

Case Study

1. Title of Case Study: Direct Numerical Simulation analysis of localised forced ignition and spherical flame propagation in turbulent droplet-laden mixtures

2. Grant Reference Number: EP/J021997/1, EP/K025163/1, EP/R029369/1

3. One sentence summary: Carrier phase Direct Numerical Simulations of localised forced ignition and spherically expanding flames propagating in monodispersed n-heptane droplet laden mixtures have been performed for different initial turbulence intensities, droplet diameters and overall (i.e. gas+liquid) equivalence ratios under laminar and turbulent flow conditions to analyse the reaction zone structure and flame propagation statistics.

4. One paragraph summary: Combustion of droplet-laden mixtures depends on the complex interactions between flame, flow field and liquid fuel droplets. Thus, a detailed understanding of combustion of droplet-laden mixtures remains a challenging task considering its wide range of applications (e.g. internal combustion engines, gas turbines and explosion hazards). In this study, a three-dimensional carrier phase Direct Numerical Simulations (DNS) data has been utilised to analyse edge flame speed statistics in igniting turbulent droplet-laden mixtures. Furthermore, flame structure and flame propagation characteristics for spherically expanding spray flames have been investigated and results have been compared with the corresponding gaseous premixed flames with the same initial burned gas radius, overall equivalence ratios, and statistically similar fluid flow conditions. It has been found that the reacting mixture within the flame for droplet cases exhibit fuel-leaner conditions than in the corresponding gaseous premixed flame and this behaviour strengthens for increasing droplet diameter due to slower evaporation rate of larger droplets. The predominantly fuel-lean combustion has implications on the flame structure, flame thickness, scalar gradient, and extent of burning and flame surface area generation.

5. Key outputs in bullet points:

- Influences of liquid droplet diameter, overall equivalence ratio and turbulence intensity on flame wrinkling and the reaction zone structure.
- Statistical behaviour of edge flame speed, displacement speed, consumption speed, surface density function (i.e. modulus of reaction progress variable gradient) and the evolution of flame surface area and burned gas volume.
- Fundamental physical insights into the interactions between droplets, flame and flow field in terms of flame surface topology
- Collaboration with international colleagues (see section 7) whose field of expertise coincides with the study have expressed interest in this research and in utilising the projects datasets.
- The project has given rise to 5 high-quality journal papers and 5 international conference proceedings to date
- So far, two PhD students have benefitted from this project (e.g. received extensive training in combustion theory and modelling, high-performance computing etc.)

6. Main body text

Fuel is introduced as dispersed liquid droplets in many engineering devices such as Internal Combustion (IC) engines [e.g., Direct Injection (DI) and Compression Ignition (CI) engines] and gas turbines. Although turbulent combustion of droplet-laden mixtures has significant practical interests, it remains as one of the most challenging topics in thermo-fluid mechanics due to the complex interaction of fuel droplet evaporation, heat and mass transfer, fluid dynamics and combustion thermo-chemistry. Therefore, gaining a thorough understanding of turbulent spray combustion is of pivotal importance for the purpose of designing and developing low-emission and fuel-efficient combustion devices. Simulations of spherically expanding turbulent spray flames and premixed flames (see Fig. 1) and localised forced ignition have been conducted using the DNS code SENGAs+ [1-4] (i) to analyse and explain the effects of droplet size, overall equivalence ratio and turbulence intensity on the flame structure, flame wrinkling induced by flame-droplet interaction (see Fig. 2), mode of combustion, the evolution of the flame surface area and volume of burned gas in laminar and turbulent spherically expanding spray flames [1,2]; (ii) to demonstrate and understand the influences of initial droplet diameter and the overall equivalence ratio on displacement speed and consumption speed statistics in spherically expanding turbulent flames propagating into initially mono-sized droplet-laden mixtures [3]; (iii) to investigate the effects of turbulence intensity and droplet diameter on the strain rates, which affect the evolution of the Surface Density Function in turbulent spherically expanding flames in droplet-mists [4]; (iv) to demonstrate the effects that the droplet size and the overall equivalence ratio (or number density of droplets) have on the edge flame speed (see Fig. 3) and its various components [5].

