NUMERICAL STUDY OF LARGE SCALE HYDROGEN EXPLOSIONS AND DETONATION

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Numerical studies were conducted for large scale hydrogen explosions and detonation. For explosions, the configuration of a full-scale test of Tanaka et al. (2007) in a simulated hydrogen refill station model was used. Predictions for the same test condition achieved reasonable agreement. On this basis, further simulations were conducted to study the overpressures in the refill station model for a range of hydrogen concentrations from 15% to 60% in volume. Analysis was carried out to derive the dependence of overpressure on hydrogen concentrations. The detonation studies were conducted for the full-scale test conditions of Efimenko and Gavirkov (2008) at the RUT tunnel facilities in Russia. Comparison is made between predictions and measurements. Reasonable agreement has been obtained on pressure decay and the propagation speed of detonation wave. The study has demonstrated the potential of the present models to effectively assess the explosion and detonation hazards in hydrogen facilities.

KEYWORDS: Hydrogen, deflagration, detonation

INTRODUCTION

Hydrogen is one of the possible candidates as major energy carriers in the future. Hydrogen as fuel has the highest energy content by mass but the lowest energy content by volume. Future widespread use of hydrogen as vehicle fuel requires development of safe handling guidelines for production, transportation and utilization. Potentially widespread use of hydrogen is expected in fuel cell powered vehicles supported by a network of hydrogen refill stations. The full scale tests conducted by Tanaka et al. (2007) in a simulated refilling environment provided insight into the explosion hazards in the event of an accidental fuel release. The paper contained data for overpressures generated at various locations from the ignition sources and forms the basis of comparison with modelling.

Due to its high reactivity, an accidental release of hydrogen in an industrial facility can lead to deflagration and transition to detonation, which is a supersonic combustion wave with destructive effects, Lee (2008). The possibility of hydrogen-air cloud detonations in industrial facilities and the resulting severe damage and life loss makes it an important subject to be studied in the field of hydrogen safety. Some large scale tests have been carried out to study the behaviour and impact of detonation in large scales, but full scale testing is costly. Hence, only a limited number can be conducted in highly specialised facilities. Predictive tools, validated against experimental measurements, offer an alternative for such studies. Several numerical simulations of detonations have been carried out in the past, but most of these investigations have focused on small scales with domain sizes typically in the order of centimetres. An approach to numerically simulate large scale detonation has been developed by the authors. The modelling approach has been validated against data from the large scale detonation tests at the RUT facility in Russia, Efimenko et al. (2008).

NUMERICAL METHODS FOR DEFLAGRATION MODELLING

The explosion modelling is conducted with the traditional CFD approach based on Reynolds averaged Navier Stokes equations. For combustion, the Turbulent Flame Closure (TFC) model is used. This model is also referred to as the Burning Velocity Model (BVM) in the literature. It solves an additional transport equation for reaction progress variable (c) for the progress of the global reaction, which is given as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}) + \frac{\partial}{\partial x_k}(\bar{\rho}\,\tilde{u}_k\tilde{c}) + \frac{\partial}{\partial x_k}\left(\bar{\rho}D_t\,\frac{\partial\tilde{c}}{\partial x_k}\right) + (\rho_u\, s_t)\,|\,grad\,\tilde{c}| \quad (1)$$

where $\tilde{c}$ is Favre averaged progress variable
$\bar{\rho}$ is averaged density
ρ_u is density of unburned mixture
s_t is turbulent burning velocity
D_t is turbulent diffusion coefficient

The closure developed by Zimont (2001) is used for the turbulent burning velocity (s_t), which is given below

$$s_t = A\,G\,u'^{3/4}\,s_L^{1/2}\,\lambda_u^{-1/4}\,l_t^{1/4} \quad (2)$$

where A is a modeling coefficient
λ_u is molecular heat transfer coefficient of fresh mixture
s_L is laminar burning velocity
G is the stretching factor

u' is integral velocity fluctuation
l_t is turbulent length scale

Stretching factor accounts for the reduction of the flame velocity due to large strain rates (i.e. large dissipation rate). This effect is modeled in terms of the probability for turbulence eddy dissipation ε, being larger than a critical value ε_{cr}. For $\varepsilon > \varepsilon_{cr}$ flamelet extinction takes place, while for $\varepsilon < \varepsilon_{cr}$ the stretching effect is ignored. A log normal distribution is assumed for ε, the stretching factor is given by

