Hydrogen Explosion Study in a Confined Tube: FLACS CFD Simulations and Experiments

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1 Introduction and Previous Work

In recent years, there has been a lot of focus on predicting gas explosions involving hydrogen. This is driven by the ongoing development of hydrogen-fuelled vehicles, which are deemed to be the symbol of a future hydrogen economy. Further, there has been an increasing interest from the nuclear industry, as many new nuclear reactors are planned for the first time since the Chernobyl and Three Mile Island accidents in the 1980s. Many experiments have been carried out in recent years for studying the various important parameters that govern hydrogen explosions. Nonetheless, Computational Fluid Dynamics (CFD) tools are being used increasingly due to the time and cost benefits, and the possibility to carry out exhaustive studies and to access regimes that are not possible in experiments. CFD tools offer the possibility to properly describe explosion physics and obtain realistic numerical results. However, for simulating large-scale scenarios, many phenomena occur at scales smaller than realistic grid resolution. Therefore, sub-grid models are required, but these must be validated using dedicated experiments. DNS and other detailed simulation approaches are not very useful as they can take prohibitive amount of time for geometries such as those found in reality and are thus not possible to validate.

This paper describes the numerical simulations of experiments in a confined tube geometry carried out by SRI International, which concerned hydrogen explosions in a 10-m long tube with square cross-section [1] using the commercial CFD tool FLACS. FLACS has been developed specifically for carrying out gas explosion (and dispersion) modelling. As a result of a more than 25-year history of model development and experimental validation, it is used widely in petrochemical industry and elsewhere for explosion predictions for input to risk assessments and design load specifications. More details about FLACS can be found in references [2] and [3]. A dedicated project was carried out between 2001 and 2004 to improve the modelling and validation of hydrogen explosions in FLACS wherein many small and large-scale experiments combined with simulations and model improvements were carried out [2], and reasonable precision can be expected while simulating hydrogen explosions using the latest version.

For hydrogen explosions, deflagration to detonation transition (DDT) can be a significant threat. Transition to detonation can occur in a variety of situations, many of which are commonly found in industrial settings. Detailed description of all processes following ignition that may lead to DDT is extremely challenging. This is due to a complicated interaction of compressible flow, chemical reaction, and turbulence that needs to be described at very high spatial and temporal resolution. Much theoretical effort has been focused on development of criteria for DDT (see Ref. [4] for a summary) but these criteria and scaling arguments are difficult to apply in a process setting where numerical results are much more valuable. There have been many attempts to simulate

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DDT/detonation directly (e.g. [5]) but most of these are limited small-scale, 2D scenarios and are impossible in a "practical" situation. Although the validation of the current version of FLACS in simulating flame acceleration and high-speed deflagrations is good, a model for detonations is lacking. As a part of the activity supported by the Norwegian Research Council (NFR) to improve the ability of FLACS to predict DDT and model detonations in a simplified way, many different experiments have been simulated and the simulations are able to match the observations reasonably well [6]. This has included diverse experiments such as detonation tube experiments at McGill University [7], large-scale channel experiments at the Sandia FLAME facility [8] and jet ignition experiments at the KOPER facility [9].

More recently, large-scale experiments carried out at Fh-ICT have been simulated. The test set up consisted of a rectangular driver section with a square spaced opening in the front side followed by a "lane" which consisted of 2 parallel walls. The whole volume was filled with H_2-air mixture. In general, the modeling results are able to capture the experimental observations, including maximum pressures, flame and pressure arrival times, and locations of DDT, reasonably well (see reference [10] for details). However, the speed of the flame front was somewhat smaller than that seen in the experiments due to the absence of a shock ignition model. Another study carried out recently has been the simulation of vented tube experiments as a part of the HYCOM project. This involved hydrogen explosion simulations in a 12.2 m circular tube (174 mm diameter) closed at one end with a vent of different sizes relative to the tube diameter at the ignition end. Figure 1 presents the flame positions as a function of time for both experiments and simulations for five different venting ratios ranging from 0 (closed) to 100% (fully open). It can be seen that the simulations are able to represent the slow start-up and the subsequent flame acceleration phase reasonably well for all cases.

