

SIMULATION OF DETONATION AFTER AN ACCIDENTAL HYDROGEN RELEASE IN ENCLOSED ENVIRONMENTS

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ABSTRACT

An accidental hydrogen release in equipment enclosures may result in the presence of a detonable mixture in a confined environment. Numerical simulation is potentially a useful tool for damage assessment in these situations. To assess the value of CFD techniques, numerical simulation of detonation was performed for two realistic scenarios. The first scenario starts with a pipe failure in an electrolyzer, resulting in a leak of 42 g of hydrogen. The second scenario deals with a failure in a reformer where 84 g of hydrogen is released. In both cases, dispersion patterns were first obtained from separate numerical simulation and were then used as initial condition in a detonation simulation, based upon the reactive Euler's equations. Energy was artificially added in a narrow region to simulate detonative ignition. In the electrolyzer, ignition was assumed to occur 500 ms after beginning of the release. Results show a detonation failing on the top and bottom side but propagating left and right, before eventually failing also. Average impulse was 500 Ns/m². For the reformer, three cases were simulated, with ignition 1.0, 1.4 and 2.0 seconds after the beginning of the release. In two cases, the detonation wave failed everywhere except in the direction of the release, in which it continued propagating until reaching the side wall. In the third, the detonation failed everywhere at first but later, a deflagration-to-detonation transition occurred, resulting in a strong wave that propagated rapidly toward the side wall. In all three cases, the consequences are more serious than in the electrolyzer.

1. INTRODUCTION

Detonations in enclosed environments are a safety concern. The structure of a detonation wave results from coupling between shock and chemistry. The leading shock produces a significant increase in temperature. Since chemistry is very temperature sensitive, the reaction rates increase by orders of magnitudes across the shock. Finally, expansion due to the heat released by combustion supports the shock. In a planar model in a uniform concentration gradient, this structure propagates at a fixed speed, at least equal to a minimum value usually referred to as the Chapman-Jouguet (CJ) speed. The CJ Mach number is higher than unity by a fixed, nonzero margin that depends only upon the heat release. The leading shock can cause serious mechanical damage, hence the safety concerns [1, 2].

Hydrogen detonates over a much wider range of concentrations than hydrocarbon fuels, and it requires very little energy to ignite [3, 4, 5]. Therefore, the risks linked to the use of hydrogen as an automotive fuel are of concern. Numerical simulation was used for two realistic situations related to production and distribution of hydrogen, to evaluate its usefulness and limitations for damage assessment.

There are two strategies of choice used to prevent detonations. The first is to avoid all sources of ignition, but with hydrogen, it appears that statics, shock compression and possibly viscous effects [3,4, 5,] may lead to ignition, therefore this strategy may be of limited value. The other approach is to insure that concentrations cannot reach the lower detonability limit. However, in the current leak scenarios, at the location of the leak, hydrogen concentration is 100%, and it drops all the way across the detonability range, down to 0% at locations where no hydrogen has reached yet. Therefore, in leak scenarios, there will be a time window during which presence of detonable mixture is unavoidable.

Two realistic scenarios were modeled, using as initial conditions dispersion patterns obtained from separate simulations of the leak and dispersion process [6]. The first scenario follows from a pipe failure in an electrolyzer, in which the total content, of 42 g of hydrogen, were released at 1 MPa. Ignition was assumed to occur 500 milliseconds after the beginning of the release. The other case corresponds to a similar failure in a reformer, in which the 84 g of hydrogen contained in a reservoir at 1 MPa leak. In both scenarios, detonative ignition was artificially induced by adding energy in a small region. For the reformer, three cases have been investigated, corresponding to a detonative ignition 1.0, 1.4 and 2.0 seconds after the beginning of the release. Initial pressure was atmospheric.

Given the disparity in scale between the enclosure size and the thickness of the reaction zone, appropriately resolving the latter entails a large grid. Although clearly the problem is three-dimensional, simulations were only performed in two dimensions to limit the simulation within a manageable size. This is quite conservative; on the other hand, all equipment inside the enclosure were neglected in the detonation simulations (but not in the dispersion simulations). Reflections on equipment would likely increase the risk of Deflagration-to-Detonation-Transition (DDT).

2. FORMULATION

The flow is described by the inviscid, nonconducting, reactive Euler's equations in conservative form. In both scenarios, the enclosure is represented as a rectangular box, with dimensions corresponding to the dimensions of the enclosure in a vertical plane.

Dispersion patterns were obtained from numerical simulation of a leak, using a commercial code [6], and these patterns are used as initial conditions in the detonation simulations reported here. After ignition, further dispersion was neglected. Except in the very close neighborhood of the hole, velocities associated with the dispersion process are very slow compared to the speed of the wave, which is supersonic. Thus the dispersion pattern changes very little over the very short simulation time. Non-Reynolds-averaged patterns might lead to additional localized spots where DDT could occur, but this could not be dealt with in the current simulations.