$$G = \frac{1}{2}\, erfc\left[-\frac{1}{\sqrt{2\sigma}}\left(\ln\left(\varepsilon_{cr}/\,\tilde{\varepsilon}\right) + \frac{\sigma}{2}\right)\right] \tag{3}$$

where *erfc* denotes the complimentary error function and $\sigma = \mu \ln(l_t/\eta)$ is the standard deviation of the distribution of ε with μ being an empirical model constant. The critical dissipation rate ε_{cr} is computed from a specified critical velocity gradient g_{cr}, and the kinematic viscosity of the fluid (ν), according to

$$\varepsilon_{cr} = 15\,\nu\, g_{cr}^2 \tag{4}$$

The integral velocity fluctuations, integral turbulent length scale, and Kolmogorov length scale resp. are evaluated as given below, where k is turbulent kinetic energy.

$$u' = \sqrt{2\,k/3}, \quad l_t = k^{3/2}/\varepsilon, \quad \eta = (v^3/\varepsilon)^{1/4}$$

The accurate estimation of ε_{cr} is necessary to correctly account for the bending of s_t at the high turbulent intensity regions. The model constants used in the present numerical simulation are

$$A = 0.65\,,\ \mu_{str} = 0.28\,,\ g_{cr} = 8000\,s^{-1}$$

The laminar burning velocity s_L is modelled using the equivalence ratio (ϕ) correlation developed by Metghalchi and Keck (1982). Laminar burning velocity is expressed as a base value at reference condition $s_{L,0}$, multiplied by a correction factor for preheat and pressure dependencies.

$$s_L = s_{L,0}\left(\frac{T_u}{T_{ref}}\right)^{\alpha}\left(\frac{p}{p_{ref}}\right)^{\beta} \tag{5}$$

The exponents for preheat (α) and pressure (β) dependency are given as

$$\alpha = 1.524 + 0.026\,\phi \tag{6}$$

$$\beta = 0.26 \tag{7}$$

with temperature and pressure reference states as

$$T_{ref} = 291\,\mathrm{K},\ P_{ref} = 1\,\mathrm{atm}$$

The reference laminar burning velocity $s_{L,0}$ is specified as a polynomial given below

$$s_{L,0} = -1.482 + 6.174\,\phi - 2.632\,\phi^2 + 0.32\,\phi^3 \tag{8}$$

The above polynomial is evaluated on a fit range {0.5, 3.0} equivalence ratio, outside the range the burning velocity is modelled to decay linearly to zero at the flammability limits {0.1,7.1}.

NUMERICAL METHODS FOR DETONATION MODELLING

For the numerical simulation of detonations the reactive Euler equations are solved with a set of chemical reaction equations for the underlying combustion process. These reactions model the consumption and production of each chemical element present during the detonation process. By using the rate of production and consumption of each element and the resulting change in the enthalpy it is possible to calculate the energy source term and the progress rate of the phenomenon.

For accurate simulations of the fine structures in detonation, it is generally necessary to capture the shock waves. This would require very fine grid resolutions typically in the order of microns. The current computer power still prohibits the use of such fine resolutions in large scale detonation studies. On the other hand, if a model can be tuned to obtain the correct pre/post detonation states and the correct energy release from the combustion, the speed of the detonation wave can be computed as part of the overall coupled fluid/reaction simulation.

It should be acknowledged that a coarse-grid simulation will not capture the internal structure of the detonation wave, e.g., the von Neumann spike, but if adequately tuned, it should be able to capture the moving detonation front and hence the detonation wave speed. However, the downside of using relatively coarse grids is that the shock wave will be smeared over at least that distance – and more typically 3 or 4 cells once a curved shock wave is (inevitably) captured oblique to the mesh. In such case, it would also be necessary to implement treatment to avoid artificial acceleration of the detonation wave due to numerical diffusion. Because of this, and the possibility of stiffness from a detailed reaction mechanism, the best option would be to use a simple one step global chemistry which is not stiff for a coarse mesh. One could then safely run a coarse grid simulation at a CFL (Courant-Friedrichs-Lewy) number of 1 and capture the overpressure generated by the detonation wave as well as confinement pressure behind the wave so long as the energy balance (not the kinetic pathway) is maintained.

