Numerical simulation of large scale hydrogen detonation

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ABSTRACT

The present work is concerned with numerical simulations of large scale hydrogen detonations. Euler equations have been solved along with a single step reaction for the chemistry. Total variation diminishing (TVD) numerical schemes are used for shock capturing. The equations are solved in parallel in a decomposed domain. Predictions were firstly conducted with a small domain to ensure that the reaction scheme has been properly tuned to capture the correct detonation pressure and velocity. On this basis, simulations were set up for the detonation tests carried out at the RUT tunnel facilities in Russia. This is one of the standard benchmark test cases selected for HYSAFE [1]. Comparison is made between the predictions and measurements. Reasonably good agreement has been obtained on pressure decay and the propagation speed of detonation. Further simulations were then conducted for a hypothetical hydrogen-air cloud in the open to assess the impulse as well as overpressure. The effects of cloud height, width were investigated in the safety context.

Keywords: Numerical Simulation, Detonation, Large Scale

1. INTRODUCTION

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 [2]. 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 [3-5], but full scale testing is costly. Hence, only a limited number can be conducted in highly specialised facilities. Predictive tools, validated from experimental measurements, offer an alternative for such studies. Several numerical simulations of detonations have been carried out in the past [6-10], but most of these investigations have focused on small scales with domain sizes typically in the order of centimetres. Despite the theoretical values of these investigations, the results cannot be directly applied to risk assessment in real scenarios. More recently, hydrogen detonations at realistic scale have also been conducted by Bédard-Tremblay et al. [11] and Zbikowski et al. [12].

In the present study, an approach to numerically simulate large scale detonation is developed. Predictions were carried for large scale detonation tests at the RUT facility in Russia as well as hypothetical planar hydrogen cloud [1].

2. THE GOVERNING EQUATIONS

A detonation is a shock wave which is followed by a combustion wave. The shock and the combustion region are coupled and move together, in other word detonation is a supersonic combustion wave [2].

For the numerical simulation of detonations the reactive Euler equations should be solved. These equations include the conservation equations for mass continuity and energy, equations 1 to 3:
Continuity equation:

$$\frac{\partial \rho}{\partial t} = -\nabla(\rho V) \qquad (1)$$

Momentum conservation equation:

$$\frac{\partial \rho V}{\partial t} = -\nabla(\rho VV) - \nabla P \qquad (2)$$

Energy conservation equation:

$$\frac{\partial \rho E}{\partial t} = -\nabla(\rho EV) - \nabla(\mathrm{V}P) \qquad (3)$$

The above equations should be solved along with a set of chemical reaction equations for the underlying combustion process. These reactions model the consumption and production of each chemical element which is 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 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 which is used here is a single step Arrhenius form reaction which can be written as

$$\omega = A(1-\alpha)EXP(-\frac{E_a}{RT}) \qquad (4)$$

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 reactions need 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 should be 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. [13], several simulations in one and two- dimensions were carried out to tune the reaction constants in Eq. (4). 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 [14], which gave CJ pressure and propagation velocity of 15 atm and 1970 m/s respectively, the CJ results of the equilibrium code are validated against experimental results for detonations [14].

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

$$\omega = 11^9 \times (1-\alpha) EXP(-\frac{23000}{T}) \qquad (5)$$

The other equations that should be added to the governing equations are as follows:

Reaction progress equation:

$$\frac{\partial \rho\alpha}{\partial t} = -\nabla(\rho\alpha V) + \rho\omega \qquad (6)$$

Energy equation:

$$E = -\alpha\mathbb{Q} + \frac{P}{[\rho(\gamma-1)]} + \frac{V^2}{2} \qquad (7)$$

Equation of state:

$$\frac{P}{\rho} = \frac{RT}{M} \qquad (8)$$

In Eq. 5, α is the reaction progress variable and is zero where all the mixture is unburned and 1 where the mixture is burnt. $\mathbb{Q}$ is the heat of chemical reaction per unit mass. The relation between ω and α is as follows:

$$\omega = \frac{d\alpha}{dt} \qquad (9)$$

3. NUMERICAL SOLUTION

The above equations are discretized using finite volume method [15]. Explicit Euler scheme is used for the time derivatives. For shock capturing, the Van Leer scheme which is a total variation diminishing scheme, is used.