The wave thickness is about 1.5 mm. This is quite thin compared with the enclosure, which is nearly 3 m long. A mesh size covering the whole domain and that can resolve the wave properly would entail a huge computation. Although such a large computation might be doable in a research environment, it would not be economically practical in the context of risk assessment. Consequently,

chemistry was modelled using a single-step Arrhenius rate recently used by Gamezo et al. [7] (including heat release and gas properties). All freely propagating waves tend to travel at the minimum (Chapman-Jouguet) wave speed (CJ-speed). This speed depends only upon the heat release, but it is not affected by the details of the kinetic scheme [1]. A more complex scheme could easily be used, as in Liang & Bauwens [8, 9, 10] including features such as chain branching [11, 12], but the effect of the concentration gradient due to dispersion on propagation speed is handled by the single step model. Given that the resolution used provides with no more than one or two grid points across the wave thickness, any advantage of a more detailed scheme would be illusory. The reactive Euler's equations effectively consist of Newton's law coupled with an Arrhenius rate equation, which are fundamental and as such do not require "validation" by comparison with experimental data. This model will naturally yield the correct CJ wave structure, consistent with the heat release.

The walls of the reformer are assumed to be rigid. Shock reflection will be affected by wall rupture and motion. However, because of inertia, the time scale describing wall motion is long compared to the time scale associated with wave propagation. The equipment inside the reformer was neglected; it is likely that the equipment would cause more reflections, which might help triggering deflagration-to-detonation transition (DDT).

The simulation was performed in two dimensions, taking the dispersion cloud in the vertical symmetry plane in the longitudinal direction. Performing the simulation in 2D is a conservative assumption but is in some way compensated by neglecting the equipment inside. As seen below, resolution is already a major concern in 2D; a three-dimensional simulation of comparable cost would be useless because of lack of resolution. Likewise, there is no reasonable way to translate the actually three-dimensional internal obstacles into a 2D equivalent; instead, it was elected to neglect them.

To simulate detonative ignition, an amount of energy sufficient to produce a shock stronger than the CJ wave is added to four simulation cells that are meant to correspond to the ignition location.

3. NUMERICAL SOLUTION

The code that was used for the numerical simulation is based on an ENO ("Essentially Non-Oscillatory") algorithm. It was originally developed by Xu et al. [13]. That code was extensively modified; it was parallelized using the MPI ("Message-Passing Interface") protocol, and optimized for parallel computer architectures. It is well-validated and it has been used extensively for numerical studies that dealt with the relationships between chemical kinetics models and detonation cells [8, 9, 10, 14]. It is second order accurate in space and time except for flux limiting, near shocks.

4. RESULTS

4.1 Electrolyzer

The process described above has been used to simulate detonation in an electrolyzer [15]. The electrolyzer enclosure is taken to be a box having a width of 4 m and a height of 2.54 m. It has been discretized into 2000 cells in width, and 1778 cells in height. A leak of 42 g of hydrogen results from a pipe failure. The dispersion pattern after 500 ms, obtained from a separate simulation [6], is shown in Fig. 1. Results from the detonation simulation are shown in Figs. 2 and 3, for ignition 500 ms after beginning of hydrogen release. The results are shown as Schlieren-like pictures, for mass fraction,

pressure and temperature gradients, respectively. Schlieren-like quantities represent the first derivative of the primitive variables obtained from the simulation. This means that those quantities are one order of accuracy lower than the primitive variables. For the pictures to have a high resolution requires that the computation be done using a very fine mesh. On the pictures, faint traces observed in the unburnt region are simply a result of the numerical noise coming from the initial concentration gradient.

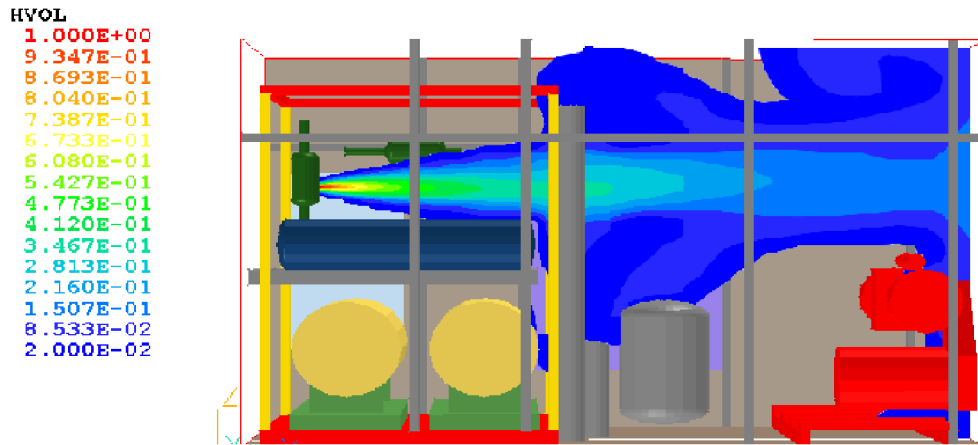


Figure 1. Hydrogen dispersion in the electrolyzer after 500 ms

The ignition location corresponds to the center of the burnt region in Figure 3. After ignition, the detonation propagates into the rich mixture, towards the right on the pictures, in the direction of the release, until it encounters leaner mixture, at which point it fails. (Detonation occurs when the shock and the reaction zone are coupled; this is only observed to occur on the right and left on the results.) At the top and bottom, the detonation fails; the shock, represented by the outer dark line, easily visible on the temperature gradient plots, is now no longer at the same location as the concentration jump. Between the second and third image (between 352 and 704 μ s), the shock and the reaction front decouple also on the right side. Finally, the detonation on the left side also fails, meaning that it has now failed everywhere. After failure, the leading shock weakens since it is no longer supported by chemistry. As a result, temperature behind the shock drops, causing the chemistry to slow down.