A modelling approach is hence developed on the above basis which combines the use of single step chemistry with grid resolutions in the order of millimetres. The chemical reaction used here is a single step Arrhenius form

reaction and can be written as

$$\omega = A(1-\alpha)EXP\left(-\frac{E_a}{RT}\right) \tag{10}$$

where α, ω, A and E_a are progress variable, reaction rate, pre-exponential factor and chemical activation energy, respectively. Standard forms of these reactions can be found in the literature. However for the present study, which involves very large scales and relatively coarse mesh, the reaction needs to be tuned to find the right pre-exponential factor and activation energy. During this process, it is essential to ensure that the rate of energy release is correct. Feeding the right energy release rate into the governing equations is essential to obtaining correct results. This rate should be consistent with theoretical and experimental data.

Following Sichel et al. (2001), several simulations in one and two-dimensions were carried out to tune the reaction constants in Eq. (10). The predictions for pressure, velocity and other static parameters of detonation were compared with Chapman Jouguet (CJ) parameters calculated from an in-house equilibrium code by Heidari et al. (2007) which gave CJ pressure and propagation velocity of 15 atm and 1970 m/s, respectively.

By comparing the predictions with the above CJ parameters, appropriate coefficients for the reaction were selected as shown below:

$$\omega = 11^9 \times (1-\alpha)EXP\left(-\frac{23000}{T}\right) \tag{11}$$

The other equations added to the governing equations are as follows:

Reaction progress equation:

$$\frac{\partial \rho\alpha}{\partial t} = -\nabla(\rho\alpha V) + \rho\omega \tag{12}$$

Energy equation:

$$E = -\alpha\mathbf{Q} + \frac{P}{[\rho(\gamma-1)]} + \frac{V^2}{2} \tag{13}$$

Equation of state:

$$\frac{P}{\rho} = \frac{RT}{M} \tag{14}$$

In Eq. 13, α is the reaction progress variable and is zero where all the mixture is unburned and 1 where the mixture is burnt. **Q** is the heat of chemical reaction per unit mass. The relation between ω and α is as follows:

$$\omega = \frac{d\alpha}{dt} \tag{15}$$

THE EXPLOSION SIMULATIONS

EXPERIMENTS CONSIDERED AND NUMERICAL SET UP

A numerical study was conducted for the semi-confined explosion tests of Tanaka et al. (2007) in a simulated hydrogen refilling station. The test chamber of 8.25 m × 3 m × 2.7 m is open only on the front. All the other sides are closed as shown is Fig. 1. The chamber was partitioned along its length into three sections each with a volume of 22 m^3. In each test, only one of the sections was filled with hydrogen-air mixture. The ignition source was placed at the centre of the gas mixture volume.

Considering the symmetric nature of the chamber, only half of the test volume is included in the numerical simulation. Overpressure measurements were carried out at 5, 10, 15 and 20 m over the distance of 30 m from the open end of the chamber as shown in Fig. 2. The dimensions of the simulation domain were chosen in such a way that the effect of end boundary condition were minimal on the predictions at the monitoring locations.

RESULTS AND DISCUSSIONS

It is known that the TFC combustion model is sensitive to the turbulence parameters for calculations of the turbulent burning velocity. Preliminary simulations were carried out to fine tune the turbulence parameters for the 30% H_2 concentration case to match with the experimental results and ascertain other input parameters for the combustion

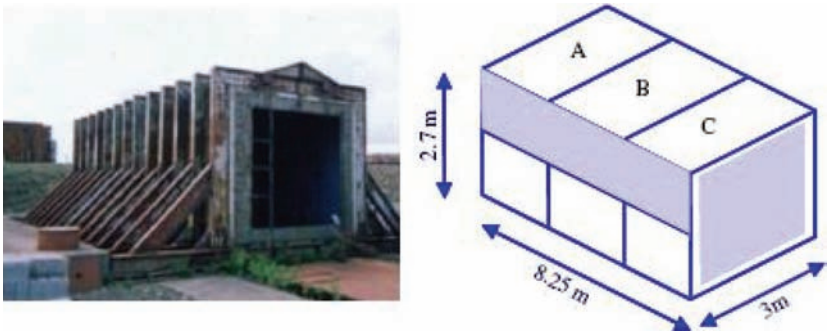

Figure 1. Test chamber structure (Reproduced from Tanaka et al., 2007)