The possibility of DDT is indicated in terms of a normalized spatial pressure gradient across the flame front as it is hypothesized that this parameter is able to visualize when the flame front captures the pressure front, which is the case in situations when fast deflagrations transition to detonation [5,11,12]. Comparison of the characteristic geometrical dimensions with the detonation cell size is also carried out in order to ensure that the geometrical dimensions are sufficient for the propagation of any initiated detonation front. Although the SRI experimental results presented in reference [1] do not discuss DDT and detonations, the maximum pressures and flame speeds observed seem to indicate that DDT occurred in many of the scenarios. We investigate this by simulating the tests with the FLACS CFD model.

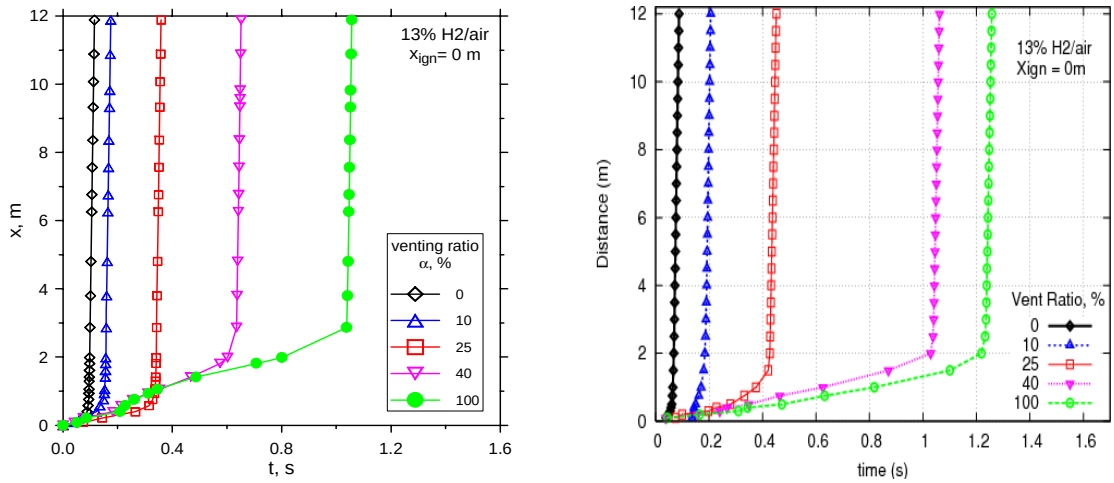

Figure 1. X-t diagram of the flame propagation from the open end (X_{ign} = 0 m) and at various vent ratios α = 0-100%

2 Brief description of experiments

The experimental facility comprised of a 9.9 m long square section (dimension 38.1 cm) steel tube. The ignition end of the tube was closed, while the opposite end was opened prior to ignition. Different obstacle

configurations were used to induce turbulence during the flame propagation. A schematic of the tube with the layout of the obstacles is presented in Figure 2. All the steel obstacles were 6.35 cm thick and were attached to a steel floor that was 1.27 cm thick on top of 1.91-cm-thick risers. Blocks with heights of 11.43 cm, 16.51 cm, and 22.86 cm were used to obtain three different blockage ratios (BR) of 0.32, 0.47, and 0.65. The regular spacing between the blocks (38.1 cm, 76.2 cm, or 152.4 cm) depended on the number of blocks (25, 13, or 7 respectively). The first block was always located at 38.1 cm from the initiation end. Pressure, ionization, and thermocouple measurements were made at 10 locations along the top of the tube as shown in Figure 2. More details of the experimental apparatus are available in Ref. [1].

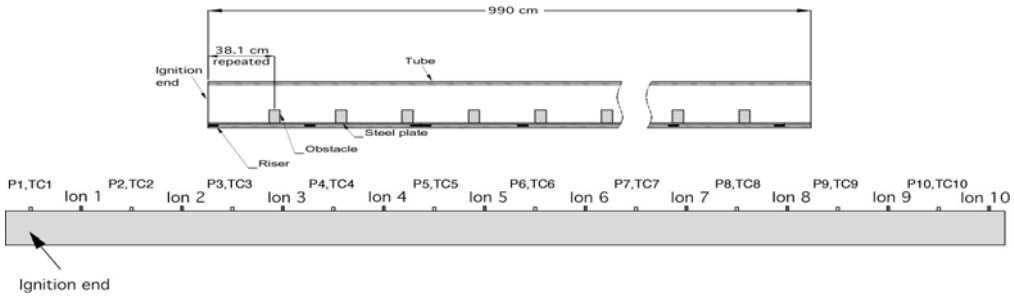

Figure 2. A schematic of the experimental geometry: Tube, obstacle configuration, and sensor details

3 Results and Discussion

There were a total of 8 tests in the experiment. The test matrix is summarized in Table 1. As mentioned above, the tests studied the effects of concentration, blockage ratio, and the number and separation of obstacles on flame acceleration, and hence pressure loads.

