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Numerical simulation of flame acceleration and deflagration-to-detonation transition in hydrogen-air mixtures with concentration gradients

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ABSTRACT

The present study aims to test the capability of our newly developed density-based solver, ExplosionFoam, for flame acceleration (FA) and deflagration-to-detonation transition (DDT) in mixtures with concentration gradients which is of important safety concern. The solver is based on the open source computational fluid dynamics (CFD) platform OpenFOAM® and uses the hydrogen-air single-step chemistry and the corresponding transport coefficients developed by the authors. Numerical simulations have been conducted for the experimental set up of Ettner et al. [7], which involves flame acceleration and DDT in both homogeneous hydrogen-air mixture as well as an inhomogeneous mixture with concentration gradients in an obstructed channel. The predictions demonstrate good quantitative agreement with the experimental measurements in flame tip position, speed and pressure profiles. Qualitatively, the numerical simulations have reproduced well the flame acceleration and DDT phenomena observed in the experiment. The results have revealed that in the computed cases, DDT is induced by the interaction of the precursor inert shock wave with the wall close to high hydrogen concentration rather than with the obstacle. Some vortex pairs appear ahead of the flame due to the interaction between the obstacles and the gas flow caused by combustion-induced expansion, but they soon disappear after the flame passes through them. Hydrogen cannot be completely consumed especially in the fuel rich region. This is of additional safety concern as the unburned hydrogen can be potentially re-ignited once more fresh air is available in an accidental scenario, resulting in subsequent explosions.

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Introduction

The energy landscape is gradually shifting from fossil fuels to alternative renewable energy resources such as solar, wind,

hydroelectric, etc. This change is also driven by the need to reduce pollution from the combustion of fossil fuels, greenhouse effect and acid rain, etc. Hydrogen is seen as a promising clean energy carrier. This in turn requires the associated safety issues to be addressed.

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The accidental release of hydrogen into confined or semi-confined enclosures can often lead to a flammable hydrogen-air mixture with concentration gradients. Accidental ignition of this mixture could result in flame acceleration and deflagration-to-detonation transition (DDT). This phenomenon was experimentally investigated by Kuznetsov et al. [1,2]. They showed that flame acceleration in mixtures with concentration gradients may be determined by the maximum local hydrogen concentration in semi-confined geometries. Vollmer et al. [3,4] and Boeck et al. [5,6] reported that a strong positive effect of concentration gradients can be found on flame acceleration, especially in a channel without obstructions. In other words, concentration gradients can result in significantly stronger flame acceleration compared to the homogeneous mixtures. Ettner et al. [7,8] developed a density-based code to simulate flame acceleration and DDT process within OpenFOAM® toolbox. Although their grid resolutions were insufficient to resolve the flow details, the predictions showed good agreement in flame tip velocity, position and pressure, etc. with the measurements of Vollmer et al. [3,4] and Boeck et al. [5,6]. Apart from these limited investigations, FA and DDT in hydrogen-air mixtures with concentration gradients have largely been overlooked despite their relevance to safety in hydrogen energy applications and nuclear installations.

The present study is motivated by the above background and takes advantage of ExplosionFoam, a density based CFD solver newly developed within the frame of OpenFOAM® toolbox. The numerical predictions were carried out for the experiments of Ettner et al. [7]. Comparison of the key parameters with the data will be presented, and the predicted details for flame evolutions will be used to uncover insight of the phenomena.

Mathematical modelling

Governing equations

In the process of flame acceleration and DDT, the reactants are assumed to behave as an ideal gas together with the products. The flow is governed by the compressible reactive Navier-Stokes equations as written below:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{U}) = 0 \quad (1)$$

$$\frac{\partial \rho \vec{U}}{\partial t} + \nabla \cdot (\rho \vec{U} \vec{U}) + \nabla \cdot p = \nabla \cdot \tau \quad (2)$$

$$\begin{aligned} \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho \vec{U} E) + \nabla \cdot (\vec{U} p) &= \nabla \cdot (\tau \cdot \vec{U}) + \nabla \cdot (\lambda \nabla T) \\ &+ \nabla \cdot \left(\sum_{k=1}^{NS} \rho D h_k \nabla Y_k \right) \end{aligned} \quad (3)$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho \vec{U} Y_k) = \nabla \cdot (\rho D \nabla Y_k) + \omega_k \quad (4)$$

where ρ , \vec{U} , p , E , and Y_k are the density, velocity, pressure, total internal energy, enthalpy and mass fraction of the i th species,

respectively. t is time, τ is stress tensor and NS is species number. The source term, ω_k , is chemical reaction production rate. D and λ denote diffusion coefficient and thermal conductivity.

Chemistry model

Ideally full chemistry needs to be used in the DDT simulations. The widely used hydrogen-air chemistry models typically have 9 species and dozens of reactions, e.g. Oran et al. [9] used a scheme with 9 species and 48 reactions, O'Conaire et al. [10] used a scheme with 9 species and 21 reactions. For the simulations of most shock tube tests, the computational mesh would need to be in the order of million to even tens of million because of the size of the tubes. It would be computationally too expensive to use detailed kinetic schemes. A single-step chemistry model is a viable alternative and already adopted by a number of investigators [11–13]. In this paper, to provide the source terms in equations (3) and (4), the one step chemistry model developed by Wang et al. [14] was employed for hydrogen-air combustion:



The reaction rate in Arrhenius form can be expressed as

$$\frac{d[\text{H}_2]}{dt} = 1.13 \times 10^{15} \exp\left(\frac{-112957.41}{RT}\right) [\text{H}_2][\text{O}_2] \quad (6)$$

Numerical scheme

Within OpenFOAM® toolbox, ExplosionFoam, a density based CFD solver has been developed to solve the above governing equations (1)–(4) using the finite volume method. This solver assembles the famous Godunov type schemes such as Roe [15] and Roe and Pike [16], advection Upstream Splitting Method (AUSM) [17–19] and Harten-Lax-van-Leer_contact (HLLC) [20], etc. For the present study, the HLLC method was used to integrate the convective terms. For time integration, the second-order Crank-Nicholson scheme was adopted. The viscous terms are evaluated with second-order central differencing discretization. The governing equations are then solved using the parallel ExplosionFoam solver with adaptive mesh refinement (AMR). The entire computational domain was initially covered by coarse grids, and along with the computation, fine grids were imposed on the coarse grids in the regions with large temperature gradients. Sharpe [21] reported that more than 20 cells per reaction zone length are required to ensure numerical convergence. Many published papers show that grid resolutions are sufficient with 16–64 grid cells in the reaction zone length. So we have confidence that, the finest grid is around 1/32 half reaction length, which is sufficient for flame acceleration and detonation simulations.

Case setup

Numerical simulations were conducted for the experimental set up of Ettner et al. [7] for flame acceleration and DDT in hydrogen-air mixture with concentration gradients in an obstructed channel, which is 5.4 m long and 0.06 m high. Seven

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