Numerical modelling of deflagration to detonation transition in hydrogen air mixtures

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ABSTRACT

For over half a century, combustion researchers have studied the phenomenon of Deflagration-to-Detonation Transition (DDT). DDT phenomenon lies at the intersection of chemical kinetics, flow turbulence and compressible gas dynamics; and presents a formidable and challenging conundrum. In the nuclear industry, DDT is a known risk in accident scenarios involving unintended release and combustion of hydrogen. Through use of sophisticated measurements, experimentalists have clearly elucidated the mechanisms underlying DDT. More recently, numerical modeling has also been adopted as one of the methods for studying DDT. In this article, the multitude of effects involved in DDT have been presented from a physical standpoint. Then, numerical challenges and strategies to model DDT are described along with key validation results. Finally, the mechanistic aspects of DDT are also discussed.

Keywords: Numerical Modeling, Flame Acceleration, Shock Wave, DDT, Detonation

Introduction

During severe accident in water-cooled nuclear power reactors, large quantities of hydrogen can be released into the atmosphere of the containment. The main source of hydrogen generation is the oxidation of zirconium clad and other metallic components in presence of steam, and Molten Corium Concrete Interaction (MCCI) after failure of reactor vessel. This hydrogen can get transported into the containment through a break in the reactor cooling system or during corium-concrete interaction. The hazard potential of hydrogen can be attributed to its physical properties as described in Table 1 [1]. Compared to a typical industrial gas like methane, hydrogen has a wider flammability limits, lower minimum ignition energy and higher reactivity (i.e. higher energy release and burning velocity). As a result, any unintended electrostatic discharge, hot surface, mechanical friction or an increase in local temperature above the minimum ignition threshold may lead to ignition.

Upon ignition, combustion usually starts locally but can quickly intumesce into a global deflagration. Under certain conditions, an abrupt transition called Deflagration-to-Detonation Transition (DDT) may occur. Combustion in hydrogen-air mixture shows a particularly high propensity for DDT. Both deflagration and detonation are significant risks to containment integrity. The loading associated with detonation is of the impact type and may be more severe than the quasi-static loading of deflagrations. In the worst case scenario, if the containment design safety margin is crossed, the structural integrity of the containment may be breached. The potential risk associated with hydrogen combustion was first realized after the Three Mile Island (TMI) accident in 1979 where burning of a hydrogen cloud affected the integrity of the reactor containment. The Fukushima-Daiichi accident in 2011 reasserted that the hydrogen combustion issue cannot be neglected and control of hydrogen risk is still a key safety issue for operation of nuclear power plants.

Physical Considerations of DDT

Across a combustion wave, the stored chemical energy of the reactants is converted into thermal and kinetic energy of the products. Broadly, combustion waves can be categorized as deflagration or detonation. Deflagrations propagate at subsonic speeds relative to the reactant mixture. These are expansion waves, across which the density decreases and the products are accelerated in a direction opposite to wave propagation. On the other hand, detonations are supersonic compression waves. The Mach number of a detonation wave relative to the reactants is

Table 1: Comparison of physical properties between hydrogen and methane [1]

Property	Hydrogen (H_2)	Methane (CH_4)
Flammability limits in air (%v/v)	4 -75	5 -15
Minimum ignition energy (mJ)[1,2]	0.02	0.33
Lower heating value (MJ/kg)[1,2]	118.8	50.0
Laminar burning velocity (m/s)[1,2]	3.06	0.39
Minimum ignition temperature (K)[1,2]	845	905
Density at STP (kg/m^3)	0.0808	0.6430

[1]At stoichiometric conditions and STP
[2]Source: Sandia National Laboratories

Table 2: Properties of deflagration and detonation

Parameter	Deflagration	Detonation
Mach number[1]	< 1 (subsonic)	> 1 (supersonic)
Density ratio[1,2]	< 1 (expansion)	> 1 (compression)
Pressure ratio[1,2]	~1 (constant pressure process) >1 (constant volume process)	> 1
Temperature ratio[1,2]	> 1 (exothermic)	> 1 (exothermic)

