

Numerical simulation of diverging cylindrical detonation in hydrogen air mixtures

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Abstract

Propagation and stability of diverging cylindrical detonation in hydrogen air mixture is numerically simulated and the mechanism of the transverse waves is analysed. For the numerical modelling, a new solver based on compressible, transient, reactive Navier–Stokes equations is developed which can simulate detonation propagation and extinction in hydrogen-air mixture. A single step reaction mechanism is tuned to ensure the detonation and deflagration properties (in case of detonation failure) can be simulated accurately. The solver is used for modelling various detonation scenarios, in particular cylindrical diverging-detonations, because most of accidental industrial detonations start from a spark and then a diverging-detonation propagates outwards. The diverging-detonation, its cellular structure and adoption with the increased surface area at the detonation front, as well as interactions with obstacles leading to detonation failure and re-initiation are studied.

Introduction

Studying the propagation mechanism of diverging cylindrical and spherical detonation is particularly important because most unconfined accidental detonations in industries starts from weak ignition source which then leads to a cylindrical or spherical detonation wave propagating outwards. Studying the propagation mechanism can help the researchers understand how the detonation wave can cope with the increase in the surface area and sustain which in turn could facilitate understanding the most effective ways to mitigate and control these types of detonation waves. This is particularly important for hydrogen industries due to the rapid growth in the development of hydrogen fuelled industries [1] and the fact that an accidental release of hydrogen can create a highly reactive mixture with air which can easily detonate and cause severe damage to the facilities and the people.

In the past a number of theoretical studies have been carried out [2-4] to analyse the propagation mechanism of diverging detonations, but most of these works are based on assuming a simple CJ condition for the detonation. However the curvatures and instabilities at the leading front of the detonation waves mean that they cannot be described with a steady CJ detonation. A more general approach [5, 6] towards CJ condition can be adopted to incorporate the effects of the surface curvatures leading to a more realistic description of diverging detonations. Polley et al. [7], experimentally studied the necessary condition for transforming a planar detonation into a cylindrical diverging detonation in four different mixtures including hydrogen and oxygen mixture.

Jackson et al. [8] studied the evolution of detonation shock front in a weakly unstable cellular detonation both numerically and experimentally and analysed the structure of expanding and shrinking detonation cells.

In diverging detonation, as the surface area of the detonation front increases, new transverse waves, which in turn form new triple points and cells, must be generated to keep a constant cell size and consistent cell pattern [12]. This phenomenon is also referred to as “cellular cell bifurcation” and is demonstrated in studies by Lee et al. [9, 10]. This phenomenon in a cylindrical detonation of acetylene and oxygen mixture is illustrated experimentally by Qian et al. [11] by using a series of self-luminous, open-shutter photographs. Wang et al. [12, 13] simulated and studied the propagation mechanism of diverging cylindrical detonations by solving two dimensional Euler equations and a single step reaction mechanism and concluded that the local curvature of the cylindrical cellular detonation is a key parameter in propagation of cylindrical cellular detonations. Jiang et al. [14] solved two dimensional Euler equations and a two-step reaction mechanism. In their numerical work they identified four mechanism of transverse wave generation and showed that the propagation of diverging detonation is maintained through the growth of transverse waves in a manner that match with the rate of surface area increase in the detonation wave front [14].

In the present work a solver which was previously developed by the author, to model deflagration to detonation transition [15, 16], is adopted and modified to simulate diverging detonations and their diffraction and failure in presence of obstacles and the possibility of detonation re-initiation.

