Case Study 4

1. Title of Case Study: Numerical Study of Deflagration-to-Detonation Transition in Homogenous and Inhomogeneous Hydrogen-Air Mixtures

2. Grant Reference Number: EP-K025236

3. One sentence summary: Numerical study flame acceleration and transition to detonation in homogeneous and inhomogeneous hydrogen-air mixtures

4. One paragraph summary:

Explosions in homogeneous reactive gas mixtures have been widely studied both experimentally and numerically. However, in accident scenarios, combustible mixtures are usually inhomogeneous. The present numerical investigation aims to study flame acceleration and transition to detonation in homogeneous and inhomogeneous hydrogen-air mixtures with two different average hydrogen concentrations in a horizontal obstructed channel, filled with hydrogen-air mixture. A density-based solver was implemented within the OpenFOAM CFD toolbox. The Harten–Lax–van Leer–Contact (HLLC) scheme was used for accurate shock capturing. A high-resolution grid is provided by using adaptive mesh refinement, which leads to 30 grid points per half reaction length (HRL) in the finest regions near the flame and shock fronts. In agreement with the experimental measurements and observations, it was found that transverse concentration gradients lead to stronger flame acceleration and promote transition to detonation for an average hydrogen concentration in air of 20%, whereas gradients slightly retard both phenomena for a 30% mixture.

5. Key outputs in bullet points:

- Developed and validated a density-based solver within the OpenFOAM CFD toolbox.
- This study confirms previous experimental findings that transverse concentration gradients in channels can lead to substantially stronger flame acceleration and a higher propensity for transition to detonation in comparison with homogeneous mixtures at the same average hydrogen concentration.
- New collaboration with California Institute of Technology.
- Trained an early stage researcher in an EU Marie Curie Innovative Doctoral Program.
- Two conference papers, one book chapter. One paper submitted to ICDERS 2017 and another one under preparation for Combustion and Flame

6. Main body text

A density-based numerical code has been developed based on the OpenFOAM computational fluid dynamic (CFD) toolbox. To evaluate the convective fluxes contribution, Harten–Lax–van Leer–Contact (HLLC) scheme is used for accurate shock capturing. Compressible Navier–Stokes equations with a flame wrinkling combustion model are solved. For turbulence modelling the Large Eddy Simulation (LES) technique with one eddy equation subgrid scale model is adopted. The solver and numerical schemes were initially tested by solving the Sod's shock tube problem.

Previous experiments of Boeck et al. [1] of DDT in homogeneous and inhomogeneous hydrogen-air mixtures in a horizontal partially obstructed channel were numerically simulated using either a homogenous mixture of 30% hydrogen in air or an inhomogeneous mixture with vertical concentration gradients of hydrogen giving an average volumetric concentration of 30% and 20%.

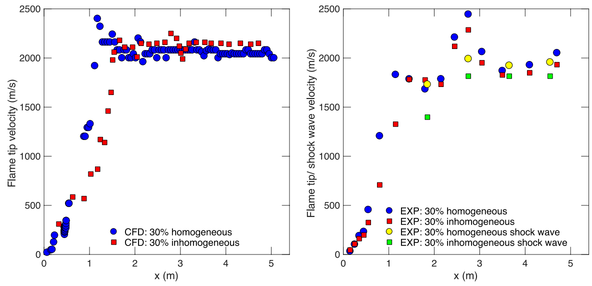

Fig. 1 Comparison between the predicted and measured flame tip velocities in the 30% homogeneous and inhomogeneous mixtures.

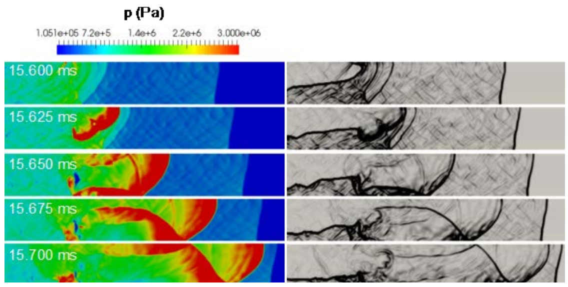

Figure *2*. Pressure (left) and numerical schlieren (right) fields of detonation onset in the inhomogeneous 20% hydrogen mixture.

Some sample results are shown in Figures 1 and 2. In summary, the predicted flame tip velocities and locations of detonation onset are in reasonable agreement with the measurements. For both homogeneous and inhomogeneous 30% hydrogen cases, onset of detonation occurs within the obstructed channel section. The homogeneous mixtures show slightly faster flame acceleration and earlier onset. For the 20% case, transition to detonation is observed only for the inhomogeneous mixture, where the concentration gradient enables stronger flame acceleration, especially in the unobstructed channel section in comparison with the homogeneous mixture. This study confirms previous findings that transverse concentration gradients in channels can lead to substantially stronger flame acceleration and a higher propensity for transition to detonation in comparison with homogeneous mixtures at the same average hydrogen concentration.

[1] Boeck LR, Katzy P, Hasslberger J, Kink A & Sattelmayer T. Shock Waves, Vol. 26 (2): 181-192, 2016.

7. Names of key academics and any collaborators:

Jennifer X Wen, Warwick FIRE, University of Warwick
Lorenz R. Boeck, California Institute of Technology, USA

8. Sources of significant sponsorship (if applicable):

Part of " Numerical characterization and simulation of the complex physics underpinning the Safe Handling of Liquefied Natural Gas (SafeLNG)" (2014-2017), an Innovative Doctoral Programme (IDP) funded by the Marie Curie Action of the 7th Framework Programme of the European Union with 1.77M Euros.

9. Who should we contact for more information?

Jennifer X Wen Jennifer.wen@warwick.ac.uk Mobile (+)4407796707950

10. Please indicate if you would like this case study to be included on the Consortium's ARCHER web-page.

Yes