[1]The actual values will depend on the gas mixture and initial conditions

[2]Ratio of product value to reactant value

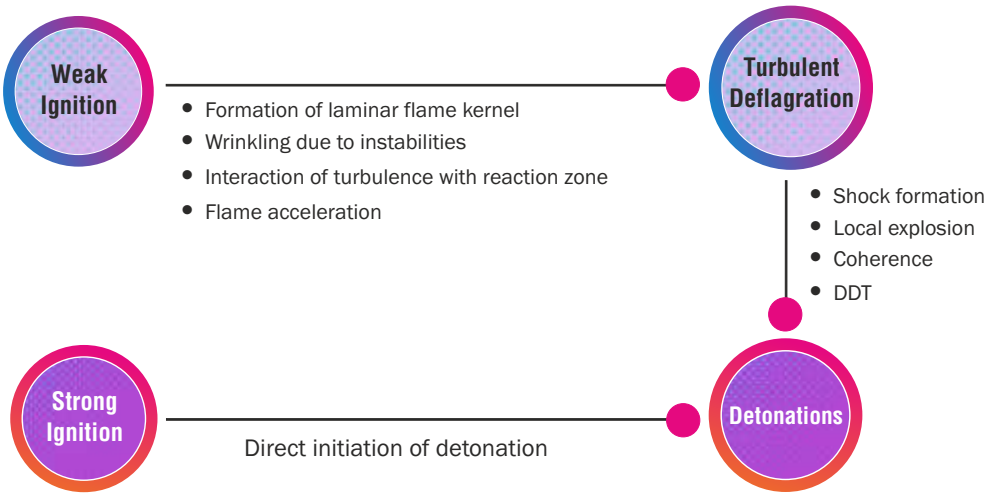

Fig.1: Overview of the mechanisms leading to DDT

greater than one. Across a detonation front, there is a significant increase in density, and the products follow the direction of wave motion. Theoretical change in thermodynamic properties across a combustion wave (deflagration or detonation) can be computed using the Rankine-Hugoniot relations [2]. The properties of deflagration and detonation are summarized in Table 2.

Thermodynamic analysis merely tells us the existence of two types of waves and their properties, but it provides no information on which of these waves will actually persist in a domain. Whether a deflagration or detonation will initiate in a mixture primarily depends on the ignition source. In a weak ignition such as a spark discharge, a minute energy of the order of 10^{-5}J or higher is deposited in a very localized volume [3]. This leads to formation of a laminar flame kernel at the location of the ignition. If the mixture is flammable and quenching does not occur, a self-sustained deflagration wave can propagate. In a strong ignition, a gargantuan energy source of the order of 10^{4} J or higher is deposited, for example through a high explosive charge [3]. Direct detonation can be initiated through a strong ignition.

Hydrogen deflagrations can undergo flame acceleration due to thermo-diffusive and hydrodynamic instabilities and turbulence [4]. An initially smooth laminar kernel gets wrinkled and entrains more of the reactant mixture; causing an increase in the flame surface area. An increase in flame surface area further augments instabilities leading to higher flame wrinkling. This positive feedback loop ultimately leads to a fully developed turbulent deflagration. The primary propagation mechanism is turbulent transport and depends on the interaction between turbulence and heat release in the reaction zone. The average rate of propagation of a turbulent deflagration is characterized through turbulent flame speed, which for hydrogen flames can be 1-2 orders of magnitude higher than the laminar burning velocity [5].

During propagation of deflagration, acoustic disturbances can travel into the reactant mixture and coalesce into shocks waves. Shock waves may reflect from the domain boundaries and pre-compress the reactant mixture to high temperature and pressure. In the absence of driving force, such shocks may get quickly attenuated. But, under certain critical conditions, a local explosion (strong ignition) can take place in the vicinity of a shock front. If the magnitude and rate of energy released from the local explosion are sufficient to sustain the shock propagation, then a spontaneous coupling can take place between the shock and the trailing explosion (coherence), eventually leading to a transition from deflagration to detonation. DDT is associated with an abrupt increase in local pressure and flame speed. Subsequently, a detonation wave propagates into the reactant mixture. Detonations are essentially self-sustained shock waves driven by a trailing local explosion. The various mechanisms leading to DDT are illustrated in Fig.1.

During a severe accident, the possibility of strong ignition and direct detonation can be ruled out. However, weak ignition sources are abundant and the formation of detonation through DDT cannot be precluded. Thus, modeling of DDT is essential to calculate the design safety margin of equipment, internal structures and containment. Such studies also help in optimum design and placement of hydrogen mitigating devices.