Numerical model

The diffusive and viscous effects are less significant in supersonic flow especially in Detonation waves which have an extremely high velocity. Therefore it is possible to simulate detonation waves by solving reactive Euler equations (Navier-Stokes equations simplified for inviscid flow). However the current work intends to investigate detonation failure and re-initiation meaning that at some stages high velocity deflagration waves with significant contributions from diffusive terms must be simulated. To model this range of combustion regimes e.g. deflagrations and detonations properly, full Navier-Stokes equations must be solved. These equations represent the conservation of mass, momentum and energy:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho U_i)}{\partial x_i} = 0 \quad \text{Mass conservation equation (1)}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial(\rho(U_i + V_{k,i})Y_k)}{\partial x_i} + \nabla \cdot (D_i \nabla Y_k) = \omega_k \quad \text{Spices conservation equation (2)}$$

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial(\rho U_i U_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left(\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial U_j}{\partial x_j} \right) \quad \text{Momentum equation (3)}$$

$$\frac{\partial \rho h_0}{\partial t} + \frac{\partial(\rho h_0 U_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(k \frac{\partial T}{\partial x_j} \right) + \frac{\partial p}{\partial t} + \mu \left[\frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)^2 - \frac{2}{3} (\nabla \cdot \vec{U})^2 \right] + S \quad \text{Energy equation (4)}$$

In the above equations, D_i and S represent species diffusion coefficient and the energy source term.

Employing a suitable reaction mechanism is one of the most crucial steps in order to ensure a reliable prediction.

Tuning the reaction mechanism

The right amount of chemical energy needs to be injected, through the reaction mechanisms, in the right place at the correct timing otherwise the dynamic of the flow would be adversely affected. There are a number of chemical reactions proposed in the literature e.g. [17, 18] for flame and detonation propagations. Preliminary simulations carried out by the author have, however, shown that some of the proposed reactions in the literature fail to reproduce reasonable behaviour in some ranges of

combustion regimes that is of interest in this study. Therefore, in order to overcome these problems, it is necessary to develop a reaction mechanism which is able to reproduce reasonable behaviour for both deflagrations and detonations.

In the present work the Arrhenius equation presented in Eq. 5 is used to describe production rate of the products.

$$\dot{\omega} = A[O]^{n_O}[F]^{n_F} \exp\left(\frac{-E}{RT}\right) \quad (5)$$

[O] and [F] represent the oxygen and fuel molar concentrations, n_O and n_F show the reaction empirical orders.

Eq. 5 is tuned in this work using the approach proposed by Bane, Ziegler and Shepherd [19] for detonation, and the approach proposed by Oran et al. [17] for deflagrations. Wang et al. used this approach to derive a model for hydrogen reaction [20]. This method is adopted in the present work.

and the resulting single step chemical reaction is presented in Eq. 6.

$$\dot{\omega} = 9.3 \times 10^{10} [H_2][O_2] \exp\left(\frac{-43.67RT_0}{RT}\right) \quad (6)$$

The approach to derive the chemical reaction is discussed by Wang et al. [20] in more details.

Reaction validation

In order to validate the derived reaction mechanism a set of test simulations for flame and detonation propagation in a 1-D domain with 1 μm grid spacing are carried out to verify the flame temperature, propagation velocity, detonation pressure and detonation propagation velocity. The predicted flame velocity, temperature and detonation pressure and velocity are listed in Table 1:

Table 1 Flame and detonation parameters, predictions compared with measurements.

Stoichiometric mixture	Current work	Experimental
Flame temperature	2491 K	2483 K [23]
Burning velocity	2.95 m/s	2.9 m/s [23]
detonation pressure	15.9 atm	15.447 atm [22]
Detonation velocity	1997 m/s	1980 m/s [22]

The predicted temperature, pressure and velocities are in agreement with the experimental results from literature [21-23]. This verifies that the derived reaction mechanism can be used for the deflagration and detonation predictions. However in case of detonation, the pressure and velocity (and other statics parameters) are known to be driven by thermophysical properties, therefore validation of detonation dynamic properties are also required to verify the applicability of the proposed reaction mechanism. Therefore simple 2D detonation propagation is simulated to evaluate the formation and size of the detonation cellular structure. Formation of the detonation cellular pattern is recorded by tracking the position of the triple point, figure 1. The recorded cell width varies from 0.5 to 2 cm and the average recorded cell width is $\lambda \approx 1.5$ m/s which is within the expected range.

