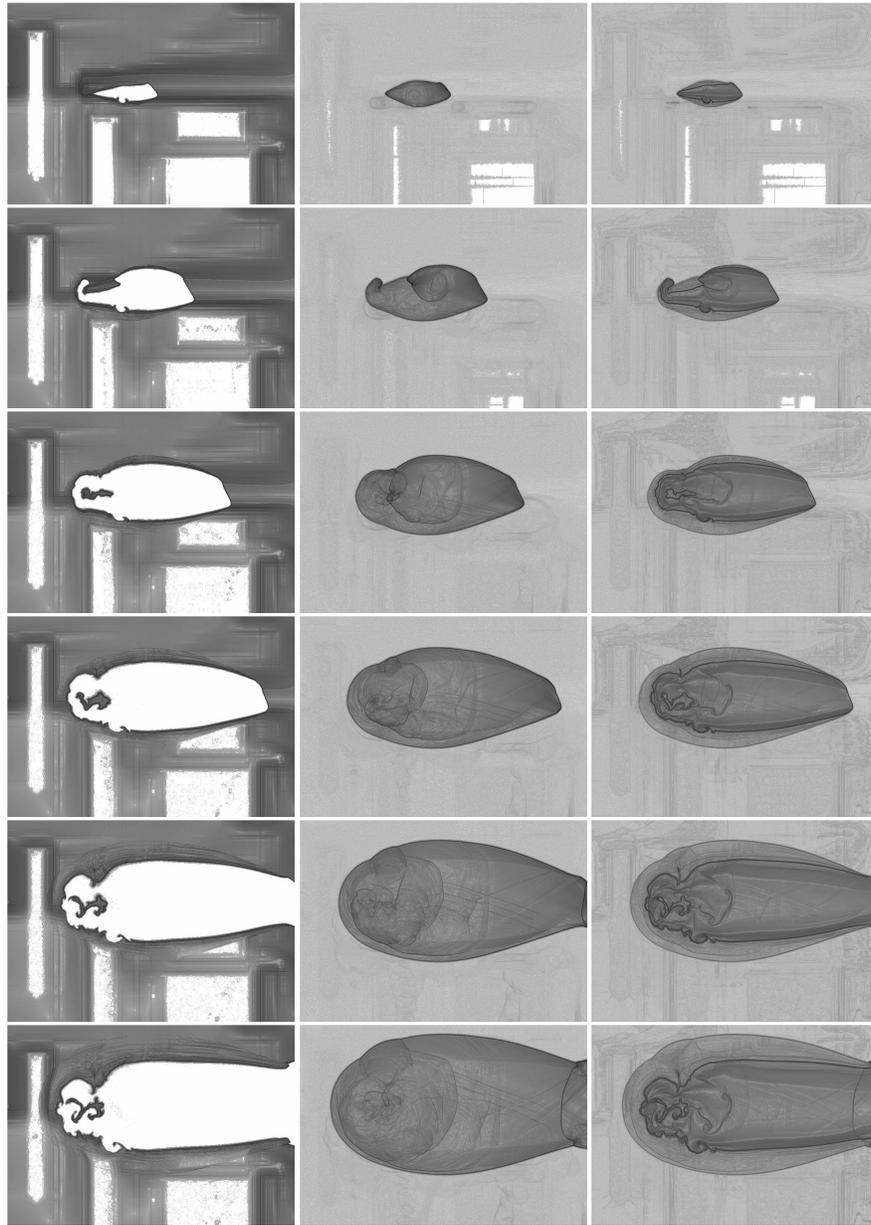


Figure 1: Mass fraction (left), pressure (center) and temperature gradients (right), from top to bottom, 1.76, 3.52, 5.28, 7.04, 8.80 and 10.56 ms after ignition, for ignition 1.0 s after release