The Van Leer flux limited method can be expressed by the following formulation:

$$u_i^{n+1} = u_i^n - \lambda(\hat{f}^n_{i+\frac{1}{2}} - \hat{f}^n_{i-\frac{1}{2}}) \qquad (10)$$

$$\hat{f}^n_{i+\frac{1}{2}} = \frac{1+\eta_i^n}{2}\hat{f}^{L-W}_{i+\frac{1}{2}} + \frac{1-\eta_i^n}{2}\hat{f}^{B-W}_{i+\frac{1}{2}} \qquad (11)$$

$$u = \begin{bmatrix} \rho \\ \rho u \\ \rho e_T \end{bmatrix} \qquad (12)$$

$$f = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_T + p)u \end{bmatrix} \qquad (13)$$

Further details about the scheme can be found in reference [16]. The courant number is kept under 0.1 to avoid large time steps during the solution.

3.1 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 263 m^3 volume [1]. Schematic of the test channel is shown in Figures 1 and 2.

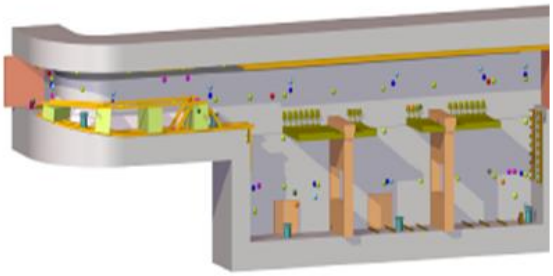

Figure 1. The experiment channel (reproduced from [4])

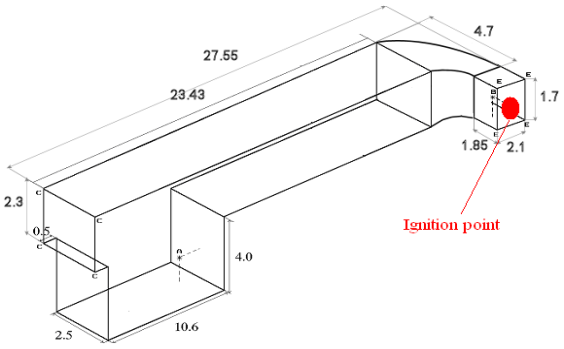

Figure 2. The tunnel dimensions (reproduced from [4])

The dimensions of the tunnel and the ignition location are shown in the Figure 2.

The tunnel was filled with hydrogen-air mixture. Ignition was started at one end of the tunnel as shown in Figure 2. The detonation was started by direct initiation [17] with a high explosive charge of 200 g weight as the initiator [1].

Overall, twelve monitoring points were selected where pressure gages were used to record pressure-time history. As shown in Figure 3, the gauges were place at the opposite end of the tunnel with regard to the ignition point.

Pressure measurements are available for 5 of the 12 monitoring points, i.e. points 7 to 11. The present predictions are compared with these measurement as well as the numerical predictions of Kotchourko [4] for the same set up.

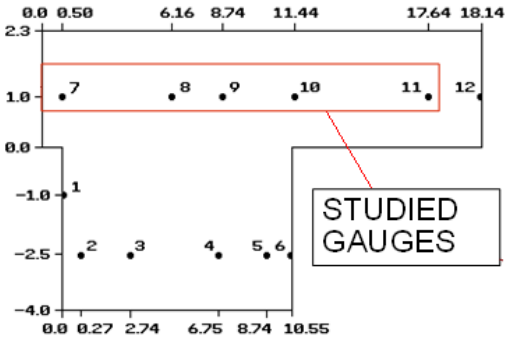

Figure 3. Locations of the monitoring gauges (reproduced from [4])

3.2 Numerical setup 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 Figure 4 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.