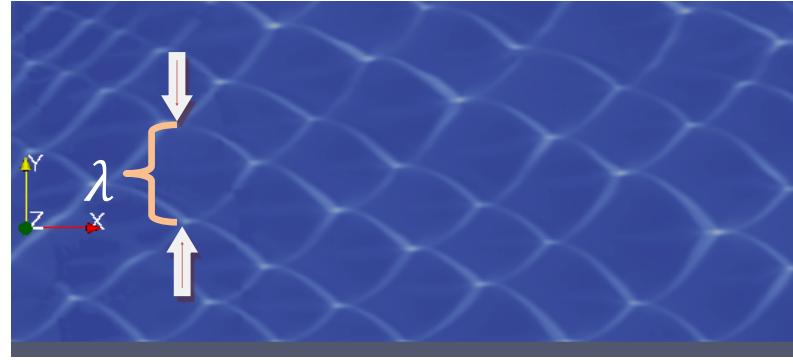


Figure 1: Recorded detonation cellular pattern

Turbulence model

Over the past years it is observed that monotone fluid-dynamic algorithms produce results that are in good qualitative and quantitative agreement with experimental results [24]. Monotone fluid-dynamic algorithms do not use explicit turbulence models. Even in some studies which include significant turbulence in sub-grid scales, the monotone fluid-dynamic algorithms have been found to produce reasonably accurate predictions [24-27].

There are interesting physical reasons which explain good performance of these methods as described by Oran [24] and Grinstein et al. [27].

Apart from the physical justifications discussed in the literature, the numerical nature of the nonlinear monotone numerical methods exhibits some uniquely valuable properties which can be summarised in: conservation, and positivity which can be called monotonicity. It means this numerical methods, through their local dissipation, can smoothly connect the large scale, energy carrying, resolved eddies to the smaller unresolved scales, and this is done by the natural dissipation effects which exists in these methods. While using these methods in LES one can trust that the larger scales are resolved with the minimal influence from the numerical errors from the smallest resolved scales [24].

For simulating detonation failure and re-initiation a wide range of time and space scales must be resolved to produce a reliable solution, however, the information about these scales and instabilities involved can be used to make the simulations efficient. As a compromise between computational requirement and accuracy, it is decided to base the present study on monotone fluid-dynamic techniques and Implicit Large Eddy Simulation (ILES), meaning that the sub-grid scale turbulence wouldn't be modelled explicitly; instead the numerical diffusion is used to compensate the sub-grid scale effects.

A solver is developed by the author and based on OpenFOAM CFD toolbox [28] to solve the governing equations, the same solver was used previously by the author to simulate DDT and reasonable result were achieved [15, 16]. The finite volume method with the explicit Euler scheme for the time derivatives [29] is used. For shock capturing, the Van Leer flux limited method which is a total variation diminishing scheme and a monotone fluid-dynamic scheme is used [24].

Diverging cylindrical detonation and diffraction over the obstacles

The solver is used to simulate the propagation of diverging detonation firstly in unconfined free space and secondly in presence of obstacles. In Figure 2 the numerical prediction of the present work are qualitatively compared against the open-shuttle photograph of a diverging cylindrical detonation by Soloukhin [30]. Although the two cases are not identical, the two intersecting sets of logarithmic

spirals which are formed by trajectories of the transverse waves creating the detonation cell structure can be compared qualitatively. At the ignition centre, initially a slightly overdriven detonation is formed which quickly disappears and the diverging detonation grows outwards, leaving the cellular pattern behind. Therefore the recorded cellular pattern around the ignition centre may not be consistent with the rest of the domain.