Numerical Modeling of DDT

Numerical modeling of DDT has specific challenges which are highlighted below:

- Combustion of hydrogen happens through a network of elementary reactions involving several intermediate species. The individual reactions occur at vastly different time scales and are coupled non-linearly. So, a direct modeling approach which resolves all the chemical time scales is highly computationally intensive.
- Due to presence of multiple species including steam, all the thermodynamic and transport properties have to be specified for multi-component mixtures. Some important properties like laminar burning velocity in presence of steam are not known in the existing literature and have to be derived from first principles.
- Modeling of combustion instabilities which is critical for the initial flame propagation from laminar flame kernel is a difficult problem. This is due to the sub-unity Lewis number and multiple instability mechanisms which are prevalent.
- Different turbulent intensities from low to high and associated length and time scales can exist during flame propagation. While turbulence modeling of non-reactive flows is well established, several gap areas exist for reacting flows due to the non-linear coupling between flow turbulence and heat release in the reaction zone. Modeling of this turbulence-chemistry interaction is of critical importance to accurately predict turbulent flame speed and burning rate. Turbulent quenching and local flame extinction also have to be modeled.
- DDT involves formation and propagation of shock waves. To capture these accurately, fully compressible and conservative form of the Navier-Stokes equations and appropriate shock resolving numerical schemes have to be employed. This increases the grid and time discretization requirements considerably.
- Mathematically, subsonic phenomena like deflagrations exhibit parabolic behavior while supersonic flows like detonations exhibit hyperbolic behavior. Separate numerical schemes are available for these class of flow problems, but less is known about their performance in mixed parabolic-hyperbolic behavior that can be expected during DDT.
- An important physical phenomenon that has to be accounted for is the local explosion. The explosion boundary for hydrogen-air mixture is highly dependent on the mixture composition and pressure, both of which can show significant gradients during DDT. Modeling the location of local explosion and the energy released therein is an important and challenging aspect.
- A key practical challenge is the geometric scalability to larger domains. For example, a domain of $1m^3$ with a flame thickness of 0.5 mm and a modest number of 10 control volumes over the flame thickness will require 8 trillion computational cells. In the context of hydrogen safety for 700 MWe Indian PHWR, the geometric volume of the containment is of the order of $70000m^3$. As per Moores law, scaling up the fully resolved simulations to real-world containment applications will increase the grid requirement exponentially, to a limit beyond the present availability of computational and time resources. When this is combined with shock resolving numerical schemes, it will increase the complexity to intractable dimensions.

Objective of the present work is to explore models and numerical techniques that can address some of the challenges mentioned above without compromising on the accuracy of predicting key safety parameters. The generalized conservative and compressible form of Navier-Stokes equations have been considered. To account for turbulence, Reynolds Averaged Navier Stokes (RANS) or Large Eddy Simulation (LES) may be used. In the present work, the RANS approach has been chosen so that it can be scaled up to larger physical domains. Also, RANS approach provides good estimates on the macroscopic parameters of interest. Due to variation in the density field, the averaging procedure is based on Favre decomposition.

For combustion modeling, the geometric approach based modeling has been employed [5]. In the geometric approach, the flame front is identified to be a surface convected and distorted by the flow field. Combustion is then quantified in terms of effective flame speed and the available flame surface. This approach is very well suited to situations in which combustion occurs in the flamelet regime. Flamelets can be described as thin regions in which combustion occurs. Whether combustion occurs in the flamelet region is governed by the Damkohler number, which is defined as the ratio of turbulent mixing to chemical time scales. For hydrogen combustion, the elementary reactions take place very fast for temperatures higher than the ignition temperature; therefore the chemical time scale is small. Also, there are no sources for large turbulence generation, except those generated by the propagating flame itself and its interaction with the surrounding domain. As the turbulence intensity is small, the time scale associated with turbulence eddies in the flow field are large. Therefore, one can expect that the Damkohler number is much higher than unity. But this is just a heuristic argument. Detailed Borghi diagram analysis has to be carried out to actually determine the variation of the Damkohler number during flame propagation in a constricted domain like a shock tube. This entails computation of turbulent time scale and various chemical time scales in real time and map the variation of the Damkohler number on the Borghi diagram. The authors have determined through such analysis that the Damkohler number varies in the range of 10^2–10^4, thus signifying that the combustion takes place in the flamelet regime and the geometric approach is indeed justified [6].