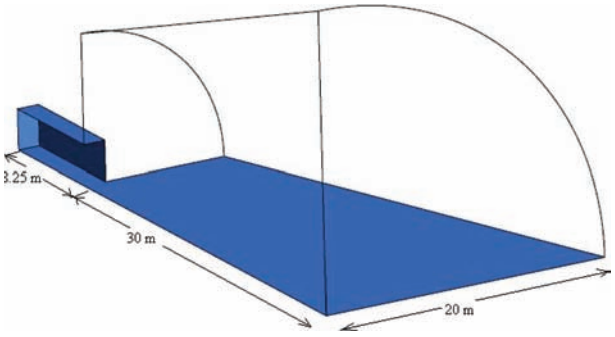

Figure 2. The computational domain (shaded region is wall)

model. Following this, for the simulations of the 15% and 50% H_2 concentrations, only the initial fuel mixture fraction was changed while the same turbulence parameters and inputs to the combustion model were used. Predictions were also carried out for two additional H_2 concentrations of 40% and 60%, which were not tested in the experiments.

As shown in Fig. 3, there is very good agreement between the predicted overpressures at the monitoring locations with the experimental measurements, i.e. 15%, 30% and 50% concentrations. The peak overpressure decrease almost inversely with distance from the front open end. The effect of hydrogen concentration on the overpressure up to10 m from the open end is shown in Fig. 4. As the overpressure is related to flame speed, the experimentally measured flame speed is shown in Fig. 5. It can be seen that below 40% H_2 concentration, the overpressure at both 5 and 10 m increases with hydrogen concentration. At 40% H_2 concentration, the overpressure reaches its peak. Afterwards, the overpressure decreases with further

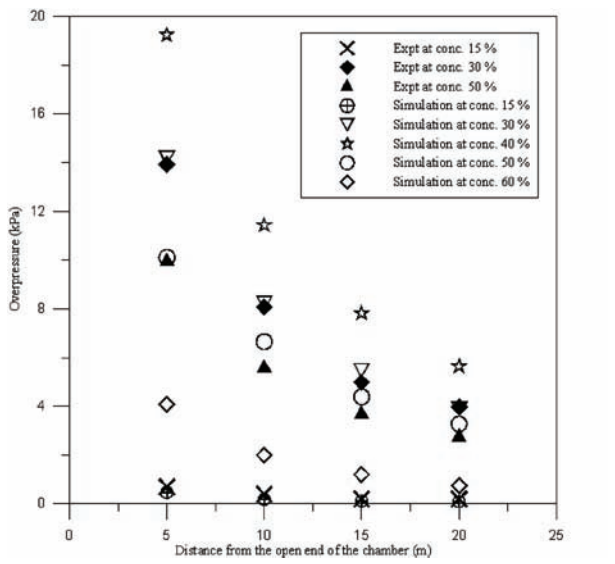

Figure 3. Variation in overpressure (kPa) with distance from open end of chamber

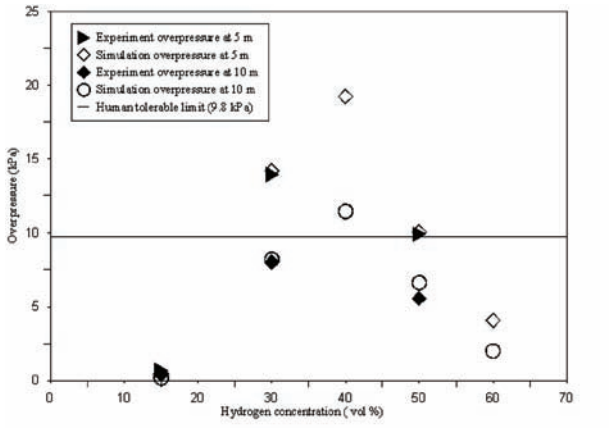

Figure 4. Effect of hydrogen concentration on overpressures generated

increase in H_2 concentration. Comparing with flame speed observed during the experiments, the hydrogen concentrations leading to the largest overpressures correlate with those which have the highest flame speed.

Considering the fact that an overpressure of 9.8 kPa is the permissible human tolerance limit, the safe distance from the simulated hydrogen fuel installation can be taken as 15 m for this particular installation. This conclusion is, however, only valid for the configuration considered. Even for the same geometry, this safety distance can be different when there is congestion. In a congested environment, flame accelerates faster due to enhanced mixing and turbulence, resulting in higher overpressures than an uncongested environment. Hence for explosion safety, it would be necessary to ensure that hydrogen refuel stations are well

