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Flame acceleration and transition from deflagration to detonation in hydrogen explosions

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ABSTRACT

Computational Fluid Dynamics solvers are developed for explosion modelling and hazards analysis in Hydrogen air mixtures. The work is presented in two parts. These include firstly a numerical approach to simulate flame acceleration and deflagration to detonation transition (DDT) in hydrogen–air mixture and the second part presents comparisons between two approaches to detonation modelling. The detonation models are coded and the predictions in identical scenarios are compared. The DDT model which is presented here solves fully compressible, multidimensional, transient, reactive Navier–Stokes equations with a chemical reaction mechanism for different stages of flame propagation and acceleration from a laminar flame to a highly turbulent flame and subsequent transition from deflagration to detonation. The model has been used to simulate flame acceleration (FA) and DDT in a 2-D symmetric rectangular channel with 0.04 m height and 1 m length which is filled with obstacles. Comparison has been made between the predictions using a 21-step detailed chemistry as well as a single step reaction mechanism. The effect of initial temperature on the run-up distances to DDT has also been investigated.

In the second part, one detonation solver is developed based on the solution of the reactive Euler equations while the other solver has a simpler approach based on Chapman–Jouguet model and the programmed CJ burn method. Comparison has shown that the relatively simple CJ burn approach is unable to capture some very important features of detonation when there are obstacles present in the cloud.

1. Introduction

Accidental release of hydrogen can result in a highly reactive mixture with air. Because of its low ignition energy and high laminar flame speed, even a weak ignition of hydrogen–air mixture can lead to rapid flame propagation and acceleration with possible transition to detonation, which is a highly destructive type of combustion.

In order to address the related safety issues, the behaviour of accelerating hydrogen flames and the criteria of DDT have to be adequately quantified. The relatively high cost and requirement for specialist facilities have put constraint on the number and physical scale of the experimental tests that can be conducted. Validated predictive tools are increasingly regarded as an alternative for consequence analysis in the development of codes and standards, facility sitting as well as development of mitigation and protection measures.

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The aim of the present work is to numerically predict the behaviour of hydrogen–air deflagration and possibility of transition to detonation in the mixture. It is specifically intended to investigate applicability of multi-step reaction mechanisms in DDT simulations and analysing the possible issues associated with reliability of the reaction mechanisms in DDT simulations. This work also assesses the performance and reliability of simple detonation models such as CJ burn method in order to shed light on the risks and deficiencies associated with such simple models.

In the past a number of numerical and experimental studies have been carried out to investigate the deflagration to detonation transition phenomenon, affecting parameters on DDT and the criteria for onset of detonation [1].

Lee and Moen [2], in a very comprehensive article investigated and explained DDT from a physical point of view. They did not simulate DDT numerically and their article is completely based on their knowledge and experimental results and it provides us with the most comprehensive qualitative description of DDT. In this article Lee explained in details his famous "Shock Wave Amplification through Coherent Energy Release" (SWACER) theory for DDT. Lee et al. [3], in an earlier work, titled "*Photochemical initiation of gaseous detonations*" had introduced his famous SWACER theory. This bears close similarity to the induction time gradient theory developed by Zeldovich in 1970 [4] but offers more physical insight. The authors mention that due to incomplete physical knowledge DDT still it is not possible to have a reliable and quantitatively correct numerical simulation. The Shock Wave Amplification through Coherent Energy Release, SWACER mechanism, implies that the formation of detonation requires amplification of shock waves through several localised auto explosion points. This mechanism was observed and suggested by Lee in his photo irradiation experiments. This mechanism is based on proper synchronisation of shock wave and chemical energy release applied to a single travelling pressure pulse. "*The SWACER is based on the principle that the time sequence of chemical energy release is such that it is coherent with the shock wave it generates, so it strengthen the propagating shock*" [2]. According to the SWACER mechanism, presence of localised auto-explosions can precondition the mixture ahead of the shock wave in a way that leads to synchronization of chemical energy release with the shock. This synchronization results in shock amplification and transition to detonation. Kratzel et al. [5] used a 2-Dto calculate flame folding in the early phase of the process after ignition, to model DDT in hydrogen–air mixture in a tube with obstacle. They used a random vortex method for the flame acceleration. As they concluded, the result of their numerical simulation for deflagration and detonation (separately) is promising in comparison with experimental data but the transition process between these two modes of combustion (deflagration and detonation) is missing in their simulation. So it is concluded further research is needed to at least have a qualitatively reasonable simulation of these combustion processes [5].

Smirnov et al. [6], carried out numerical simulation of mixture ignition and flame acceleration in 1-D and 2-D and also presented experimental tests to investigate several affecting parameters on the onset of detonation. They used a two-step chemical kinetic model for combustion and a modified Godonov numerical scheme to solve governing equations. It is concluded from their 1-D results that the flow structure differs greatly with activation energy (E_a). For high E_a a region of constant flow is created which is followed by a combustion wave. For low E_a instantly, by an ignition, a strong detonation wave is created which eventually slows down to CJ condition. For intermediate E_a, initially a combustion wave is formed and the pressure in between precursor waves and flame front increases and flame acceleration rapidly forms a detonation. In 2-D, only the flow structure of a detonation wave is presented. It is also concluded that, an acceleration of the reaction zone preceded by several shock waves can be a result of the interaction of the contact surface with the flame zone overtaking it [6].

Khokhlov and Oran [7–9], studied the role of hot spots and shock flame interactions in detonation initiation in the flame brush.

They developed a physical and numerical model to simulate the shock–flame interaction in the conditions of the reflected shock-tube experiments. The model includes a self-consistent description of processes of chemical reactions, molecular diffusion, viscosity, and thermal conduction in acetylene–air mixtures. It reproduces the laminar flame and detonation properties of acetylene–air initially at room temperature and in the pressure range 0.1–1 atm. The simulations were carried out using adaptive mesh refinement "*at a level that resolved the laminar flame and all of the chemical and physical processes associated with flame development, propagation, and interaction with shocks*" [8]. The model provides a resolved, multidimensional solution of the two-dimensional reactive Navier–Stokes equations.

Khokhlov and Oran subsequently used this model to carry out a series of DDT studies [7–9]. Initially the interaction of a single shock with a sinusoidally perturbed flame is investigated and the results are compared in two and three dimensions [8]. They examined a single shock–flame interaction and the resulting Richtmyer–Meshkov (RM) instability. The RM instability was found to form a funnel (also called a "spike") of unburned material extending into the burned region. As a result of the instability, the interaction increased the surface area of the flame, which increased the subsequent energy release. However, it is concluded that the single shock–flame interaction was not enough to create a flame brush that could lead to DDT.

Khokhlov et al. [9] reported two-dimensional simulations of shock–flame interactions, including the effects of both the incident and reflected shocks on the flame. These simulations examined how this interaction generates a flame brush, amplify shocks, and leads to the high-speed shocks observed in the experiments. It is found that the shock–flame interactions, through the RM instability, create and maintain a highly turbulent flame brush. The turbulence in these simulations was not the Kolmogorov turbulence; rather, it was driven at all scales by repeated shock–flame interactions. Multiple shock–flame interactions and merging shocks in un-reacted material led to the development of a high-speed shock that moved out in front of the turbulent flame. The region between this shock and the flame was subjected to