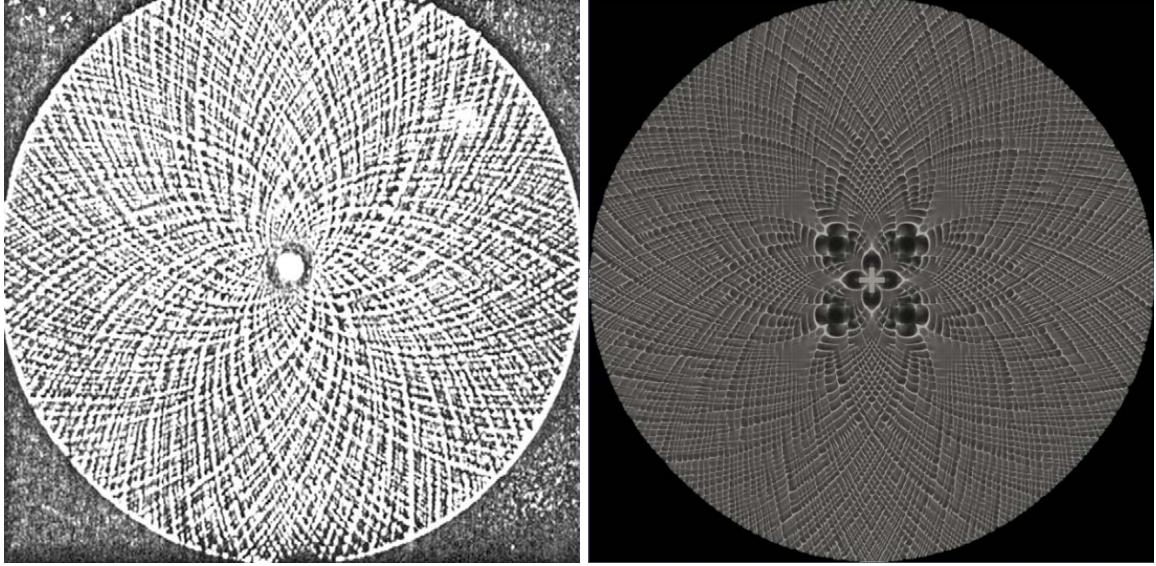


Figure 2: Numerical simulation of cellular pattern in a diverging cylindrical detonation (right image) compared against the open-shuttle photograph of a diverging cylindrical detonation [30].

Both the numerical prediction and experimental observations show that the trajectories of the transverse waves create two sets of intersecting logarithmic spirals which forms a flowery cellular pattern.

According to Lee [10], to have a self-sustained detonation the average cell size must remain the same, however, in a diverging detonation the surface area of the detonation front keeps increasing with the square of the radius, meaning that if the same number of cells remain at the detonation front, the average cell size must increase rapidly. This condition cannot sustain because if the cell size keep growing the time for the wavelets to decay would increase and at the end of the cycle when the transverse waves collide to make the new triple point, the strength of the transverse waves may be too low to create auto-ignition condition at their collision point. Therefore it is essential that more than one localised explosions are formed at the end of each cycle, leading to formation of more cells at the detonation front and keeping a constant averaged cell size as the wave propagates outwards. This phenomenon is simulated and captured in the present numerical work. Some of the areas where more than one localised explosions are formed are marked in figure 3, this clearly shows that formation of these new points results in formation of new detonation cells which in turn results in a consistent (on average) detonation cell size.