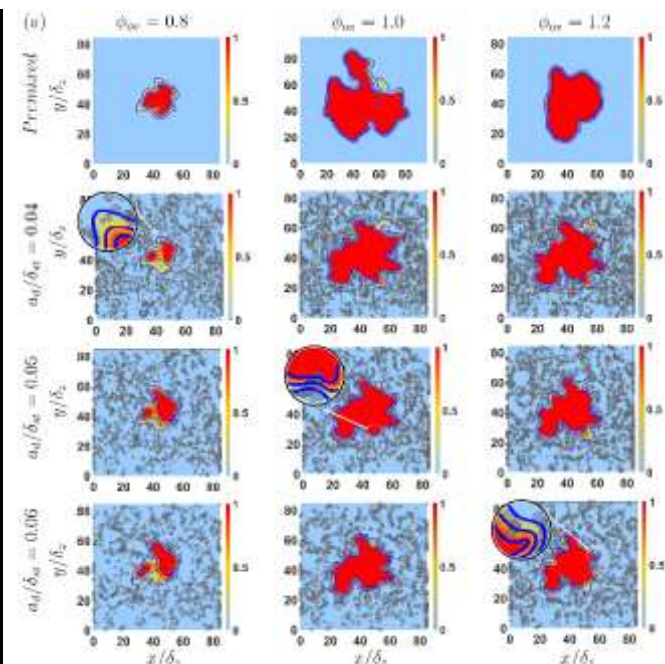


Figure 1. Distribution of reaction progress variable, c (blue lines show $c = 0.1, 0.5$ and 0.9 contours from outer to inner periphery) on the central x - y mid-plane for overall-equivalence ratio $\phi_{ov} = 0.8, 1.0$ and 1.2 cases with initial $a_d/\delta_{st} = 0.04, 0.05$ and 0.06 for initial $u'/S_{l\phi_g=1.0} = 4$ (where a_d is the droplet diameter, u' is rms turbulent velocity and $S_{l\phi_g=1.0}$ is the unstrained laminar burning velocity of gaseous stoichiometric mixture, δ_{st} is the thermal flame thickness of the gaseous stoichiometric mixture). Grey dots show the droplets residing on the plane (not to scale).

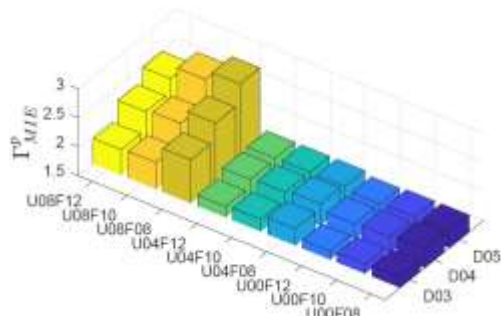


Figure 3. Normalised minimum ignition energy for successful propagation following localised forced ignition, with U00, U04 and U08 indicating $u'/S_{l\phi_g=1.0} = 0.4, 0.8$ respectively; F08, F10 and F12 indicating $\phi_{ov} = 0.8, 1.0$ and 1.2 and D03, D04 and D05 indicating initial $a_d/\delta_{st} = 0.03, 0.04$ and 0.05 , respectively.

References

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5. V. S. Papapostolou, C. Turquand d'Auzay, G. Ozel Erol, N. Chakraborty, Phys. Fluids., 31, 105108 (2019)

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

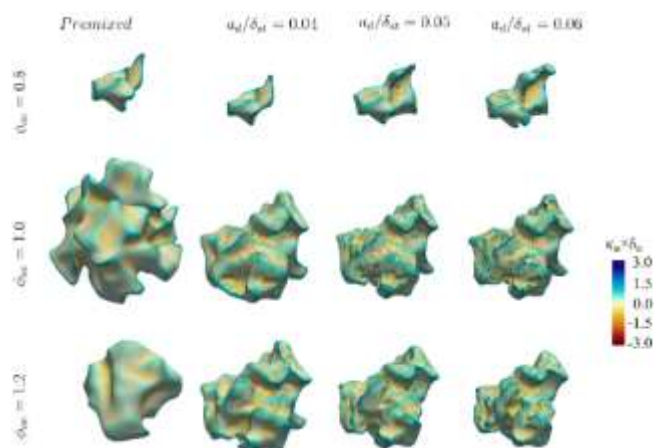


Figure 2. Instantaneous view of $c = 0.8$ isosurface coloured with normalised curvature $\kappa_m \times \delta_{st}$ for premixed gaseous (1st column) and droplet (2nd-4th columns) cases with initial $\phi_{ov} = 0.8$ (1st row), $\phi_{ov} = 1.0$ (2nd row) and $\phi_{ov} = 1.2$ (3rd row) for initial $u'/S_{l\phi_g=1.0} = 4$.

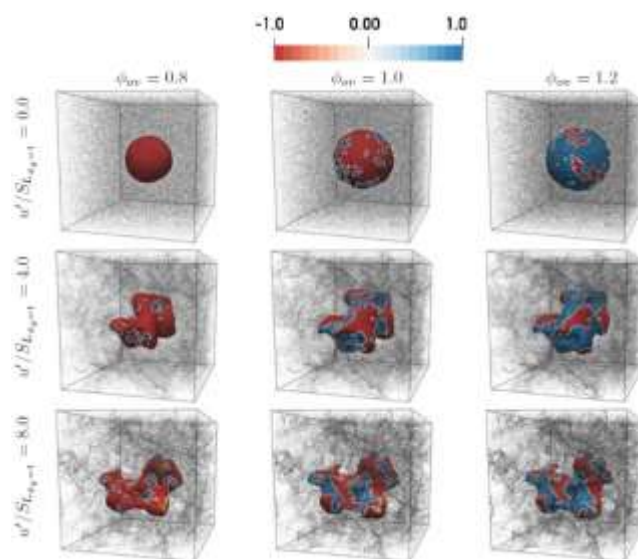


Figure 4. Instantaneous view of $c = 0.5$ isosurface coloured by the local values of flame index $\psi = \frac{1}{2} \frac{\xi - \xi_{st}}{|\xi - \xi_{st}|} \left(1 + \frac{\nabla Y_F \cdot \nabla Y_O}{|\nabla Y_F| \cdot |\nabla Y_O|} \right)$ at $t = 8t_{sp}$ for the cases with $a_d/\delta_{st} = 0.03$, with increasing initial turbulence intensity (top to bottom) and increasing ϕ_{ov} (left to right) as indicated by the labels respectively. The white line superimposed, indicates the presence of an edge flame.