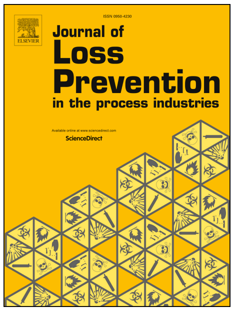

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Numerical Modelling of Deflagration to Detonation Transition in Inhomogeneous Hydrogen/Air Mixtures

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Abstract

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. There is still very limited understanding of the explosion characteristics in such situations. The present study aims to investigate deflagration to detonation transition (DDT) in such mixtures. Two cases in a horizontal obstructed channel with 30% and 60% blockage ratios filled with hydrogen/air mixture with vertical concentration gradients are numerically studied. These cases were experimentally investigated by Boeck et al. (2015), and hence some measurements are available for model validation. A density-based solver within the OpenFOAM CFD toolbox is developed and used. To evaluate the convective fluxes contribution, the Harten–Lax–van Leer–Contact (HLLC) scheme is used for shock capturing. The compressible Navier–Stokes equations with a single step Arrhenius reaction are solved. The numerical results are in good qualitative and quantitative agreement with the experiments. The predictions show that the overpressure at the DDT transition stage is higher in the non-uniform mixtures than that in homogeneous mixtures under similar conditions. It is also found that increasing the blockage ratio from 30% to 60% resulted in faster flame propagation and lower propensity to DDT. The Baroclinic torque and the resulting Richtmyer–Meshkov (RM) instability are also analyzed in relation to flame acceleration and DDT.

Keywords: *Hydrogen safety, Explosion, DDT, Inhomogeneous mixture, Instability*

1. Introduction and background

Flame acceleration (FA) and deflagration to detonation transition (DDT) in channels have been extensively studied. Most of these studies were conducted for industrial safety and intending to understanding the mechanisms of flame propagation. Much effort has been dedicated to understanding the phenomena related to FA and DDT (Ersen, 2004). Thomas (2012) has given a comprehensive study on various forms of DDT phenomena, and differentiated the terminology between the macroscopic and the microscopic DDT. He considered the large scale macroscopic DDT to include the process from accelerating deflagration up to a propagating detonation; and the small-scale microscopic DDT initiate the actual onset of detonation at the point where the combustion process changes from diffusion controlled to shock heating controlled. Looking from this standpoint, the present work concerns the large-scale macroscopic DDT.