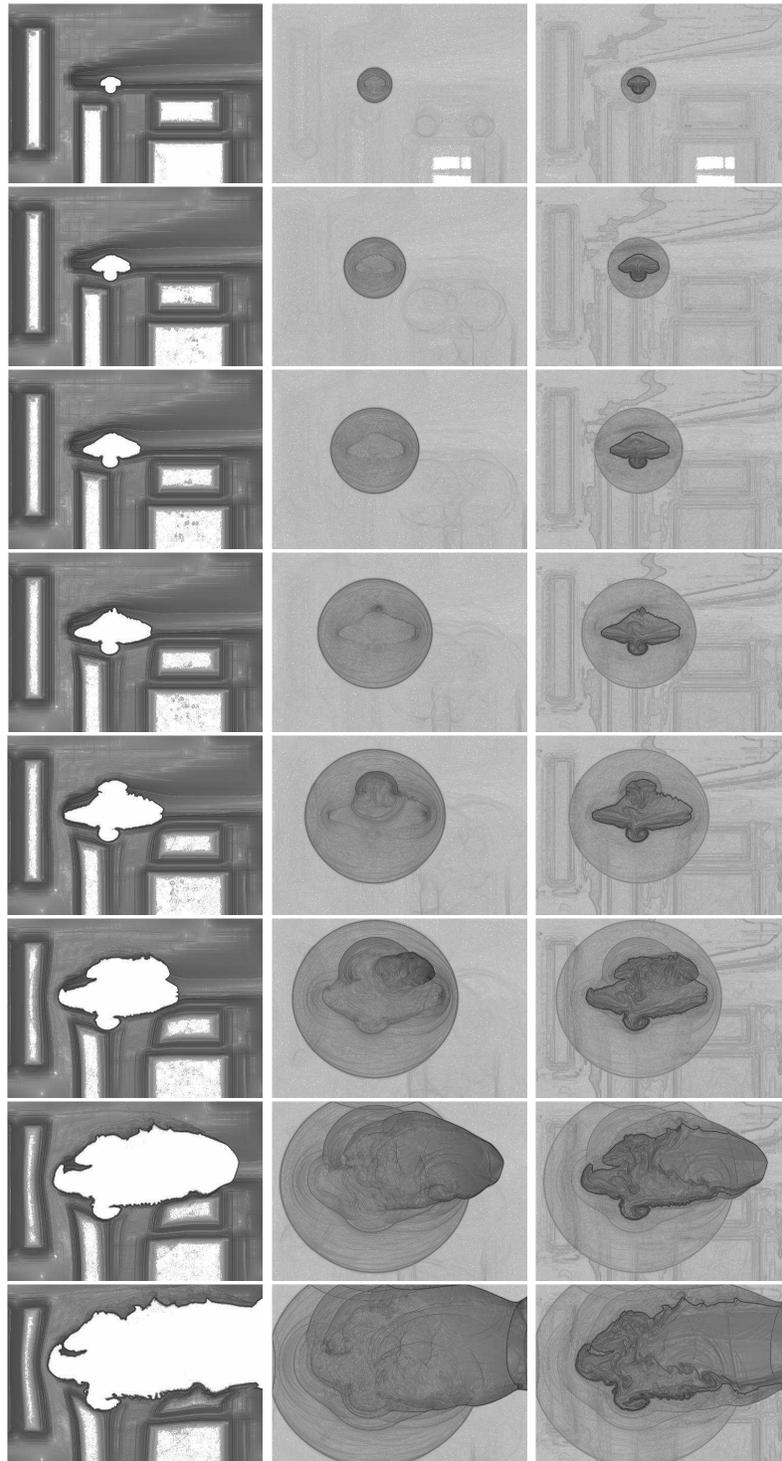


Figure 2: Mass fraction (left), pressure (center) and temperature gradients (right), from top to bottom, 3.52, 7.04, 10.56, 14.08, 17.60, 21.12, 24.64 and 28.16 ms after ignition, for ignition 2.0 s after release

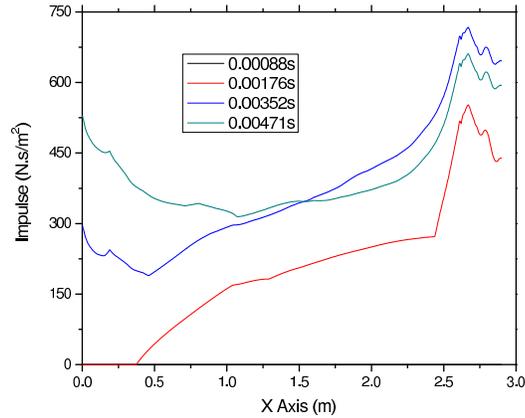


Figure 3: Impulse on the top wall, for ignition 2.0 second after release

4 Results

Results are shown in Figures 1 and 2 respectively for ignition at 1.0 and 2.0 s after release. Results for ignition at 1.4 s are similar to 1.0 s.

The figures show schlieren-like pictures, for mass fraction, pressure and temperature, in a time sequence starting from ignition. Since schlieren-like quantities are derivatives of the primitive variables used in the simulation, they are obtained at one order of accuracy lower than the primitive variables; thus obtaining schlieren-like results that look well-resolved entails a reasonable resolution.

Results appear to differ between ignition at 1.0 s and later ignition. In the latter two cases, initially the detonation fails, but eventually, a deflagration-to-detonation transition event takes place, on the upper right side of the pictures on Fig. 2, after which a detonation wave is clearly seen, propagating rapidly toward the right wall and leading to a reflection.

In contrast, in the first case, the initial detonation does not fail on the right side, but it rapidly moves and reaches the right wall, much earlier than in the other two cases.

Potential reasons for the differences include the difference in concentration fields, and the role of the location of the ignition. Given the relatively coarse resolution used compared with the thickness of the reaction zone, one must also consider the possibility that the timing of the DDT event may be grid-sensitive. Given that even for the current mesh the computation is already large, dealing appropriately with that issue will be difficult. Indeed, how fine a grid may be needed until DDT becomes grid-independent is unclear.

As to the safety issue, all three cases appear to be roughly equivalent. Results for pressure and impulse on the wall, such as for instance, shown in Fig. 3 will be discussed.

References

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