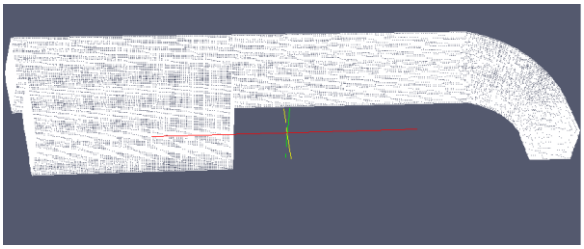

Figure 4. The Mesh pattern for RUT tunnel

The domain is decomposed into 20 sections to facilitate parallel processing. Since the domain is a closed enclosure and the reactive mixture is completely confined, all the boundary conditions are set to 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. On the other hand applying very high initiation pressure and temperature would create a strong and unstable detonation wave at the beginning before transiting to a stable detonation wave. To avoid the above mentioned oscillations it is recommended to set the ignition pressure and temperature roughly equal to the CJ values. The pressure and temperature used for initiation in the present work are 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. As mentioned earlier 200 g TNT was used to ignite the mixture in the experiments, so the hot region in the numerical work was designed to contain the same amount of energy.

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 [4].

3.3 Results for the Tunnel

The predicted pressure fields at two different moments are presented in Figures 5 and 6. In both plots, the reflection of shock waves from the side walls can be seen. In some areas these reflected shocks create regions with pressure higher than the leading detonation shock.

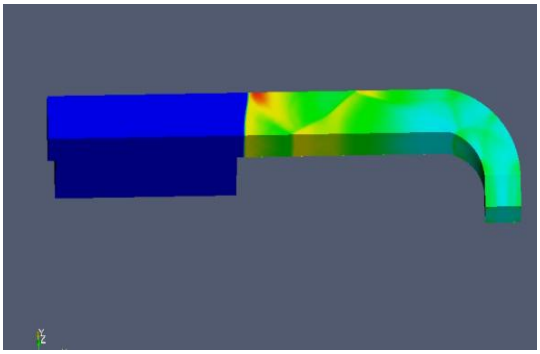

Figure 5. The predicted pressure field.

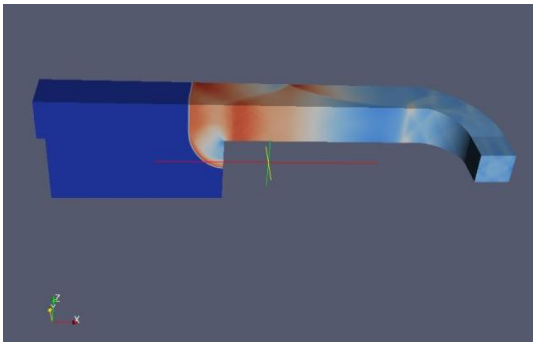

Figure 6. The predicted pressure field.

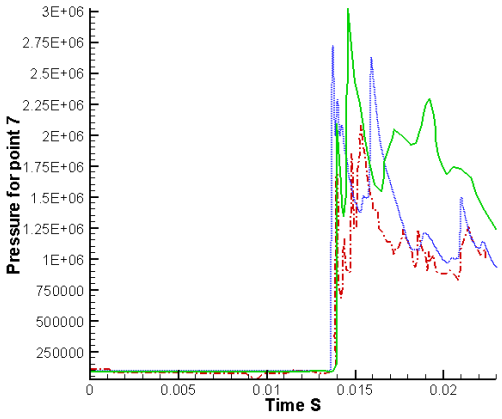

Figure 7. The predicted pressure (in Pascal) *vs* time for point 7.

The diagrams of pressure via time for the selected monitoring points are shown in Figures 7 to 11, where the red dash-dotted line represents the experimental results; the green lines are the predictions of Kotchourko [4] while the blue dotted lines are the present predictions. It can be seen that the present predictions have followed the same trend as the experiment. It is expected that the predicted peak pressure would be lower than the measurement as the grid resolution was not designed to capture the shock waves. Even at the peak, the present predictions are higher than those of Kotchourko [4]. It should also be pointed out that the measured peak pressure here was actually higher than the von-Neumann peak due to the reflections of shock waves which further amplified their strengths. 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.