The white regions observed on the mass fraction plots represent combustion products. It is clear on the results that chemistry is distinctly slower after failure, since the interface separating burnt and unburnt nearly stops propagating. The interface is subject to hydrodynamic, Richtmyer-Meshkov and Rayleigh-Taylor instabilities, which can be observed on the upper side. These instabilities result in a convoluted reaction front, which is observed later in the computation (not shown).

The shock is easy to see on both the temperature and pressure gradient plots, but the reaction front is more obvious on the temperature gradient plots. This is easily understandable since both the shock and the reaction front are the locus of large temperature jumps.

Because of the shape of the enclosure and the location of the leak, the shock quickly reaches the top of the enclosure while it is still strong. It will also eventually reach the other walls but since it is weakening after decoupling, the impulse on those walls will presumably be less damaging than on the top. It hits the top section after approximately 1100 μ s, and subjects the top cover to high peak

pressure for a very short period of time. Given that the peak pressure is so short, impulse is probably more relevant from a safety standpoint. On average, its value is around 500 Ns/m². Results for impulse on the left, right and top wall are shown in Fig. 2. Given that the ceiling panels have a mass per area of 10 kg/m², assuming that their motion is not restricted, this impulse value would result in an initial upward velocity of 50 m/s. However, this estimate is conservative because the current simulation is only two-dimensional and at worst the impulse obtained from the current simulation will apply on the centerline, while dropping toward the sides. Also, the dispersion pattern used corresponds to values in the cross-section with the highest hydrogen concentration. In summary, even though the detonation failed before reaching them, the walls were subjected to relatively strong impulse values.

Based upon current results, it appears that safety can be improved by attaching the top panels to the enclosure in a manner that will allow them to stay in place if subjected to impulse values as predicted here. Moreover, it would be advisable to use a material that will readily absorb energy and is capable of deforming plastically.