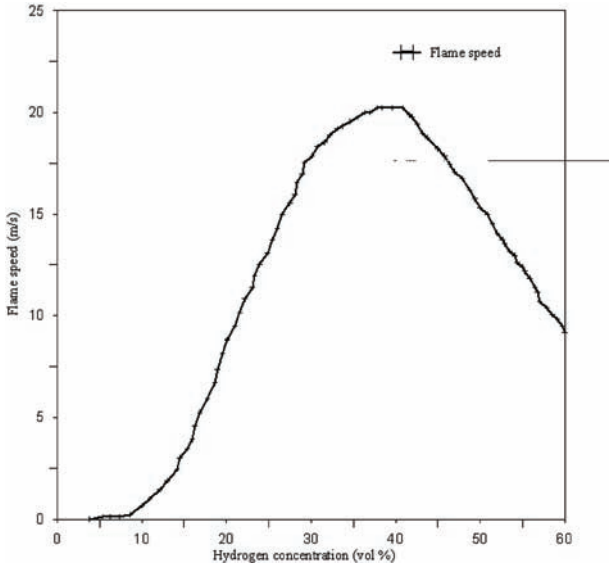

Figure 5. Flame speed *vs* hydrogen concentration (Reproduced from Tanaka et al., 2007)

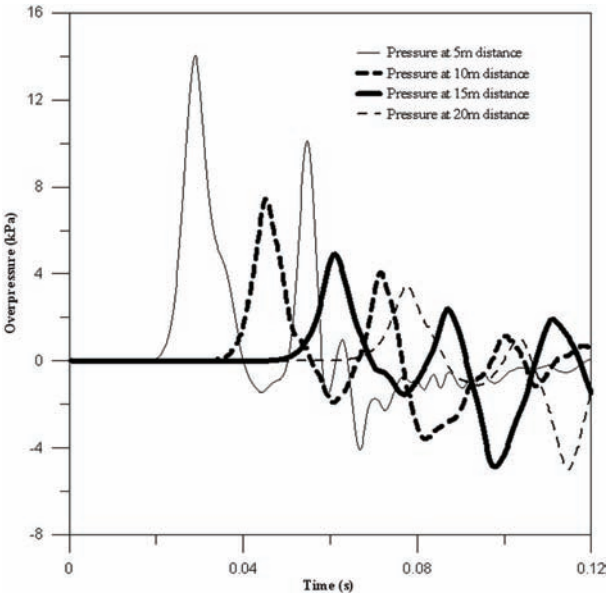

Figure 6. Pressure wave propagation at monitoring points for 30% H_2 concentration

ventilated and to reduce unnecessary congestion. The pressure wave propagation at the monitoring points along the axis of the chamber at distances of 5, 10, 15 and 20 m are shown in Fig. 6 for 30% H_2 concentration.

THE DETONATION SIMULATION

THE RUT CASE

This was a series of detonation tests carried out at the RUT tunnel facilities in Russia, which is one of the standard test cases selected for HYSAFE. A part of the RUT facilities is steel-lined reinforced concrete channel with a total volume of 263 m^3, Efimenko et al. (2008). Schematic of the test channel is shown in Figs. 7 and 8. The dimensions of the tunnel and the ignition location are shown in the Fig. 8. The tunnel was filled with stoichiometric hydrogen-air mixture. Ignition was started at one end of the tunnel as shown in Fig. 8. The detonation was started by direct

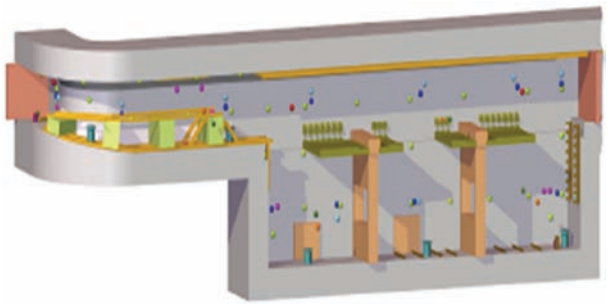

Figure 7. The experiment channel (reproduced from Kotchourko, 2007)

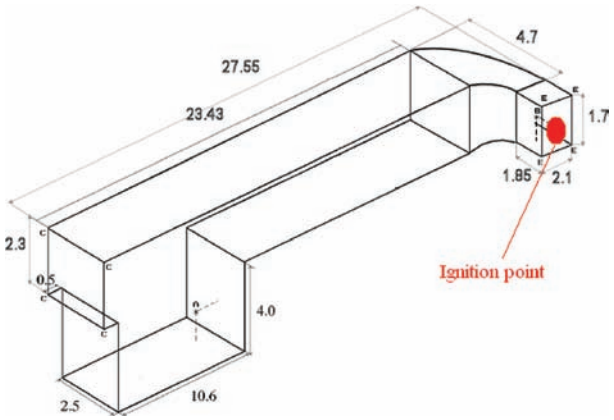

Figure 8. The tunnel dimensions (reproduced from Kotchourko, 2007)

initiation, Lee (1977) with a high explosive charge of 200 g weight, Efimenko et al. (2008).