Table 1. Summary of the test matrix

H_2 (%)	Number of Obstacles	Obstacle Spacing (cm)	BR
30	25	38.1	0.32
30	13	76.2	0.32
30	7	152.4	0.32
20	25	38.1	0.32
57	25	38.1	0.32
30	13	76.2	0.47
30	13	76.2	0.65
30	0	--	--

Figure 3 presents a comparison between the experimental and simulated scalar pressure traces at three different locations. It can be seen that the simulations agree reasonably well with observations, both in terms of maximum pressures and the time of arrival. In Figures 4 and 5, the main results obtained in the simulations are compared with those observed in the experiments. These describe the effect of number of obstacles, concentration, and blockage ratio on the flame arrival times and overpressures. Figure 3 presents the simulated flame distance as a function of time (top) and contrasts it with the experimental observations (bottom). Quite good agreement is seen in general, both in terms of arrival times and effect of various parameters, except that the flame speed at 57% H_2 is too high. Figure 4 presents the calculated values of overpressures as a function of distance along the tube (top) and compares it with experimental data (bottom). Again, reasonably good agreement is seen. However, there are a few discrepancies, which include much higher overpressures for the case of 57% H_2, and higher overpressures near the exit for the tube with no obstacles.

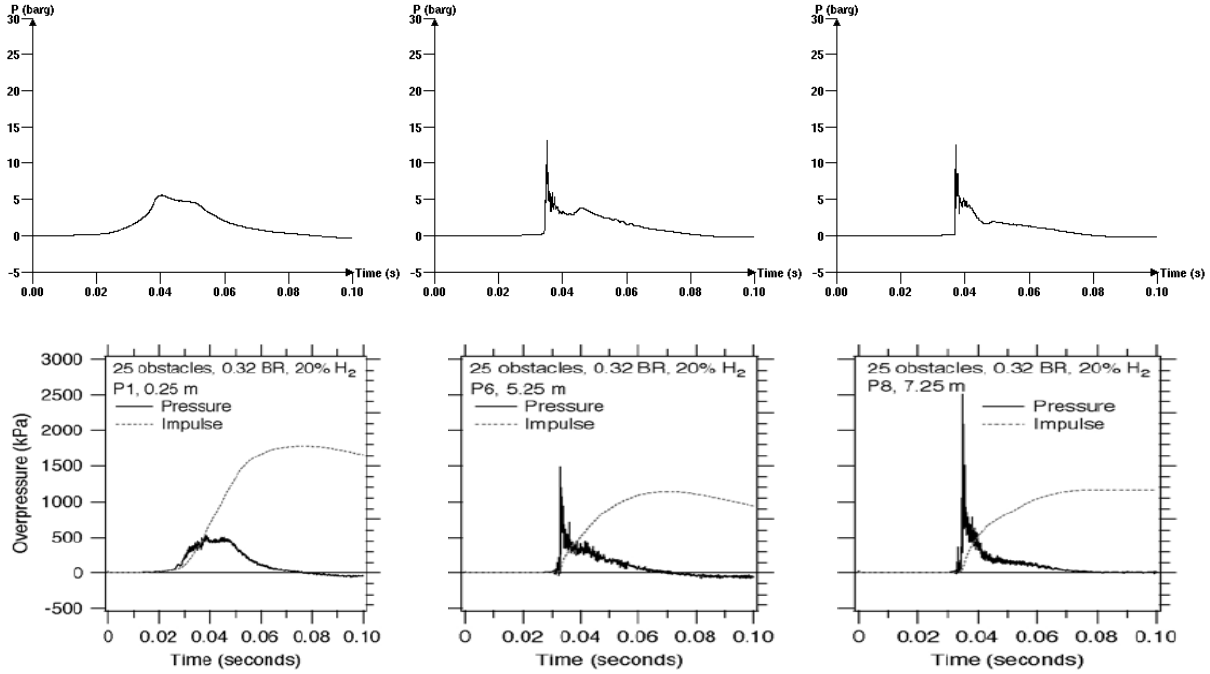

Figure 3. Comparison of simulated pressure traces (top) with experimental results (bottom) at 2 locations