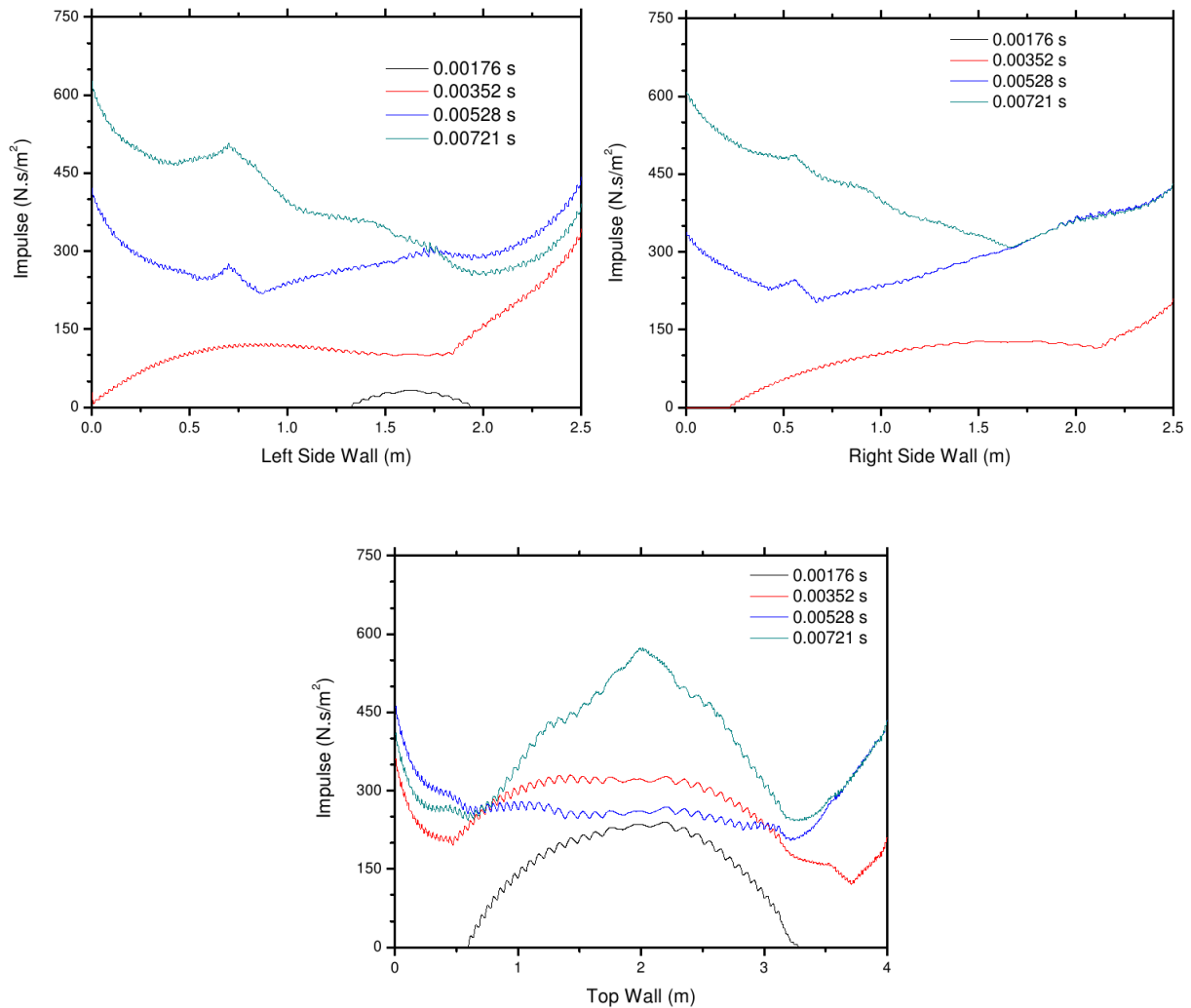


Figure 2. Impulse on left, right and top electrolyzer wall

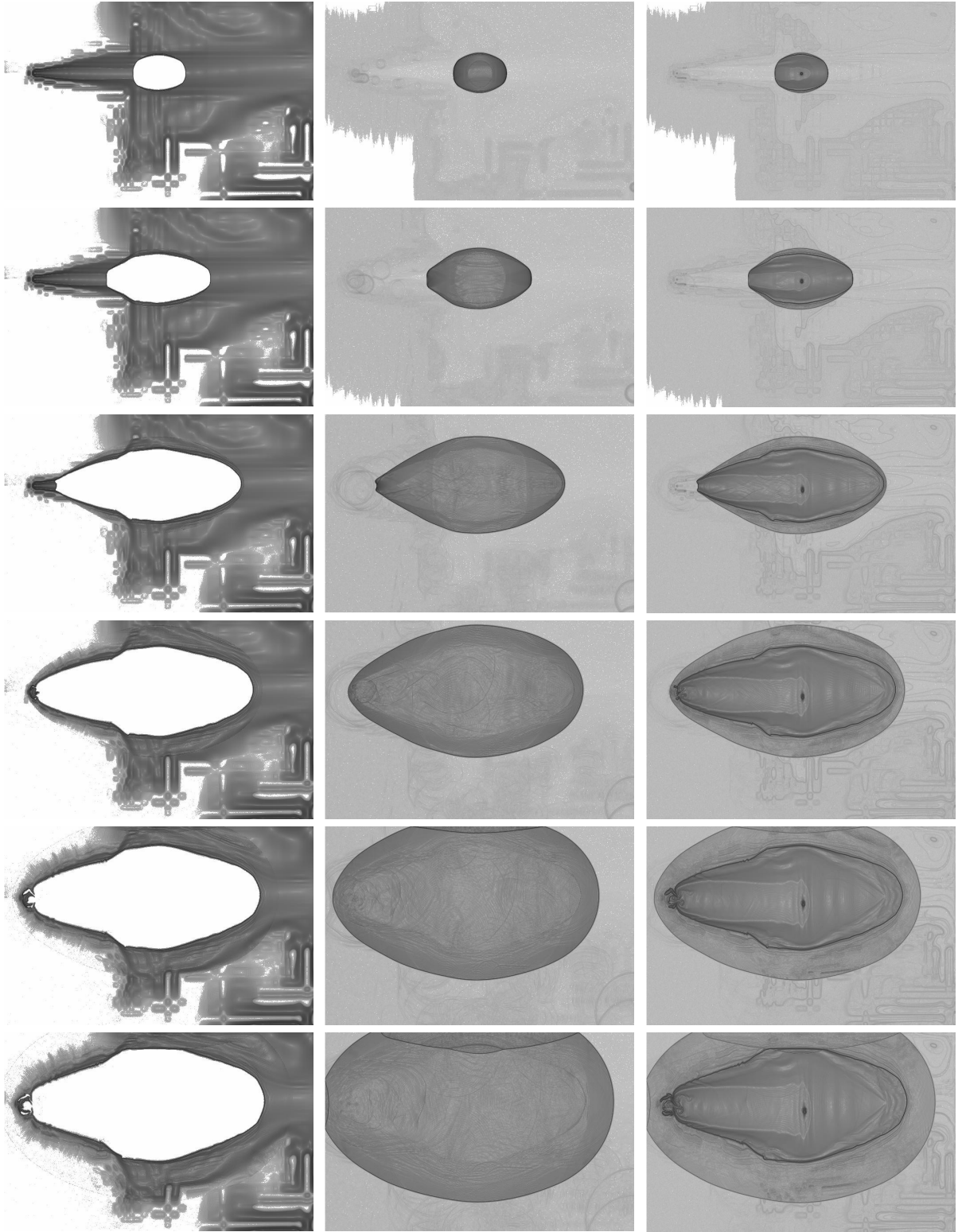


Figure 3. Mass fraction (left), pressure (center) and temperature gradients (right) in the electrolyzer.
From top to bottom, 176, 352, 704, 1060, 1410 and 1760 μs after ignition

4.2 Reformer

A more in-depth description of the reformer case can be found in Bédard-Tremblay et al. [15]. The dimensions of the reformer are 2.9 m and 2.1 m in length and height, respectively. A grid of 2000 cells in width and 1400 cells in height has been used. The simulation models a leak in a tank containing 1 Nm³ of hydrogen, or 84 g at a pressure of 10 bar into the reformer enclosure. All of the hydrogen from the tank has escaped after 1.4 seconds. From this scenario, three different cases were examined: ignition 1.0 s, 1.4 s and 2.0 s after the beginning of the release, all with the same ignition point, but each having as their initial conditions the concentration cloud at the time of ignition. Hydrogen dispersion 1.0 s after the beginning of the release is shown in Fig. 4.