Overall, twelve monitoring points were selected where pressure gauges were used to record pressure. As shown in Fig. 9, the gauges were place at the opposite end of the tunnel from the ignition point.

Pressure measurements are available for 5 of the 12 monitoring points, i.e. points 7 to 11 as shown in Fig. 9. The present predictions are compared with these measurement as well as the numerical predictions of Kotchourko (2007) for the same set up.

NUMERICAL SET UP FOR THE TUNNEL

Due to non-uniform shape of the geometry and presence of curved surfaces in the tunnel, an unstructured hexahedral mesh as shown in Fig. 10 is used. The average grid size is 5 cm while finer grids are used around the ignition point. As the domain is uniformly filled with the reactive mixture, it is necessary to keep approximately the same mesh equally throughout the computational domain. The total number of grids is around 2.2 million.

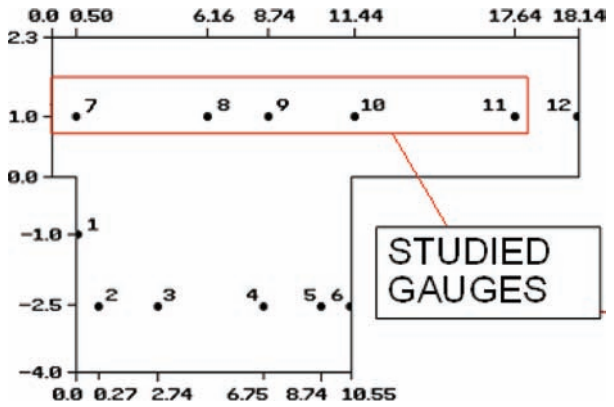

Figure 9. Locations of the monitoring gauges (reproduced from Kotchourko, 2007)

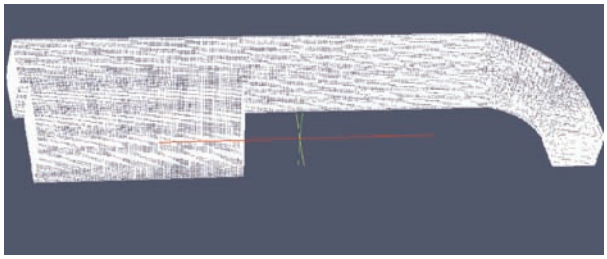

Figure 10. The Mesh pattern for RUT tunnel

The domain is split into 20 sections to facilitate parallel processing. Since the domain is enclosure and the reactive mixture is completely confined, all the boundary conditions are set as the wall. The initial temperature is 300 K and initial pressure 1 atm. Ignition was initiated by adding a small region of very high temperature and pressure around the ignition point. The values for the ignition pressure and temperature should be in a reasonable range, if the values are much lower than the CJ detonation values for pressure and temperature, it would either fail to initiate detonation or lead to oscillations prior to establishing a stable detonation wave. However, applying a very high initiation pressure and temperature would create a strong and unstable detonation wave at the beginning before transitioning to a stable detonation wave. To avoid the above mentioned oscillations we set the ignition pressure and temperature roughly equal to the CJ values: 15 atm and 3000 K. The volume of the initial hot region for ignition initiation was selected carefully such that the energy added equals to the ignition energy in the experiments. This equates to 200 g of TNT.

Following ignition, the simulation was run for 22 milliseconds, which was sufficiently long for the detonation to reach the opposite end of the tunnel and burn out all the reactive mixture. The predictions were then compared with the measurements and numerical results of Kotchourko (2007).