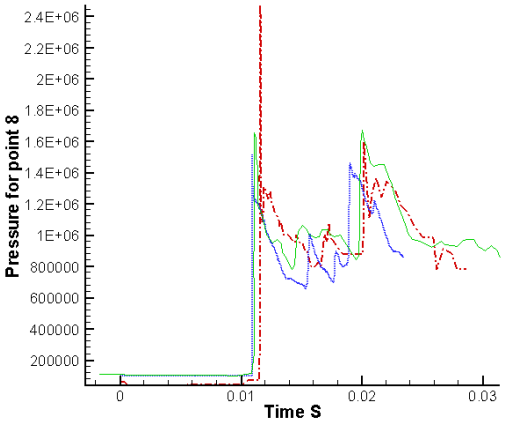

Figure 8. The predicted pressure (in Pascal) *vs* time for point 8

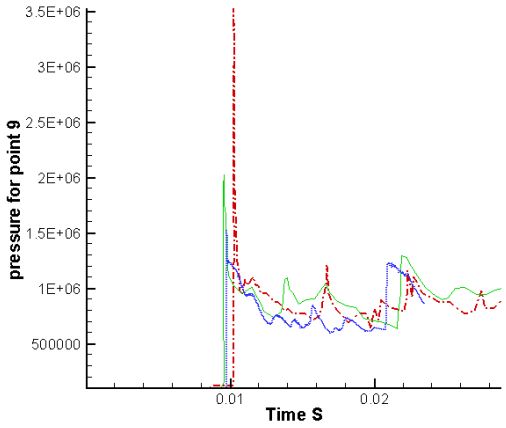

Figure 9. The predicted pressure (in Pascal) *vs* time for point 9

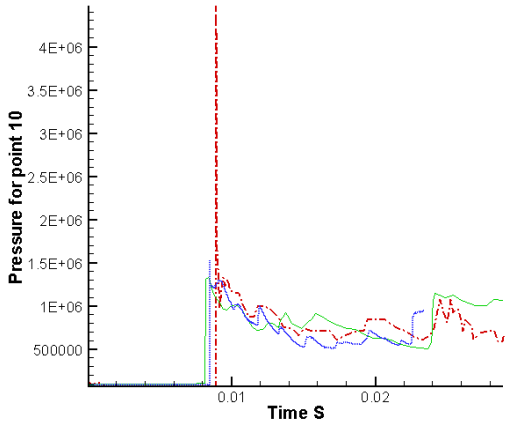

Figure 10. The predicted pressure (in Pascal) *vs* time for point 10

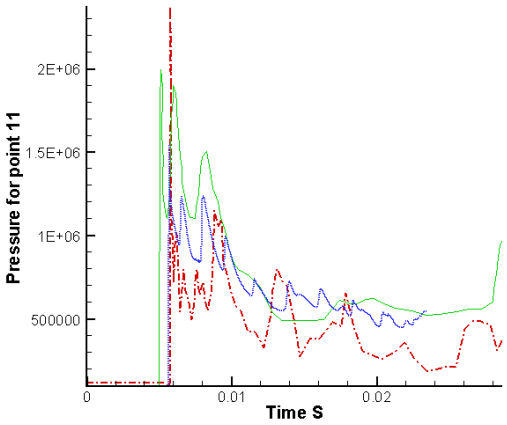

Figure 11. The predicted pressure (in Pascal) *vs* time for point 11

3.4 Numerical set up for the planar hydrogen-air cloud

Two-dimensional simulations were carried out for the detonation of a hypothetical hydrogen-air cloud to examine the propagation of the resulting blast wave in the surrounding air and the pressure impulse. Predictions were made for clouds of different aspect ratios to investigate the effect of cloud height on the rag impulse. Here just the pressure, velocity and drag impulse for one of the cases are presented.

Drag impulse is the impulse generated by high speed gasses that follow the detonation waves and in general any impulse caused by the drag force of the gas flows.

In most detonation studies, the focus has been on the pressure impulse but our study shows that high speed gasses can generate a significant drag impulse. The later has more determining influence on the damages.

