NUMERICAL SIMULATION OF FLAME ACCELRATION AND TRANSITION FROM DEFLAGRATION TO DETONATION USING OPENFOAM

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Gas explosions inside tubes have been studied from long times ago. Most of these studies were carried out for industrial safety and with a desire to describe general mechanisms of flame propagation. Therefore, most of these works concern understanding the flame acceleration (FA) phenomena and transition from deflagration to detonation (DDT) in tubes. Nowadays, in industry, transportation of hazardous materials using pipelines is a routine practice. The combustible mixtures are subject to risks such as presence of ignition sources or the pressure and temperature rising above the self-ignition condition.

One of the main hazards in Hydrogen industry is the formation of flammable vapour clouds which can propagate to kilometres with the possibly of igniting and resulting in fire and explosions. Explosions in homogeneous reactive mixtures have been widely studied both experimentally and numerically. However, in practice, combustible mixtures are usually inhomogeneous and subject to both vertical and horizontal concentration gradients. So, in this study, numerical modelling deflagration to detonation transition (DDT) in Hydrogen/Air vapour cloud both in uniform and non-uniform mixtures will be investigated using OpenFOAM CFD package.

A Recent experimental work by Böck et al. [1] for flame acceleration and DDT in a channel with vertical hydrogen concentrations, and uniform Hydrogen/air mixture, has been considered for comparison and numerical setup. The obstructed channel was horizontal with 30% and 60 % blockage ratios (BR).

Moreover, in this study, two different solvers developed in OpenFOAM have been used for the DDT modelling. A pressure based solver based on the flame wrinkling combustion model has been developed and called RMXiFoam. The solver is used for uniform hydrogen/air mixture DDT modelling as well as prediction of Baroclinic torque and Richtmyer Meshkov instabilities. According to equation (1), Baroclinic torque is a strong misalignment of the density gradient and pressure gradient. In high velocity reacting flows, such as detonations, Hydrodynamic instabilities are one of the key factors, Therefore Baroclinic vorticities have been predicted using this solver to examine the Richtmyer Meshkov (RM) instability.

RMXiFoam solver provides a reasonably good prediction of flame acceleration in the obstructed channel, but accelerated flame did not undergo transition to the detonation. Also, by checking Baroclinic torque, in the channel it has been found that the predicted Baroclinic torques are not strong enough to trigger Richtmyer Meshkov instability (Figure 1).

$$baroclinic\ term = \left(\nabla\rho \times \nabla p / \rho^2\right) \quad (1)$$

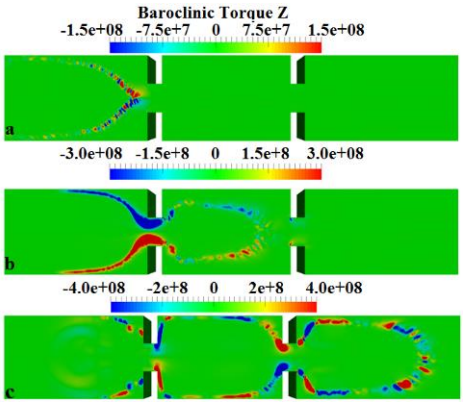

Figure 1: Baroclinic torque contour in Z direction of flame acceleration of Hydrogen flame simulation with RMXiFoam solver, for BR=60 % at a) time=1.86ms, b) time=2.16ms and c) time=2.409ms.

Figure 1 shows the Baroclinic torques during the flame acceleration, and it contains different direction of Baroclinic vorticities (red: out of the plane, and blue: into the plane). Xiao et al. [2], presented the Baroclinic torque field at different times during the initiation of the tulip flame, and predicted the magnitude of Baroclinic torque to be in the range of (-2e+8 to +2e+8) which is consistent with the current simulation (Fig 1.a). Also, they presented that Baroclinic torque increases with time (around -1e+9 to +1e+9), however, in the current simulation the predicted magnitude is smaller and as a result, no detonation and RM instability has occurred.
For better shock and detonation capturing, a density-based solver within the OpenFOAM is developed and used. The compressible Navier–Stokes equations with a single step Arrhenius reaction chemistry are solved. The numerical results were in a good qualitative and quantitative agreement with the experiments. Using the density-based method provides a good prediction of flame acceleration and transition from deflagration to detonation. Moreover, as presented in Fig. 2, the Baroclinic torque magnitude (-5e+10 to +5e+10). is considerably higher than the predictions of the first model.

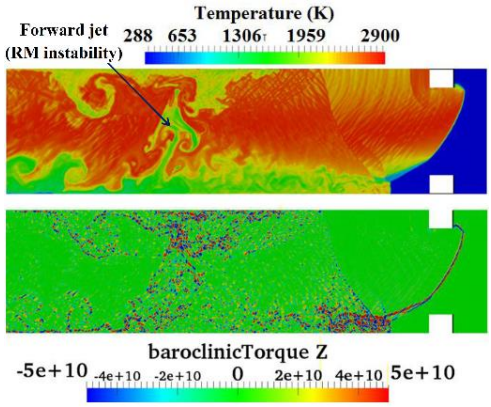

Figure2: results of density based modelling in the case with BR 30% and time=4.7ms; Top: temperature contour, Bottom: the predicted Baroclinic torque in Z direction.

Figure 2 shows that DDT has occurred in the accelerated non-uniform hydrogen flame. The temperature contour shows formation of mushroom shape forward jets in the flame surface which is known as Richtmyer Meshkov instabilities. Furthermore, the predictions show that the overpressure at the DDT stage is higher in the non-uniform mixtures compared tothe homogenous mixtures under similar conditions. Therefore, it can be found that Baroclinic torque and the resulting Richtmyer–Meshkov (RM) instability has an important effect on flame acceleration and DDT.

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