RESULTS FOR THE TUNNEL

The predicted pressure fields at two different moments are presented in Figs. 11 and 12. In both plots, the reflection of shock waves from the side walls can be seen. In some

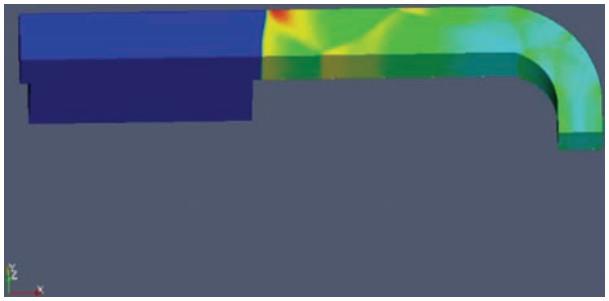

Figure 11. The predicted pressure field

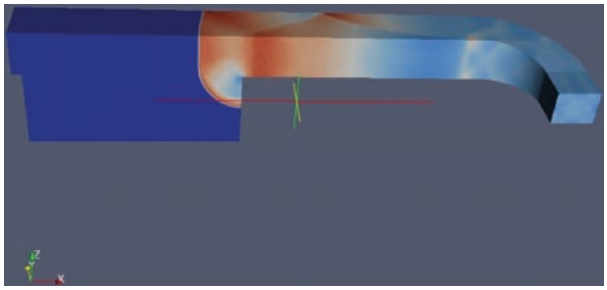

Figure 12. The predicted pressure field

areas these reflected shocks create regions with pressure higher than the leading detonation shock.

The diagrams of pressure via time for the selected monitoring points are shown in Figs. 13 to 17, where the dash-dotted line represents the experimental results; the