The geometric approach relies on the Turbulent Flame Closure (TFC) model of Zimont [7]. The TFC model is in-turn based on the transport equation for the progress variable; which can be defined as the non-dimensional temperature across the flame. The source term of this equation represents the heat release due to combustion. The turbulence-chemistry interaction is modeled using the flame wrinkling factor. As the turbulence modeling is based on RANS, all the fluctuations are averaged out. Thus the wrinkling phenomenon which is essentially a coupling between turbulent fluctuations and flame is also averaged out, and cannot be captured on a physical level and needs to be modeled. Even if the mesh is resolved to very fine levels, the inherent limitation of RANS prevents us from physical modeling of flame wrinkling. Thus, appropriate models have to be employed to include effect of flame wrinkling at the sub-grid scale. The

problem is now reduced to determining appropriate models for the sub-grid scale flame wrinkling factor. In essence, the model does not directly address various local processes occurring in turbulent flames, but assumes their universal character and accounts for the effects of such processes on the mean heat release rate. The model of Dinkelacker *et al.* has been adopted to model the sub-grid flame wrinkling factor [8]. This model accounts for the effect of thermo-diffusive instabilities through its dependence on the Lewis number. For lean hydrogen-air mixture, a sub-unity Lewis number enhances local diffusion of species thus increasing the burning rate and enhancing thermo-diffusive instability. In addition, this model captures the effects of increasing pressure on the turbulent flame speed. For the present problem, the authors have shown that the Dinkelacker model is highly appropriate [9].

To model local explosions, the induction delay times have been tabulated at various mixture compositions, pressures and temperatures using independent zero-dimensional kinetics calculations and made run-time available to the solver. This methodology has been adopted based on the work of Ettner *et al.* [10]. In locations where local explosion takes place, the heat release is augmented as an additional source term in the transport equation for progress variable. All the equations and models have been converted into a numerical framework using the open-source toolbox, OpenFOAM [11].

Numerical Setup

The experimental data used to validate the present formulation is based on shock-tube experiments conducted at the GraVent facility, which is available in the open literature[12]. This facility is an entirely closed shock tube channel of high aspect ratio with a rectangular cross-section and channel length of 5.1 m, height of 0.06 m and width of 0.3 m. The mixture is ignited at one end of the channel and the flame propagation characteristics are studied along the channel length. To enhance turbulence, the channel has a provision to include periodic obstacles along its length. There are seven uniformly placed obstacles from 0.25 to 2.05 m from the ignition end. A schematic of the experimental setup is shown in Fig.2. The setup also has a provision to create a transverse (normal to flow direction) gradient of hydrogen distribution to capture the effects of stratification of hydrogen during an accident scenario. This is achieved by injecting hydrogen through the top wall of the facility through small holes. Once hydrogen is injected, ignition is done within a certain time such that sufficient time is not allowed for uniform mixing, thus obtaining a stratified initial distribution.

Flame propagation in presence of obstacles with 30% blockage ratio has been considered. For an average concentration of 20%, if the mixing time is 3 sec, the initial stratified hydrogen concentration varies from 4.7% at the bottom wall to 37.5% at the top wall. Such distribution has been considered in the experimental work of Boeck *et al.* and available in the open literature [13]. The flame propagation in an obstructed geometry in presence of stratified initial distribution presents a realistic initial condition and is highly relevant from hydrogen safety in containment.

All numerical simulations have been carried out in a 2D domain using OpenFOAM. The initial conditions used are: T = 297 K and P = 1 atm. A grid size of 4 mm is used for all simulations after grid optimization study [14]. The grid is fully structured and orthogonal with zero skewness. The aspect ratio in all directions is unity. Such a grid setting is essential to capture shock discontinuities with minimum numerical diffusion. The mixture is assumed to be in quiescent state and hence the initial velocity in the domain is set to 0 m/s.Turbulence is modeled using the k-omega two equation model due to its good performance for both bulk and wall bounded flows. Since the flow is initially undisturbed, a low value of initial turbulent kinetic energy based on a turbulent intensity of 1% is used. The boundary conditions are described as adiabatic no-slip walls. The simulation is carried out in a transient way with implicit time discretization. The time step is determined during the solution based on the maximum acoustic Courant number of 0.3 to ensure stable progress of the solution. This resulted in an extremely small time steps of the order of 0.5 μs. Local time step convergence within a time step has been ensured. All equations are discretized with second order upwind schemes and solved with a tolerance of 10^{-6}. For high speed flows which are expected during FA and DDT, a flux-limited TVD scheme is used for better shock capturing. This scheme ensures stable convergence when the Mach number in the domain exceeds a value of 0.2. Density changes in the flow are accounted by using the ideal gas equation of state. Ignition is