The drag impulse can be determined using the Morrison equation (eq.14) [18]:

$$I = \int f_D dt = \int_0^{t_i} \left\{ \left(\frac{1}{2} C_d \times \rho \times A \times Ux^2 \right) + \rho \frac{dU_x}{dt} \right\} dt) \qquad (14)$$

The second term inside the integral is called unsteady impulse which is generally much smaller than the steady (first) term so the Morrison equation can be rewritten in the following simplified form:

$$I = \int f dt = \int_0^{t_i} (\frac{1}{2} C_d \times \rho \times A \times Ux^2) dt) \qquad (15)$$

Simulations were carried out for the detonation of a planar hydrogen cloud which is surrounded by air. The computational domain is of rectangular shape with dimensions of 160 × 70 m as shown in Figure 12. The extent of the stoichiometric hydrogen-air cloud is 10 × 7 m (red box) placed at the origin of the domain. The rest of the domain (the blue colour region) contains air.

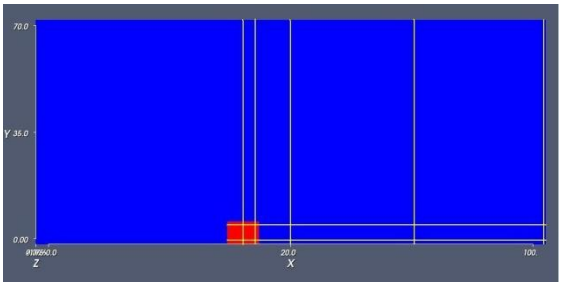

Figure12. The computational domain for the planar hydrogen-air cloud

Due to the relatively large size of the domain, it is necessary to divide the domain into several sections and use appropriate grid resolution and pattern for each region based on the its relative level of importance. For example, inside the cloud area a relatively fine structured mesh (1 cm). From the edge of the cloud and its immediate surrounding where the blast wave is expected to be strong, the mesh resolution is only decrease slightly. Further out, the unstructured mesh gradually becomes coarser. Figure 13 shows the mesh pattern in the immediate region around the cloud, where the mesh inside the cloud is so fine that the grids are almost un-distinguishable. As discussed, such grid resolution will not resolve the shock waves but should predict with reasonable accuracy the pressure decay with the tuned chemistry.

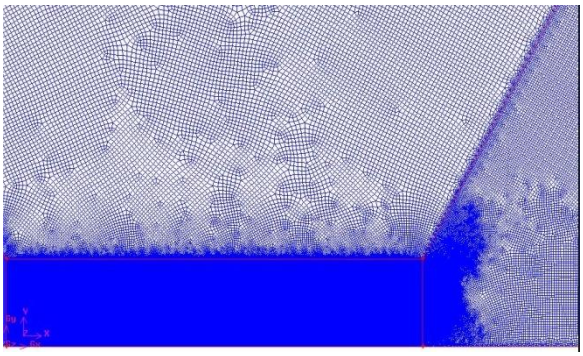

Figure13. The mesh pattern around the cloud

A hot high pressure region was used to initiate the detonation. This consisted of a vertical line of cells along the left edge of the cloud set to 3000 K and 15 atm. Pressure, density, velocity and temperature were monitored at selected points along several horizontal and vertical lines. Results will be presented in particular for several points along the monitoring line which is placed 1 m above ground for estimation of potential damage at this level through analysis of the pressure, velocity and drag impulse at 5 monitoring points. The coordinates of these points are as follows:

Table-2 Coordinates of the monitoring points

Monitoring points	Coordinates
1	(0.2 1.0)
2	(5.0 1.0)
3	(10 1.0)
4	(12 1.0)
5	(19 1.0)

3.5 Results of the planar-hydrogen cloud detonation

The pressure field for detonation and blast wave propagation are shown in Figures 14 and 15. Following initiation, a planar detonation propagates towards the right side of the domain. When the detonation reaches the right edge of the cloud, the mixture is all burned and the blast wave propagates into the surrounding air and decays rapidly with distance from the initial cloud. As the detonation wave propagates through the hydrogen-air mixture and then transmits from the cloud to air, due to the free boundary on the top of the cloud, the detonation wave diffracts. In addition, due to high pressure of detonation products, the shock wave propagates outwards from both the top and left of the cloud.