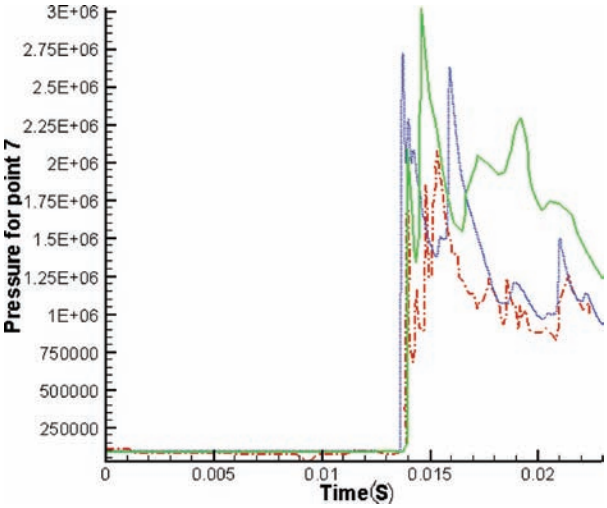

Figure 13. The predicted pressure *vs* time for point 7

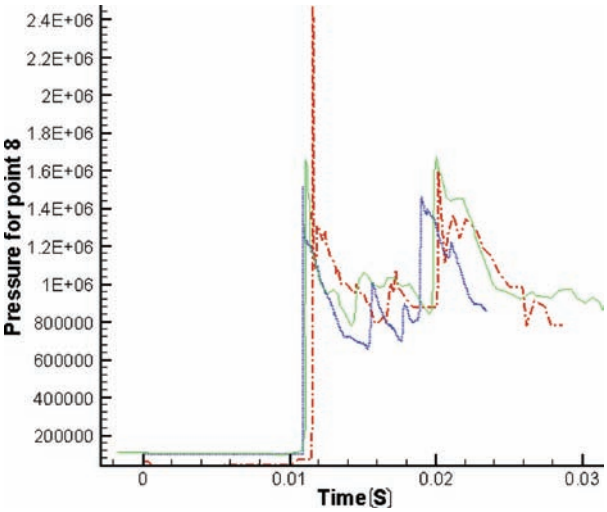

Figure 14. The predicted pressure *vs* time for point 8

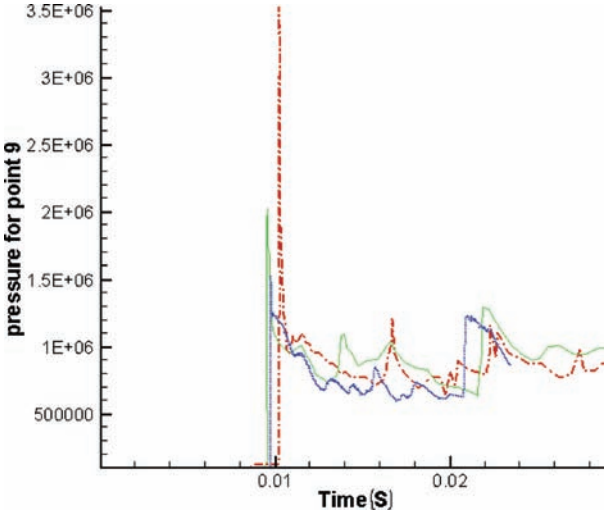

Figure 15. The predicted pressure *vs* time for point 9

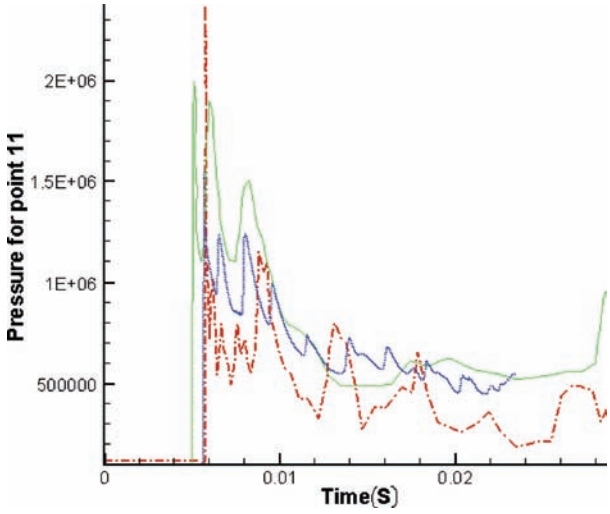

Figure 17. The predicted pressure *vs* time for point 11

continuous lines are the predictions of Kotchourko (2007) while the dotted lines are the present predictions. It can be seen that the present predictions have followed the same trend as the experiment (after the leading shock). It is expected that the predicted peak pressures of the leading shock would be lower than measurements as the grid resolution was not designed to capture the shock waves. It can be noted that the measured peak pressure was actually higher than the von-Neumann peak due to the reflections of shock waves. The predictions are broadly in line with the measurements in terms of the pressure decay following the shock, the arrival of the shock and the actual values of the overpressure at different times.

CONCLUSIONS

The predictions for hydrogen explosions in a simulated refill environment have achieved very good agreement with the experiment data. The peak overpressure decrease almost inversely with distance from the front open end. It was also found that below 40% H_2 concentration, the overpressure at the same monitoring location increases with hydrogen concentration. At 40% H_2 concentration, the overpressure reaches its peak. Afterwards, the overpressure decreases with further increase in H_2 concentration. The hydrogen concentrations leading to the largest overpressures correlate with those which have the highest flame speed. Considering the fact that an overpressure of 9.8 kPa is the permissible human tolerance limit, the safe distance from the simulated hydrogen fuel installation can be taken as 15 m for this particular configured installation. Other installation configurations would have different safe distances.

A numerical approach for the simulation of large scale detonation has been developed based on the solution of the Euler equations and single step chemistry. Predictions were firstly conducted for smaller domains of various sizes in both one and two dimensional studies to find suitable pre-exponential factor and activation energy which will predict the correct CJ parameters with the chosen grid resolution while supplying the right energy into the governing equations.

Numerical simulations were then carried out for the detonation tests conducted at the RUT tunnel facility in Russia. Comparison with the test data have shown that the model is in reasonably good agreement with the experimental data on the detonation speed judged by the time of detonation arrival at different monitoring point. The model also predicted the correct CJ pressure.

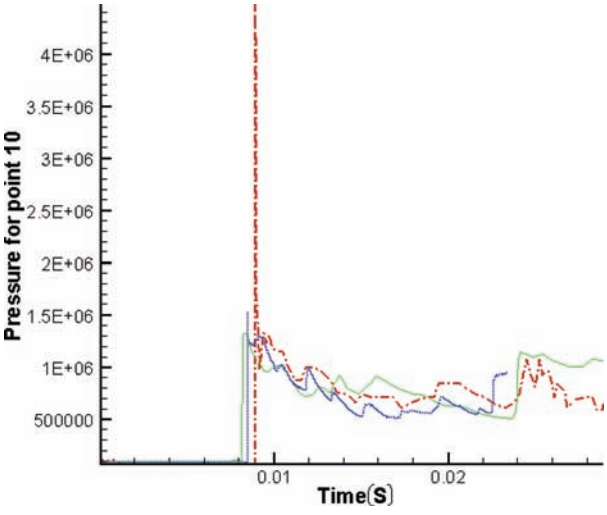

Figure 16. The predicted pressure *vs* time for point 10

ACKNOWLEDGMENTS

The authors would like to acknowledge EU FP6 Marie Curie programme for funding hydrogen research at Kingston University through the HYFIRE (Hydrogen combustion in the context of fire and explosion safety) project. We also acknowledge BP and HSL for acting as supporting groups for HYFIRE.

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