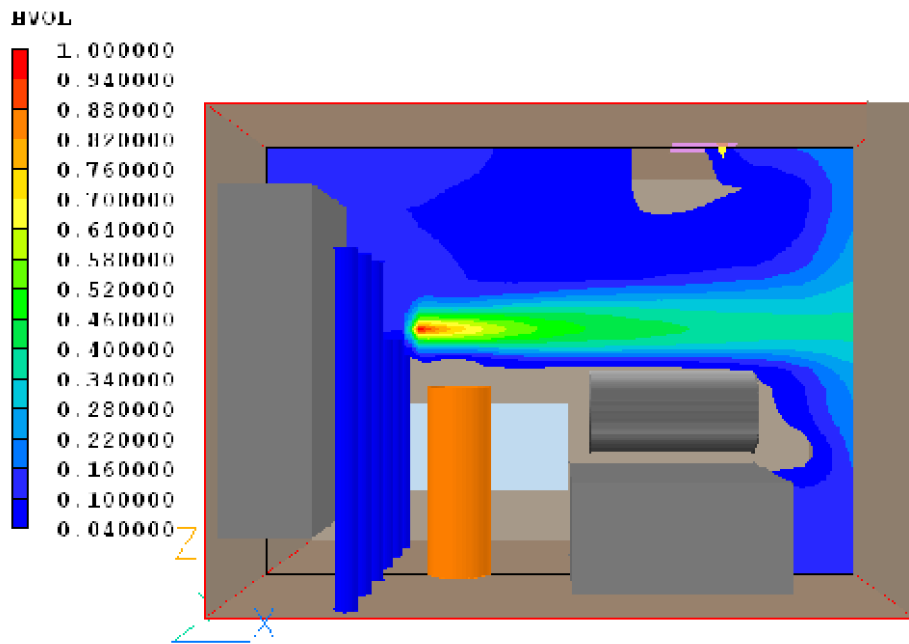


Figure 4. Hydrogen dispersion after 1 s in the reformer

The results are shown below on Schlieren-like pictures, for mass fraction, pressure and temperature gradients, in a chronological sequence from the time of ignition. Fig. 5 shows the results for the 1.0 s case.

Results for the 1.0 s and 1.4 s scenarios are somewhat similar; they show a detonation that fails everywhere except on the right hand side, where it propagates rapidly to the right wall. In the 2.0 s case the detonation first fails everywhere, but later a deflagration-to-detonation transition (DDT) occurs on the right and then the wave travels rapidly towards the right wall. As a result, in the 2.0 s case, the detonation wave reaches the wall much later than in the first two cases. The results for the 2.0 s case are shown in Fig. 6. A detonation reaches the enclosure wall on the right side in all three cases. This can be explained by observing the concentration cloud, where the right is the only region rich in hydrogen, supporting a detonation wave or at least faster chemistry. To verify whether the DDT prediction was sensitive on resolution, the 2.0 second case was repeated using a grid twice as large (4000 by 2800). Results are shown in Fig. 7.