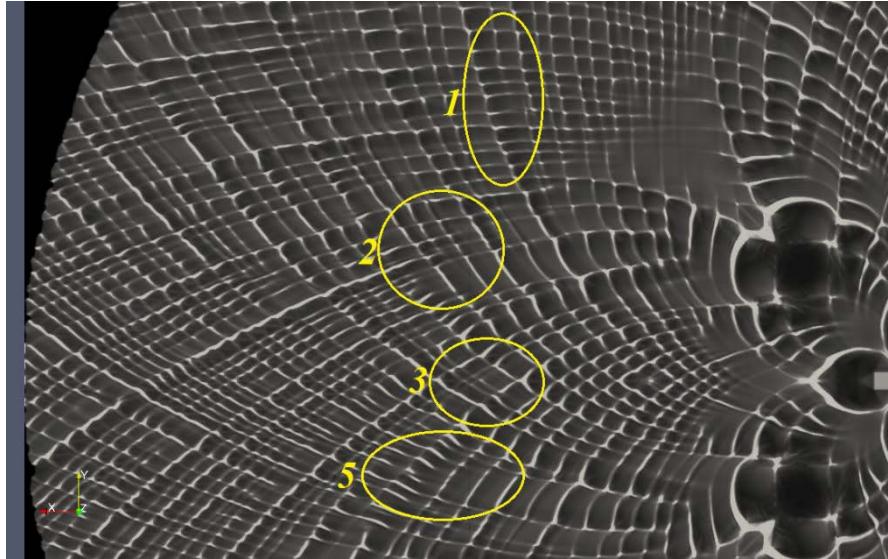


Figure 3: formation of new localised explosion points at the end of each cycle, leading to formation of more cells at the detonation front and keeping a constant averaged cell size as the wave propagates outwards

The numerical prediction of the current work are also consistent with predictions of Jiang et al. [36], which explains the mechanisms for formation of new transverse waves and localised explosion which are essential for diverging detonations to maintain their uniform propagation and stay self-sustained.

Further simulations are carried out to study the interaction of diverging detonation waves with the obstacles. This scenario is particularly of interest for risk assessments in accidental detonations in industrial facilities. In open or large geometries such as industrial facilities, a spherical or cylindrical detonation grows as it expands outwards from the ignition centre. The resulting detonation interacts with equipment at the vicinity. Therefore it is necessary to analyse the influence of obstacles on diverging detonation and the possibility of detonation failure due to diffraction.

In the present work a hypothetical 2-D domain is created to simulate diverging detonation interactions with obstacles. The results are intended to provide a qualitative description of detonation behaviour in such scenarios. The selected test case is a 0.4m by 0.4m box which includes 3 obstacles and is filled with stoichiometric hydrogen air mixture. The mixture is at standard pressure and temperature. This hypothetical cloud is ignited at the centre of the domain and consequently a diverging detonation propagates outwards. The ignition is induced by using a small region of high pressure and temperature (20 bar and 2000 K) at the centre of the domain. The induced detonation wave propagates freely downwards whereas in upward direction 3 obstacles are placed in detonation pathway.

Figure 4 shows the pressure (left image), temperature (right image) and cellular pattern (bottom image) fields for this simulation. The triple points are distinguishable in pressure field as lighter colour points (high pressure points). The wave at the top of the domain diffracts as it passes over the obstacles, this leads to flame shock decoupling which can be clearly observed in the temperature field. The decoupled pressure waves moving behind the middle obstacle hit each other at a later stage and could potentially initiate an overdriven detonation right behind the middle obstacle. Tracking the triple points as the detonation propagates outwards leaves the cellular pattern of the diverging detonation. The resulting pattern is also illustrated in figure 4 (bottom).