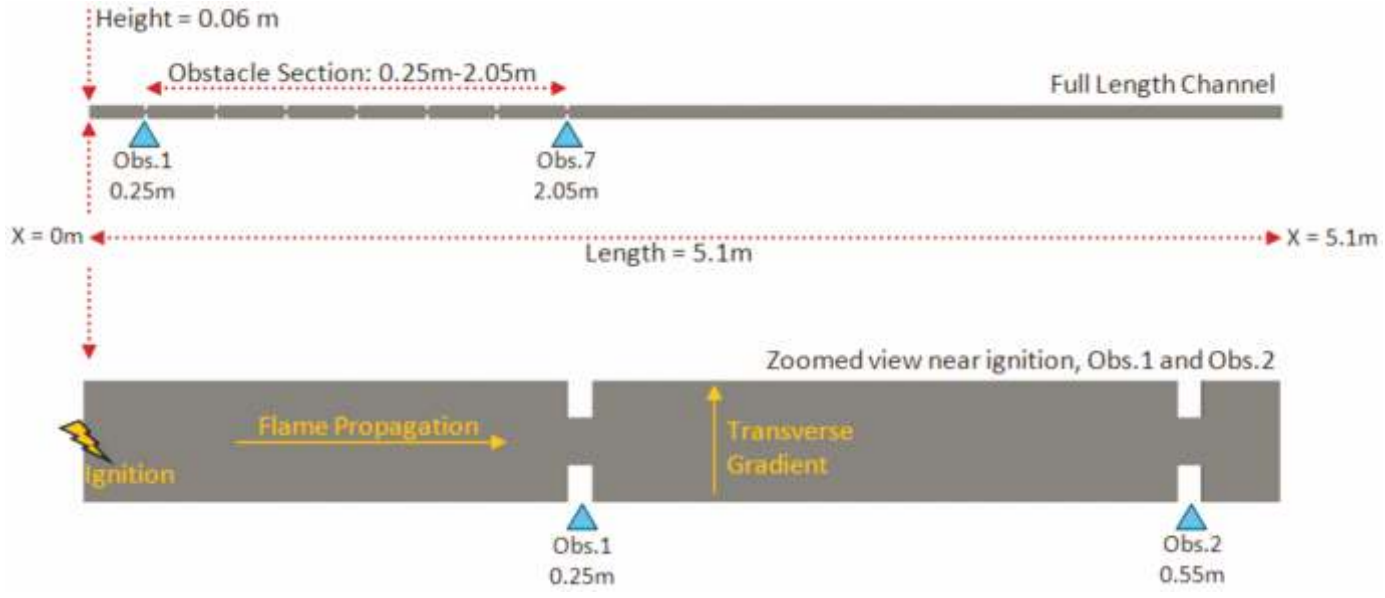

Fig.2: Schematic diagram of the GraVent experimental facility

modeled by patching a spherical region with temperature equal to the adiabatic flame temperature corresponding to 20%. Combustion modeling is based on the geometric approach i.e. progress variable equation with turbulent flame closure and tabulated ignition delay tables, as described in detail in the previous section.