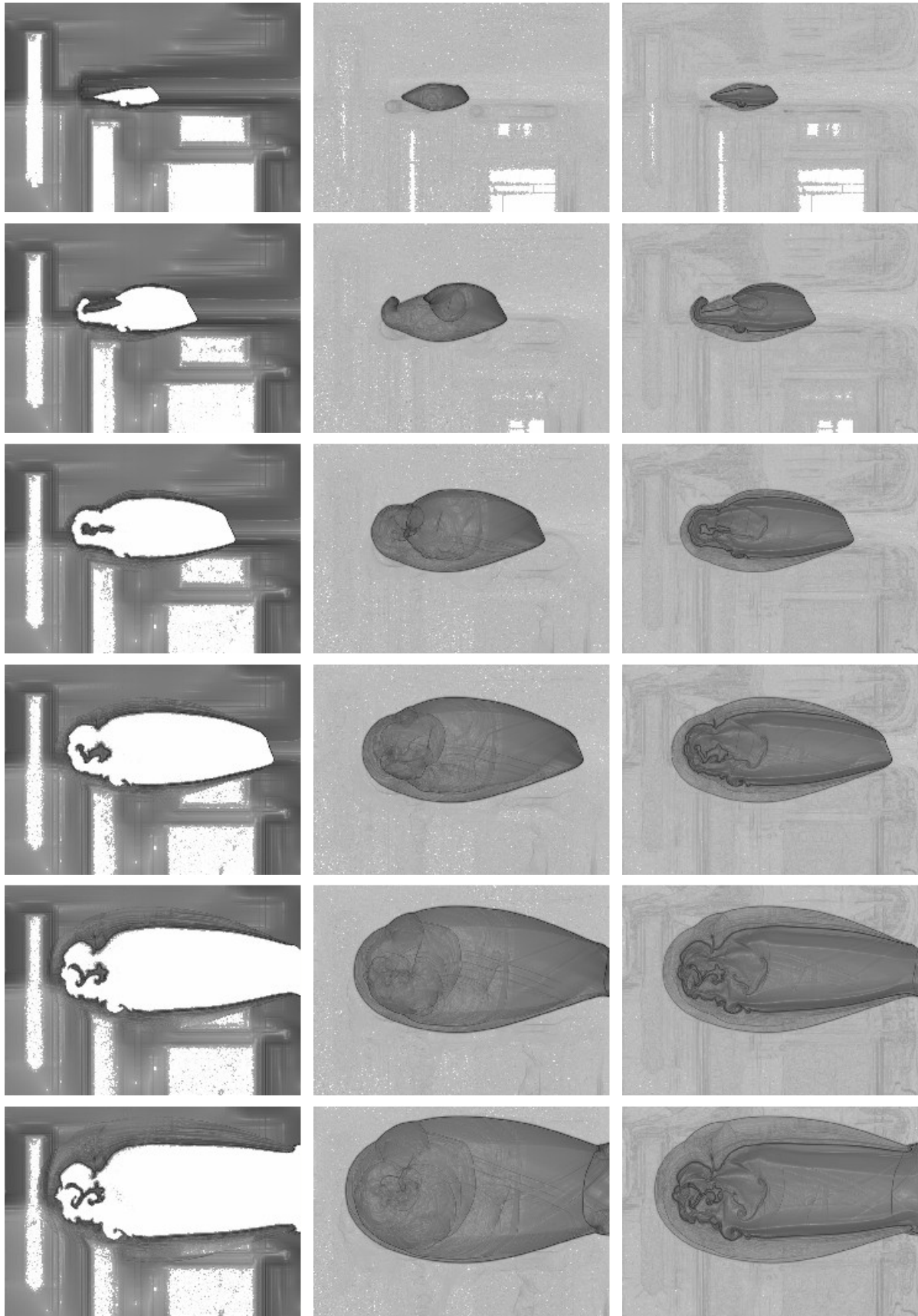


Figure 5. Reformer - Mass fraction (left), pressure (center) and temperature gradients (right), from top to bottom, 176, 352, 528, 704, 880 and 1056 μs after ignition, assuming ignition 1.0 s after release

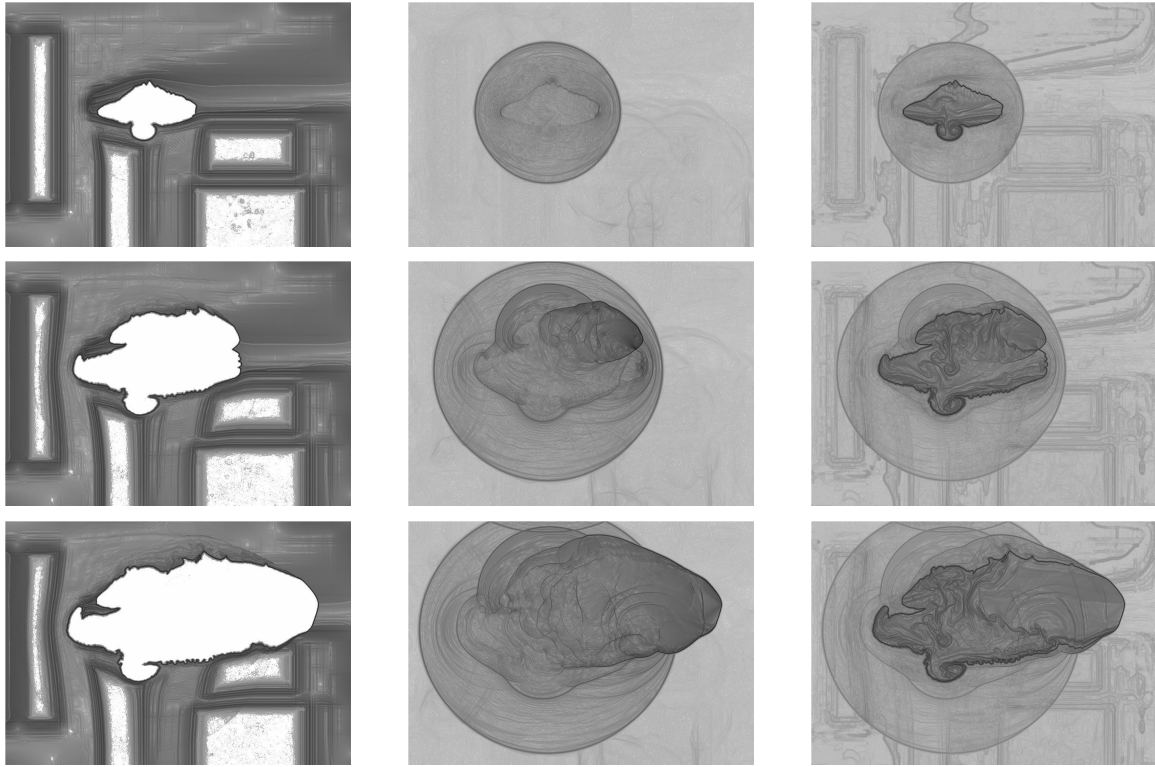


Figure 6. Reformer - Mass fraction (left), pressure (center) and temperature gradients (right), from top to bottom, 1320, 2464, 2804 μ s after ignition assuming ignition 2.0 s after release. Coarser grid