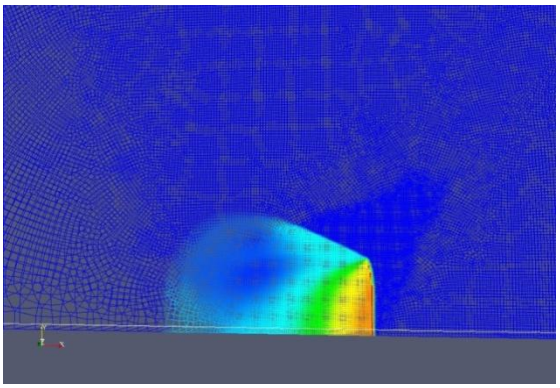

Figure14. The pressure field for the planar detonation wave

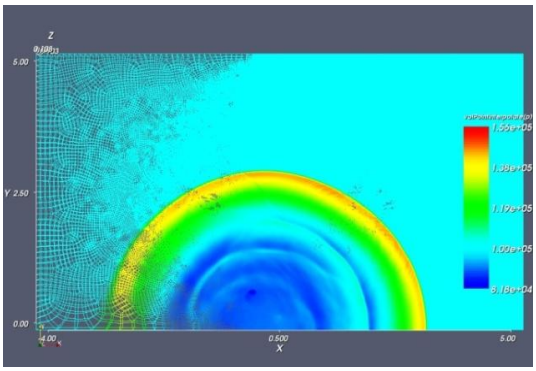

Figure 15. The pressure field for the blast wave

The pressure diagram for the monitoring points are shown in Figure 16 with predictions for points 1 to 5 are shown in red, green, purple, black and blue colour, respectively while in Figure 17, the pressure-time history for all the monitoring points at 1m above ground are shown. It can be seen that there is a sharp drop in overpressure from the edge of the cloud (point 3) where the aftershock expansion starts.

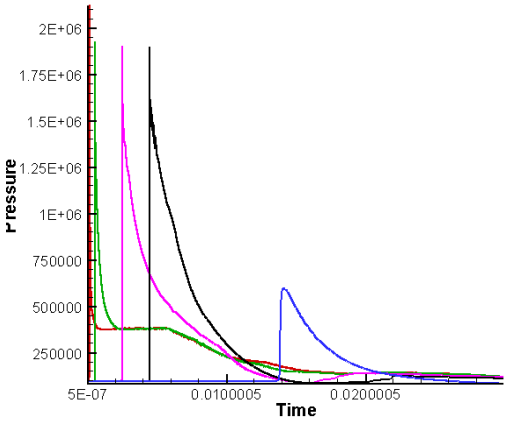

Figure16. The pressure-time diagram the line 1 m above the ground (P unit is Pascal)

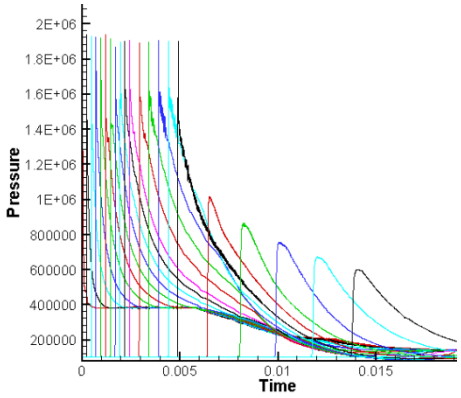

Figure17. The pressure-time diagram the line 1 m above the ground (P unit is Pascal)

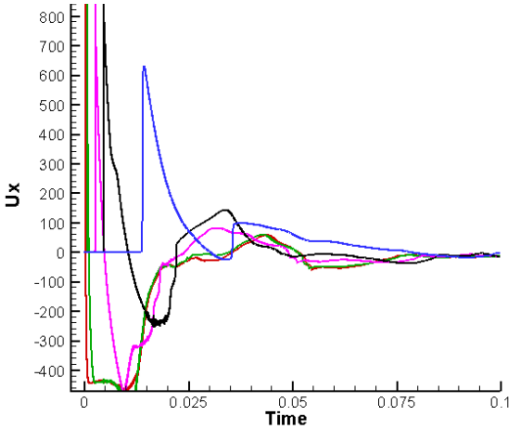

Figure 18. The velocity-time diagram at selected points 1 m above the ground (U unit is meter per second)

