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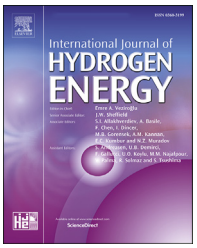

Numerical simulation and validation of flame acceleration and DDT in hydrogen air mixtures

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ABSTRACT

Combustion of hydrogen can take place in different modes such as laminar flames, slow and fast deflagrations and detonations. As these modes have widely varying propagation mechanisms, modeling the transition from one to the other presents a challenging task. This involves implementation of different sub-models and methods for turbulence-chemistry interaction, flame acceleration and shock propagation. In the present work, a unified numerical framework based on OpenFOAM has been evolved to simulate such phenomena with a specific emphasis on the Deflagration to Detonation Transition (DDT) in hydrogen-air mixtures. The approach is primarily based on the transport equation for the reaction progress variable. Different sub-models have been implemented to capture turbulence chemistry interaction and heat release due to autoignition. The choice of sub-models has been decided based on its applicability to lean hydrogen mixtures at high pressures and is relevant in the context of the present study. Simulations have been carried out in a two dimensional rectangular channel based on the GraVent experimental facility. Numerical results obtained from the simulations have been validated with the experimental data. Specific focus has been placed on identifying the flame propagation mechanisms in smooth and obstructed channels with stratified initial distribution. In a smooth channel with stratified distribution, it is observed that the flame surface area increases along the propagation direction, thereby enhancing the energy release rate and is identified to be the key parameter leading to strong flame acceleration. When obstacles are introduced, the increase in burning rate due to turbulence induced by the obstacles is partly negated by the hindrance to the unburned gases feeding the flame. The net effect of these competing factors leads to higher flame acceleration and propagation mechanism is identified to be in the fast deflagration regime. Further analysis shows that several pressure pulses and shock complexes are formed in the obstacle section. The ensuing decoupled shock-flame interaction augments the flame speed until the flame coalesces with a strong shock ahead of it and propagates as a single unit. At this point, a sharp increase in propagation speed is observed thus completing the DDT process. Subsequent propagation takes place at a uniform speed into the unburned mixture.

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Introduction

Management of hydrogen in nuclear reactors during severe accidents is very important and research in this area has attracted renewed interest. During severe accidents, hydrogen can be produced in the nuclear reactor core, primarily due to the reaction between heated zirconium present in the fuel rods and steam [1]. Hydrogen generated in the core will be released into the surrounding containment structure. Hydrogen is a highly combustible gas and has minimum ignition energies of the order of 0.02 mJ [2]. As a result, any small electrostatic discharge, hot surface, mechanical friction or a minute increase in local temperature may lead to ignition. The ignition and subsequent combustion of this mixture is a possible scenario which can lead to significant over-pressurization of the containment. In the worst case, the combustion loads may exceed the strength of the containment thereby compromising its structural integrity as demonstrated in the severe nuclear accident at Fukushima, Japan [3]. As the containment is the last barrier separating the highly radioactive fission products inside and the surrounding atmosphere, maintaining the integrity of the reactor containment is of critical importance during severe accidents.

Combustion of hydrogen can occur in different modes such as laminar flames, deflagrations and detonations with progressively increasing severity. Deflagrations are typically subsonic expansion waves that propagate through the diffusion of heat and mass from the reaction zone to effect ignition in the unburned gases. Due to expansion across the flame front, various flame instabilities set in and create a turbulent flow in the reactant mixture thus significantly enhancing the burning rate in the reaction zone. Since an increase in the burning rate results in an increase of turbulence in the unburned gases, a positive feedback loop is established between the turbulence and the reaction zone. The flame front can also interact with various geometrical features such as obstacles, which provides additional increase in the flame surface area. The net result is a continuously increasing propagation speed and is termed as weak flame acceleration. At very high turbulence levels, the reaction zone may get quenched due to high flame stretch and the rapid mixing of cold reactants with hot products. Thus, there is an upper limit on the maximum flame speeds that can be reached due to weak flame acceleration. Typically turbulent flame speeds are known to be ten times higher than the laminar burning velocity [4]. Hydrogen air flames are however known to be more resistant to turbulent quenching [5]. Flames continuously generate acoustic waves which propagate into the unburned mixture at the local speed of sound. These waves may coalesce and form precursor shocks thus pre-compressing the reactant mixture and increasing its temperature. Shock-flame interaction increases the energy-release rate and promotes further strong flame acceleration. In this regime, the propagation speed may be supersonic with respect to the unburned gases but is still subsonic with respect to the pre-compressed reactants. For the transition between weak and strong flame acceleration, the expansion factor (σ) expressed as the ratio of the densities of the unburned (ρ_u) and burned (ρ_b) gas mixtures shown in Eq. (1) has to be satisfied [6].

$$\sigma = \frac{\rho_u}{\rho_b} > 3.75 \tag{1}$$

Flow in a reactive mixture is invariably associated with gradients in mixture composition, temperature and pressure. This can lead to a spatially varying field of induction delay time. At certain critical conditions, a local explosion may take place in the vicinity of a shock front. According to the induction time gradient theory proposed by Zeldovich et al. [7] in 1970, it is postulated that a local explosion (due to autoignition) takes place in the region with the least induction time delay. The explosion process will thereafter continue at locations with longer induction times. This theory suggests that spontaneous wave formation and propagation happens in a spatial region with a gradient in induction time. Closely related but physically more insightful theory is the 'Shock Wave Amplification through Coherent Energy Release' (SWACER) concept published in the seminal paper by Lee and Moen [8]. According to the SWACER theory, DDT starts with the formation of a local explosion due to autoignition. As the speed of this explosion wave reaches the local speed of sound in the unburned gas, a local shock wave is formed. If the amount of energy released from the explosion is sufficient to sustain the local shock propagation and the rate of energy release corresponds to the local shock time scale, then a spontaneous coupling can take place between the exothermic reactions and the shock, eventually leading to a transition from deflagration to detonation. Some of the more recent reviews on the DDT phenomenon are highlighted by Shepherd and Lee [9] and Cicarelli and Dorofeev [10]. Due to highly transient behavior and dependence on geometric features, a universal criterion for DDT has not yet been established. However, a necessary condition [6] required for the transition from fast deflagration to detonation is expressed in terms of the detonation cell width (λ) as described in Eqn. (2). For complex geometries, it is difficult to define the characteristic length scale L. Also, there is no universal rule that such a length scale exists.

$$L > 7\lambda \tag{2}$$

After DDT, a detonation wave propagates into the unburned mixture. Detonations are unsteady three dimensional structures with intersecting transverse shock fronts and reacting zones whose propagation is assisted by coherent and synchronized release of chemical energy from the local explosions. The aforementioned physical and chemical mechanisms are illustrated in Fig. 1.

Oran [11] has succinctly summarized the complexity of numerically modeling the DDT phenomenon: "*The quantitative prediction of DDT in energetic gases is an extremely difficult scientific problem because of the complex nonlinear interactions among all of the contributing physical processes, such as turbulence, shock interactions and energy release and the wide range of space and time scales on which they are important.*"

Khokhlov et al. [12] have extensively used numerical modeling to study the effects of shock flame interaction in turbulent flames and its role in deflagration to detonation transition. In their work, the numerical modeling is based on fully resolved two dimensional reactive Navier-Stokes equations to study shock flame interactions under both incident

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