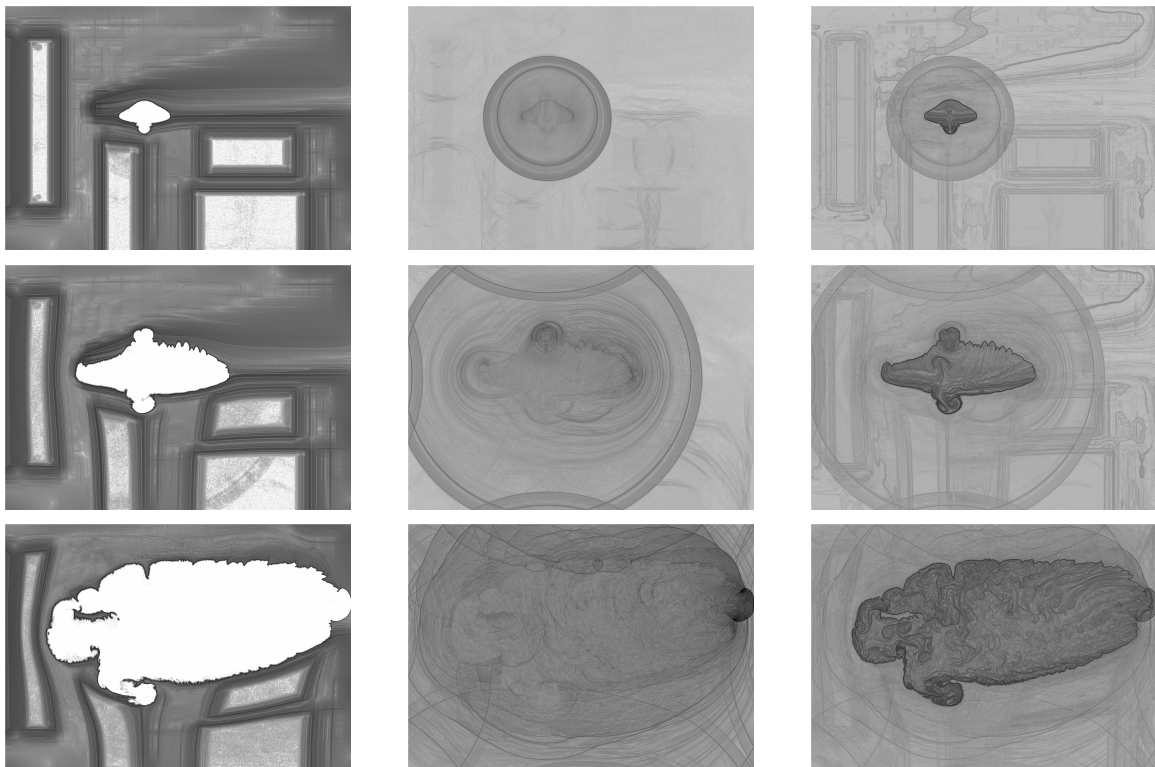


Figure 7. Reformer - Mass fraction (left), pressure (center) and temperature gradients (right), from top to bottom, 1320, 3343, 5402 μ s after ignition assuming ignition 2.0 s after release. Finer grid

Comparing Figs. 6 and 7, first, DDT occurred in both simulations. However, even before DDT occurred, the two results were already quite different in that clearly the interface separating burnt and unburnt propagate at very different speed. Thus, given that the circumstances are quite different in the two cases, it is difficult at this point to relate DDT and grid resolution. As to motion of the decoupled interface, the current physical model is not designed to handle its propagation which, over the time scale of the current computation, should be little anyway (even if accounting for turbulent flame propagation). Indeed, the diffusion processes that control flame propagation are not part of the current model, and for these slow processes to be properly resolved would require an unrealistically fine mesh. This is not realistically feasible within the scope of this project. The difference observed between the two resolutions is readily ascribed to the effect of numerical diffusion, which is admittedly not physical, and likely leads to a resolution-dependent propagation speed much larger than real, possibly by an order of magnitude. Although technically, these differences clearly show that the current simulations are not adequately resolved, motion of the interface after failure has little impact on shock motion and on the pressure field, for which the resolution used is not unreasonable. Thus the main effect is, as noted, the difference in the DDT event. Given, however, that when dealing with hydrogen, detonative ignition and DDT are frequent but unpredictable occurrences, arguably all these scenarios fall within the realm of possibility. Thus these results remain meaningful for the current purposes in that they represent realistically feasible scenarios and they give an indication of what might happen, and the order of magnitude of the damage. (Obtaining true grid convergence would entail resolving molecular diffusion, hence resolving the mean free path, which is not realistic.)