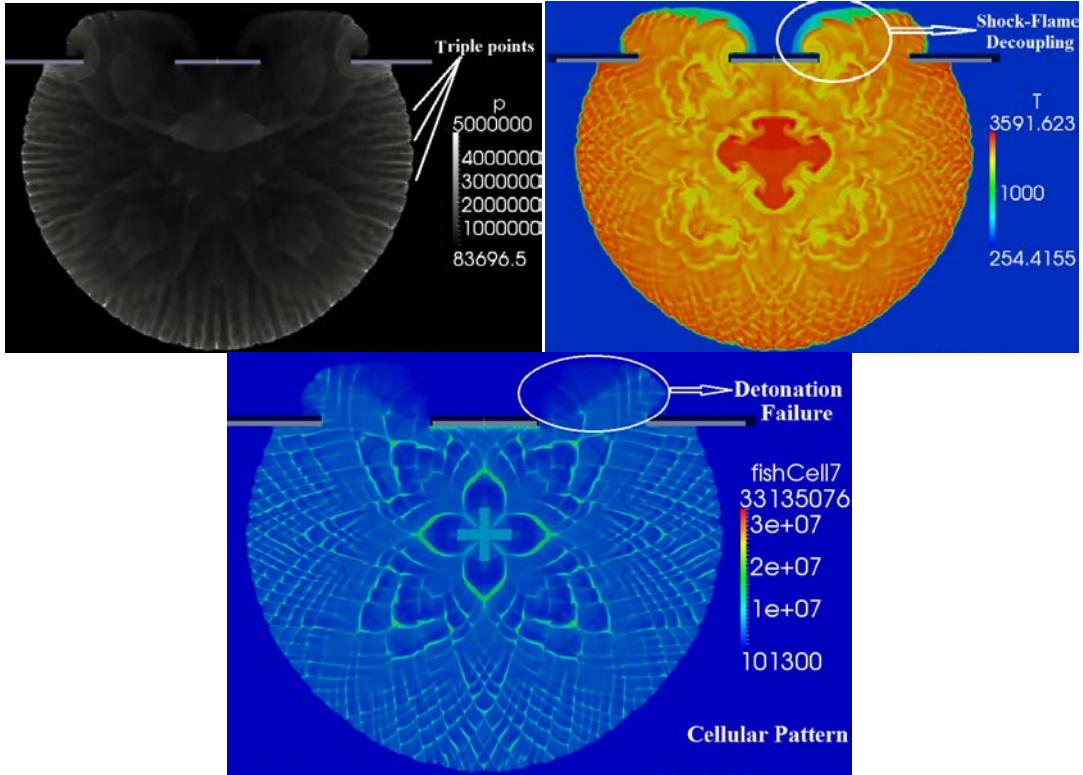


Figure 4: Pressure, temperature and cell fields for diverging detonation interaction with obstacles – flame shock decoupling after wave diffraction over the obstacles

The disappearance of the cellular pattern right over the obstacles, confirms the detonation failure at those areas which was also predicted earlier from temperature field showing flame-shock decoupling.

In figure 4, the red and yellow areas in the temperature field show the burned regions and the light green areas are the preheated regions due to shock passage. Right after the obstacle due to diffraction the shock-heated region is separated from the reacted region and moving ahead of the flame front, this represents the shock flame decoupling and detonation failure due to wave diffraction.

Conclusion

Numerical simulations of diverging detonation propagation and their interactions with obstacles leading to detonation diffraction and failure are carried out using a newly developed ILES based solver. The single step reaction mechanism is tuned and tested to ensure accurate predictions both for detonations and deflagrations (in case of detonation failure). The numerical predictions of detonation cellular pattern are in good qualitative agreement with experimental observations. As stated in literature it is essential to have new localised explosion points and transverse waves generated at the end of each cycle to form more detonation cells. This is required to keep a constant average detonation cell size which is essential for having a self-sustained detonation wave. This phenomenon is fully predicted and captured in the present numerical work. Having achieved good numerical predictions, the solver is used to simulate the interaction of diverging detonations with obstacles. The predictions show that the detonation wave diffracts and fails after passing over the obstacle however a strong decoupled shock wave keeps propagating behind the obstacle and if it collides with the shock waves from the other sides, it can potentially create a very high pressure region which could result in detonation re-initiation behind the obstacles. Therefore secondary measures such as using shock absorbent materials is suggested to accelerate the shock waves damping and lower the chance of detonation re-imitation behind the obstacles. The fine features of detonation diffraction, failure and re-initiation presented here cannot be captured using simplistic methods such as CJ burn programmed method and this was illustrated in a previous study by the authors [15].

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