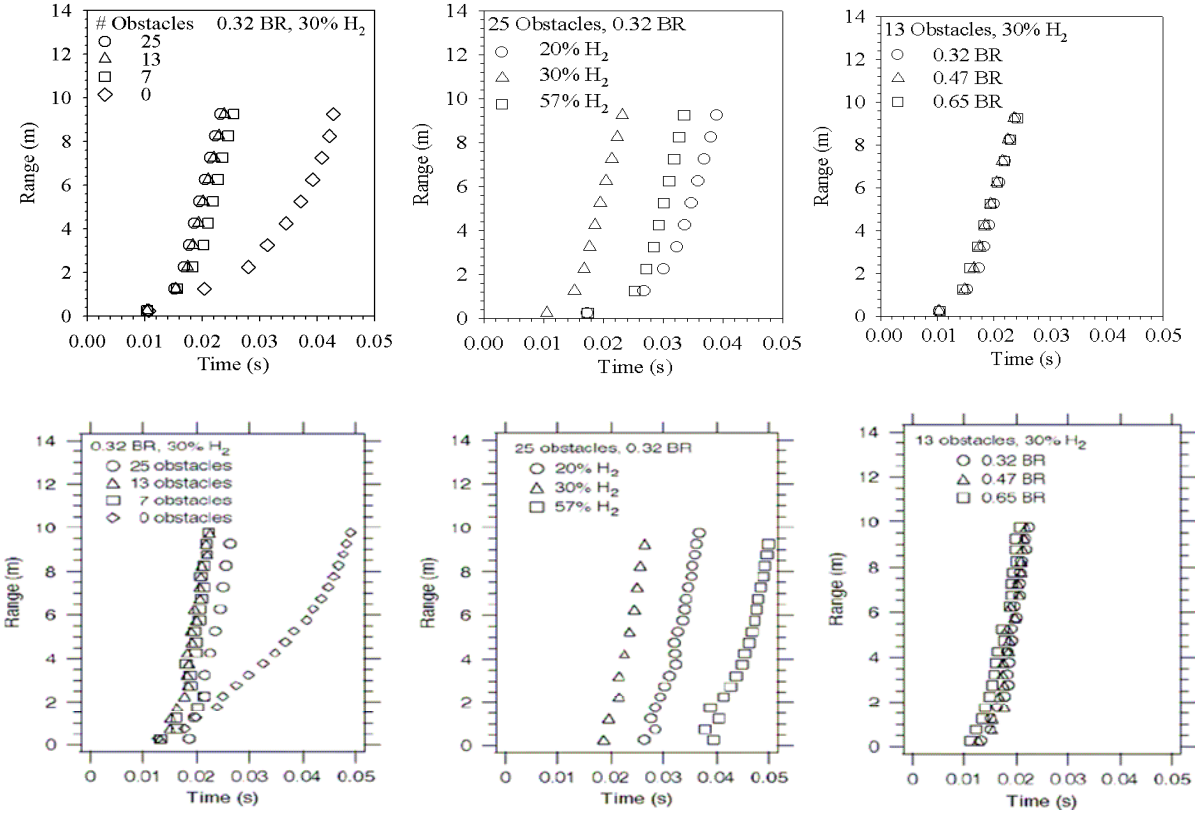

Figure 4. Comparison of simulated flame arrival times (top) with experimental measurements (bottom)

As can be seen from Figure 5, very high overpressures (sometimes 15-20 bar) and very fast flames are seen in both the experiments and numerical simulations. This indicates the possibility that DDT occurred in the experiments. This was investigated numerically using a normalized spatial pressure gradient across the flame front described above. Based on the simulation of various experiments alluded to above, we have observed that a value ≥ 10 indicates a strong likelihood of DDT. The simulations indicate the occurrence of DDT in most of the scenarios. The geometrical likelihood of the propagation of a potential detonation front was also investigated by comparison with the detonation cell size, and in each case, the geometrical size was found to be large enough. The simulations indicated a DDT at around 4-5 m from ignition for the case of 30% H_2 and BR 0.32, which is when high detonation-like pressures begin to be observed in the experiments (see the first picture below). The occurrence and values of the spatial pressure gradient were also able to distinguish the fact that very high pressures (and hence possible DDT) occur somewhat sooner for a tube with BR 0.65, and indeed, DDT was indicated at around 3 m from ignition. Detailed results are not presented here due to space constraints. As described above, FLACS still lacks a shock ignition model, which means that a detonation front cannot actually propagate, and the speed of the front is limited by the speed of sound in products. However, an "average" representation is currently being attempted in order to replicate the propagation of a detonation front for the cases that DDT is indicated and the geometrical dimensions are sufficient. Also, work is in progress to resolve the discrepancies seen for the rich H_2 mixture.