Numerical Results and Validation

The temperature contours at t = 10 ms is depicted in Fig.3. The thin region separating the high and low temperature sides may be interpreted as the flame front. The flame front is observed to elongate over the propagation distance and results in an asymmetric shape. This is attributed to preferential flame propagation towards the upper regions of the domain where the hydrogen concentration is higher. Fig.4 depicts a plot of flame speed vs. flame position from numerical simulation and the corresponding experimental data. The flame speed and flame location are based on the leading edge of the flame at any instant, as per the experimental procedure. The increasing slope clearly indicates flame acceleration. As the flame propagates, different regimes of combustion and the transition between them can be identified. The figure is overlayed with acoustic speeds corresponding to reactant and product temperatures (387 m/s and 904 m/s respectively). For flame speed lower than acoustic barrier w.r.t reactant (region A), the propagation is a slow turbulent deflagration. Good qualitative agreement can be observed between the numerical simulations and experiments. Flame speed is in the range of 0-387 m/s in region A (x < 0.85 m). As the flame propagates further, flame acceleration continues due to turbulence-flame interaction. Region B indicated in Fig.4 corresponds to fast turbulent deflagration in which shock fronts may have formed ahead of the flame. Experimental data suggests that flame acceleration here is higher than that in region A. This trend is captured from numerical simulations also. Higher flame speeds in presence of shocks can be attributed to increase in turbulent diffusivity and heat release rate from pre-compression of the reactants. As seen from the numerical simulation, the flame speed exceeds acoustic barrier w.r.t products at x = 1.65 m. At this condition, a sudden jump in propagation speed can be observed and interpreted as the transition from deflagration to detonation (DDT). Numerically predicted flame speed increases to a peak value of 2384 m/s at x = 2.06 m, while the experimental value peaks to 2448 m/s at x = 2.45 m/s. Thus, in terms of peak flame speed prediction, the numerical simulations are comparable to experimental data. Also, the slope of the numerical flame speed curve is comparable to the experimental values. Additionally, some heat loss from the enclosing walls is expected in the experiments and this can also lower the energy release rate. Due to these factors, the numerically predicted peak location may have shifted to an earlier axial location. Subsequently, numerical prediction shows a constant flame propagation at the speed of