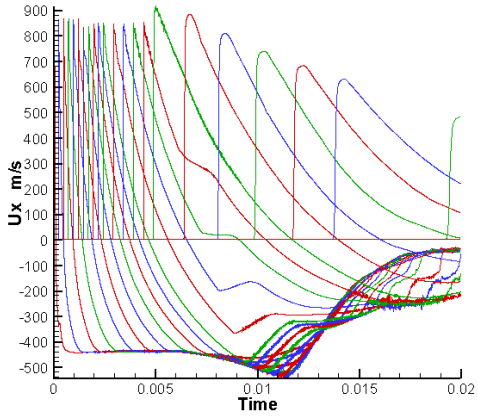

Figure19. The velocity-time diagram along the monitoring line 1 m above the ground (U unit is meter per second)

Figure 18 shows the velocity *vs* time at monitoring points 1 to 5. Figure 19 shows more points along the monitoring line 1m above the ground. It can be seen that immediately following the initiation of detonation, there is a very short period where the gas velocity shots up to very high values. This is followed by a relatively longer period of negative velocity. It is thought that while a shock propagates towards the left and a detonation propagates towards the right, the product expands and then over-expands between them. In order to match the high pressure behind the shock or the detonation wave and the over-expanding low pressure region, secondary shocks form and propagate inwards which leads to a relatively longer period of negative velocity. With time elapsing, in the product region, there exist shock-shock interaction, shock-expansion wave interaction, etc.

We further plot the drag impulse *vs* time for points 1 to 5 in Figure 20, where the sequence and colour of the curves is the same as in Figures 16 and 18. The drag impulse is calculated using the simplified Morrison equation (eq. 15) based on a cumulative total for each time step. The results show that within the cloud, the drag impulse is predominantly negative (towards the left) while outside the cloud the impulse is positive (towards the right). This finding could have important implications when examining forensic evidence following explosion accidents and to our knowledge has never been reported in previous publications. The negative impulse is caused by high negative velocities of the gasses in the opposite direction of the detonation wave which last for a relatively longer period of time in comparison with the expansion in the direction of detonation wave. This happens shortly after the detonation passage at each point. When the detonation passes a reference point, it forces the products behind it to move in the positive direction with the sound speed relative to the shock (CJ

theory). This leads to creation of high pressure gradient behind the detonation wave. When the detonation is far enough and the gasses cannot see its effect this pressure gradient forces the gasses to move in the opposite direction and compensate the pressure gradient behind the shock, which is caused by the forced movement of products by detonation. The result is a relatively long period of negative velocity after the shock passage and the generation of a strong negative impulse. Weather the overall impulse is positive or negative highly depends on the position of the monitoring point. As shown in Figures 18 and 20, nearer to the origin of detonation the negative velocities last much longer and are of higher values, leading to higher negative impulse. But for the points which are further from the origin, the positive phase is dominant producing an overall positive impulse.

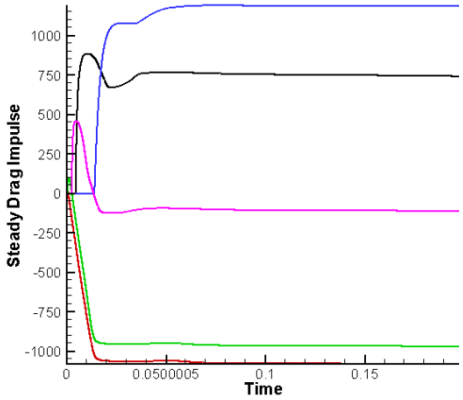

Figure 20. The drag impulse *vs* time at selected points 1 m above the ground

4. Conclusions

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. There are some discrepancies in the recorded peak pressure. This is, however, expected as the reaction constants were only tuned to produce the correct CJ parameters at the chosen grid resolution. The model has indeed predicted the right CJ pressure. Since the sharp von-Neumann peak exists only very briefly, it does not have much significance in safety studies while the CJ parameters have much more significant influence on the overall pressure and drag impulse.

Subsequently, numerical investigations were conducted for the detonation of a planar hydrogen-air cloud. In contrary to common belief that hot products will expand away from the centre of detonation, the predictions have revealed the existence of high negative drag impulse within the cloud. Such impulse was also found to vary with heights. This can be used to see the effect of such a detonation on the equipments that are mounted on different heights.

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