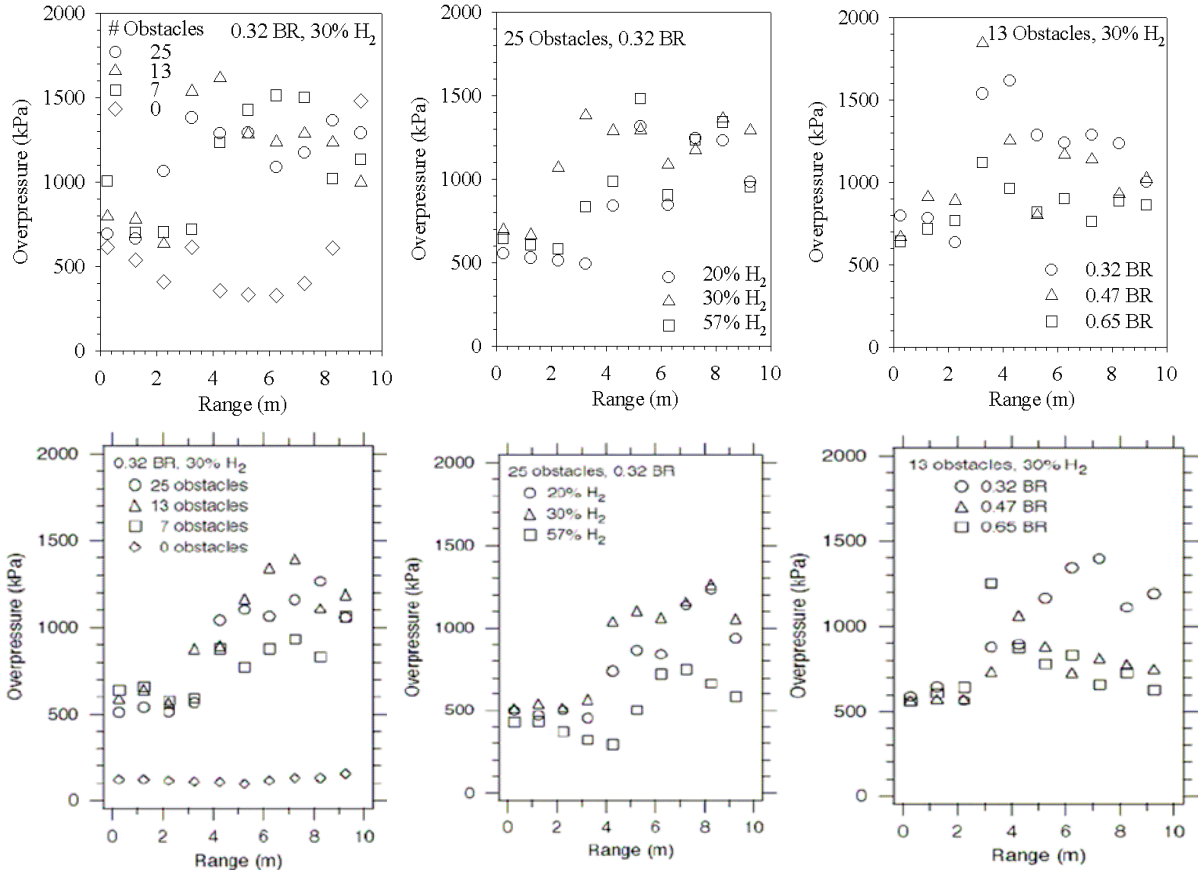

Figure 5. Comparison of simulated overpressures (top) with experimental measurements (bottom)

4 Conclusion

In general, the simulations compare reasonably well with experimental predictions. Both the values and locations of overpressures and flame are represented with reasonable accuracy. This points to the value of FLACS as a useful tool that can be employed in a predictive capacity in a process setting. Although the experiment chosen for this article is not exactly large scale, complementary work described above has proven that FLACS can be successfully employed to make reasonable estimates of the danger of an accident in a realistic geometry. Even though the description of DDT described above is approximate, we believe that useful results can be obtained and this represents an important first step to be able to bridge the gap between CFD simulations and realistic process safety studies involving the possibility of a transition to detonation.

References

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