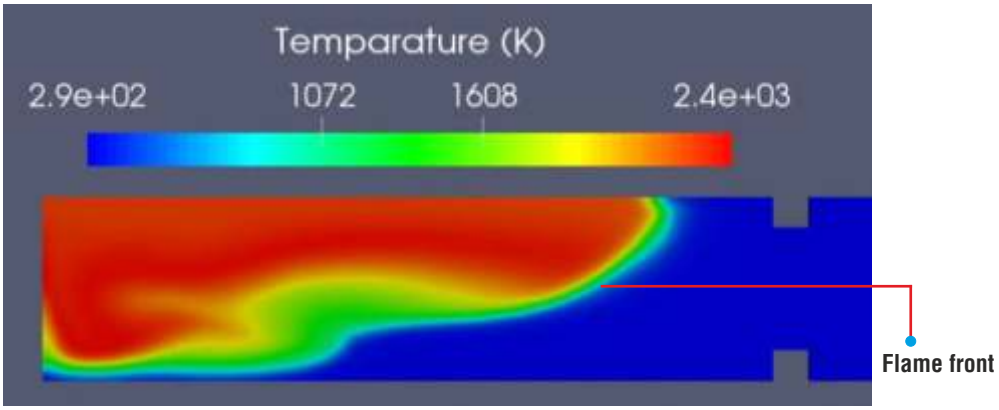

Fig.3: Temperature contours at 10 ms for stratified initial distribution

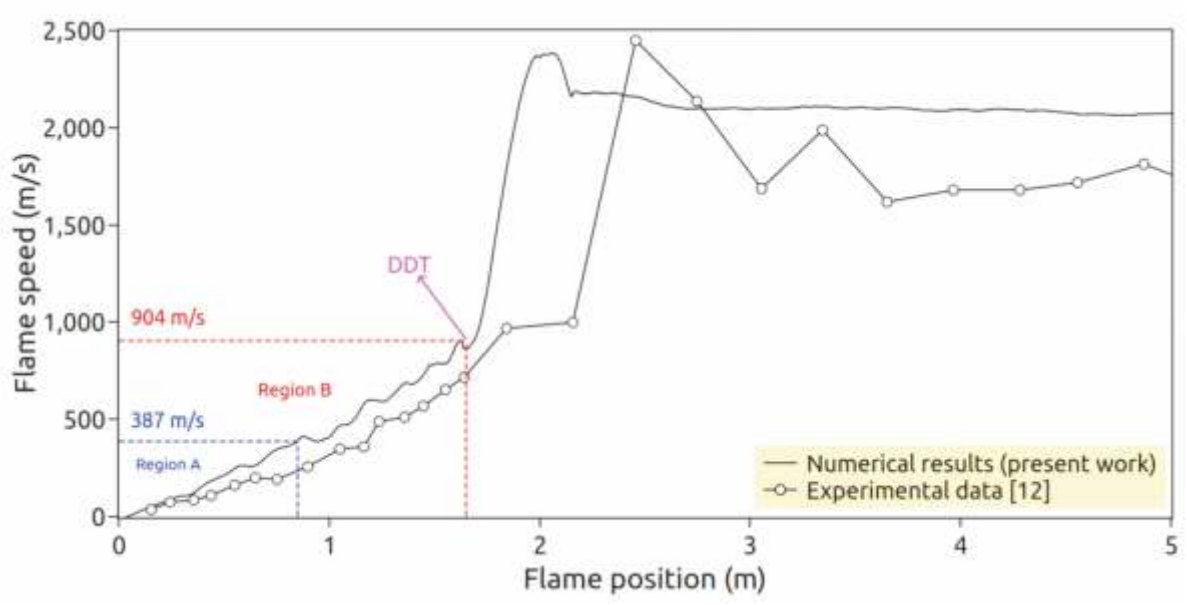

Fig.4: Different regimes of combustion, DDT and validation with experimental data