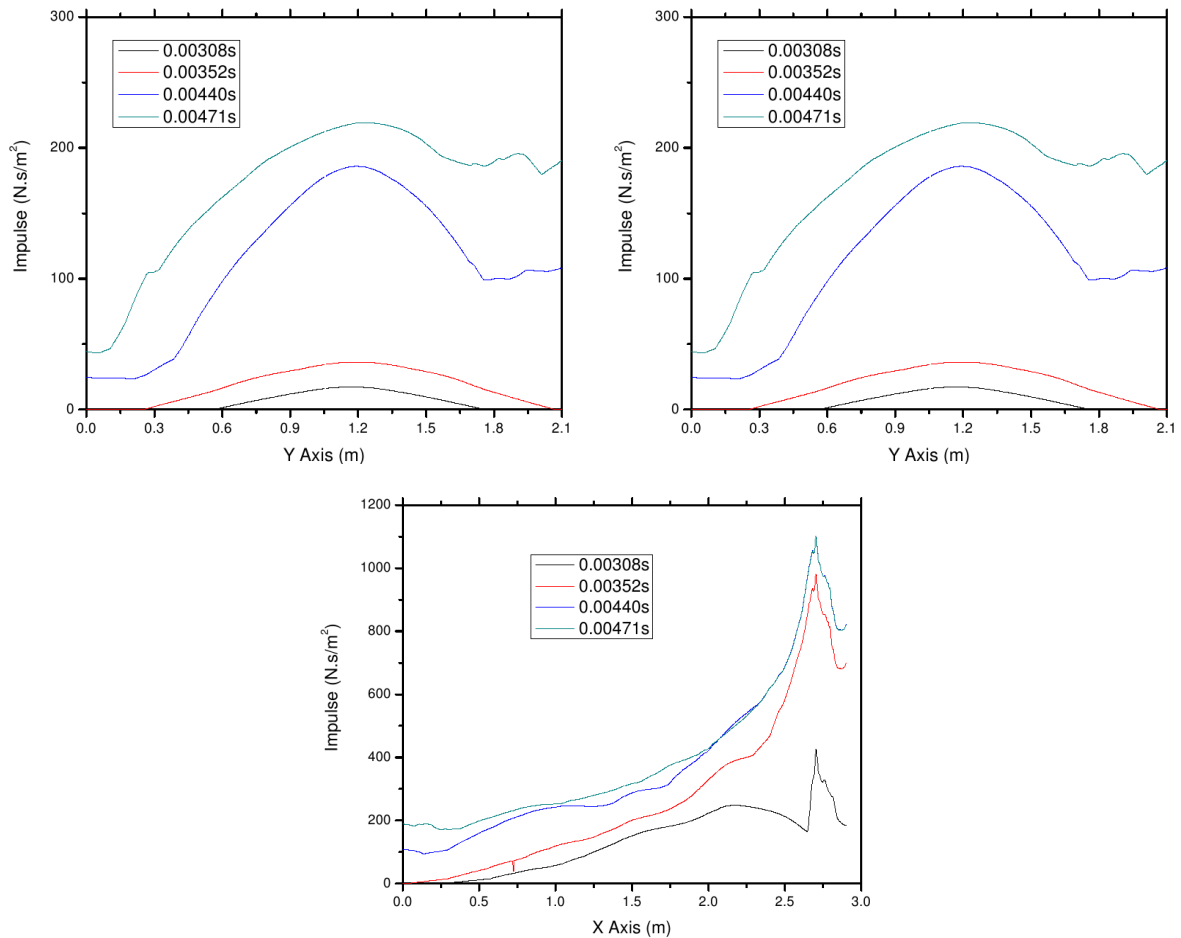


Figure 8. Impulse on left, right and top wall. Ignition 2.0 seconds after release

Comparing the results from the reformer and electrolyzer simulations, peak pressure and impulse values are quite different. For the reformer, peak pressure is 35 bar in the 1.0 s and 1.4 s cases and it reaches 80 bar in the 2.0 s case. In contrast, for the electrolyzer, peak pressure was 7 bar. Here again, the walls are only exposed to this high value of pressure for a very short period of time. For 1.0 s and 1.4 s, the largest impulse, of about 700 Ns/m², occurs at the top wall, close to the right end. For the 2.0 s case, results for impulses on left, right and top walls are shown in Fig. 8. The largest value is 1100 Ns/m², which is close to twice the 600 Ns/m² in the electrolyzer. While the peak pressures are about 10 times as high in the reformer simulation, the peak impulses are only about twice as great.

These results show that there is potential for damage. As mentioned earlier, there is no simple strategy currently available that can ensure no detonation will occur, after a hydrogen leak in an enclosed environment.

5. CONCLUSION

A study of detonation was performed for two situations where a leak occurred in an enclosed equipment. In one case, 42 g of hydrogen leaked in an electrolyzer, while in the other case, 84 g leaked in a reformer. The results show that the reformer case is distinctly worse and that if detonation occurs, it is likely to cause significantly more severe damage than the electrolyzer case.

Even though important simplifications were made in order to perform the simulations, the results give an indication of the potential damages that could occur following a hydrogen leak in an enclosure, leading to detonation. The results obtained from peak pressure and impulse may be of value when designing enclosure for equipment containing hydrogen.

There are basically three limitations causing uncertainty in these two simulations. First, the simulation was done in two dimensions to keep the computation within manageable limits; a three dimensional simulation would be unrealistically large and costly for the purpose of risk assessment. As a result, the wave thickness is poorly resolved since its is very thin compared to the mesh size.

Another limitation is regarding the flame propagation process after detonation failure, the physics of which are not included in the physical model, and indeed cannot for a realistic grid size. Instead, front propagation occurs under numerical diffusion, which likely results in faster than real front motion. Arguably, however, this has little effect on pressure and impulse results.

Still, these uncertainties are at most of the same magnitude as the uncertainties encountered in dispersion simulations of the type that were used to obtain the initial conditions for the current simulations.

Overall, results show that detonation after a hydrogen leak can lead to serious damage even if the detonation fails. Since in this two-dimensional simulation, the dispersion pattern that was used corresponds to the plane where hydrogen concentration is highest, in effect the amounts are significantly higher than the actual leaks; additionally, the two-dimensional topology provides more confinement than the actual three-dimensional enclosure. Thus although the obstacles inside the enclosure have been neglected, results obtained are likely conservative.

6. ACKNOWLEDGMENTS

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