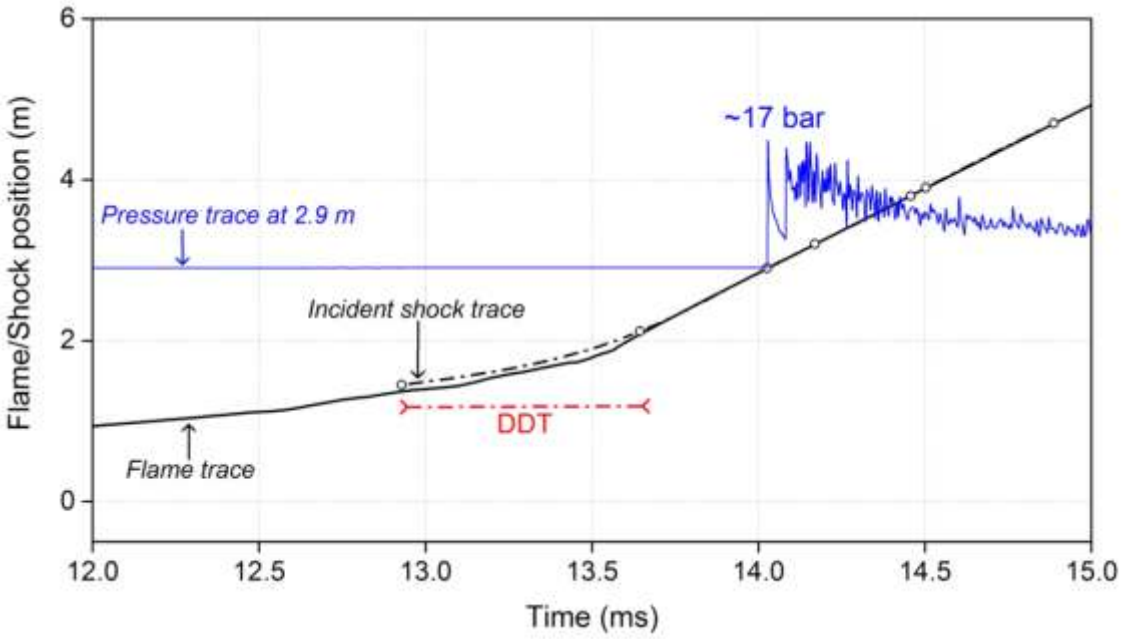

Fig.5: Flame, pressure and shock trace profiles during DDT

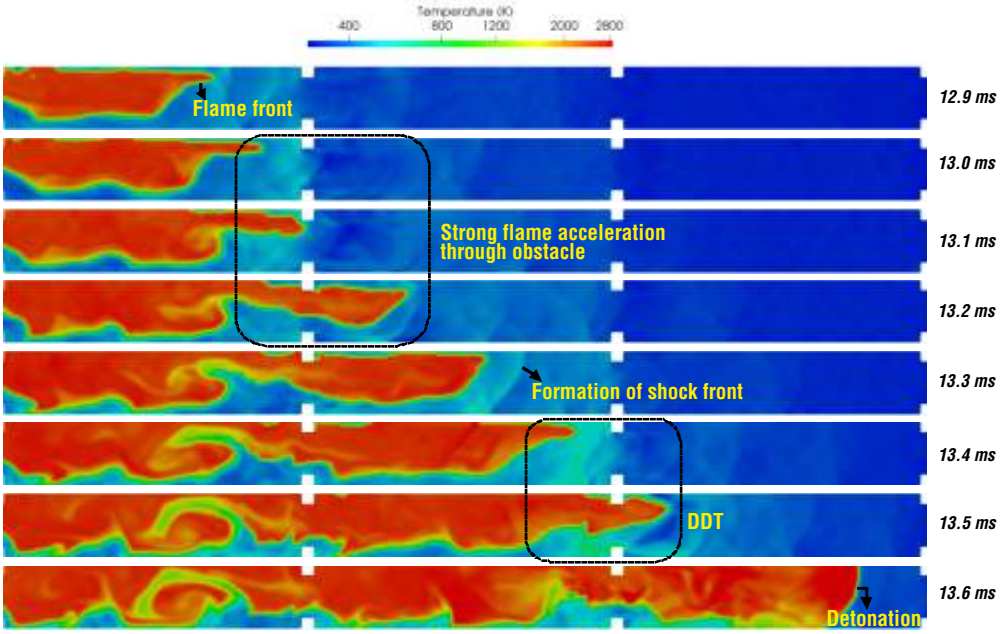

Fig.6: Visualization of flame propagation and interaction with shock front to elucidate DDT and formation of detonation wave

2069 m/s, while the experimental data suggest some oscillations. This has not been captured in the simulations and further analysis may be required to understand this behavior.

The DDT mechanism can be further explained through Fig.5 which shows flame and shock traces, both obtained from numerical simulations. Due to high flame speeds (Fig.4), shocks are expected to form ahead of 0.85 m in the domain. The first location of shock formation (incident shock) is at 1.45 m in the domain at an instant of ~12.9 ms. From the flame trace, it may be observed that the flame front is closely trailing the shock front. Thus, the reactants are pre-compressed by the leading shock before the flame zone. From the first instant of shock formation at 12.9 ms and up-to 13.6 ms, it may be observed that the distance between the flame and the leading shock front continuously diminishes. This duration may be interpreted as DDT. At 13.6 ms, the flame front and the lead shock (incident shock) coalesce to complete the DDT process. Subsequently, the spike in pressure is collocated with flame as can be seen from the pressure trace at 2.9 m and further locations, and may be interpreted as a detonation front. The theoretical Chapman-Jouguet pressure rise corresponding to 20% of hydrogen in air is 13 bar and the pressure spike obtained numerically is 17 bar. This difference may be attributed to the initially stratified hydrogen distribution.

The temperature contours during DDT (12.9-13.6 ms) are presented in Fig.6. At 12.9 ms, the flame front is seen to approach the obstacle. The flame propagation through the obstacle can be observed in the duration from 13.0-13.2 ms. This enhances flame acceleration due to turbulence and creates a higher impetus for strong shock formation. As a result, at the instant of 13.3 ms, a

shock front has formed ahead of the flame. At further instants of time, the interaction between flame leading edge and shock front leads to DDT. At 13.6 ms, the flame and the shock coalesce to form a detonation wave, which propagates further into the unburned reactant mixture, as also explained in Fig.5.

Conclusions

In this paper, a numerical method for modeling DDT has been presented. Appropriate sub-grid models have been used to account for instabilities, turbulent flame propagation, quenching and local explosion. Suitable numerical schemes have been adopted to model both subsonic deflagrations and supersonic detonations. The numerical method works on a relatively coarse grid and can be extended to larger domains. Detailed validation studies were carried out in a shock tube channel with obstacles in the flow path and with initially stratified hydrogen distribution. Different regimes of combustion like slow and fast deflagrations, DDT and detonations were observed from the numerical simulations. The numerically obtained flame speeds showed good agreement with experimental results for all regimes of combustion. Studies on pressure traces revealed the formation of a shock front in close proximity and ahead of the flame. Due to fast moving flame front, the distance between the flame and shock was observed to monotonically decrease until the flame and shock locations coincided, thereby completing the DDT process. Further modeling improvement is required to more accurately capture experimental trends and this work is in progress.

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