1. Project Title: Fundamental analysis of droplet combustion using high-fidelity numerical simulations

2. Title of Case Study: Direct Numerical Simulations of droplet-laden turbulent reacting flows

3. Summary of Case Study: In spite of extensive applicability of flame propagation into droplet-laden mixtures (e.g. Internal Combustion engines, gas turbines, as well as in hazard prediction and control), this topic has received relatively limited attention in comparison to the vast body of literature on single-phase turbulent reacting flows. As a result, engineering models for droplet-laden turbulent reacting flows are often crude and heavily dependent on empiricism in comparison to single-phase models. Thus, improved models are needed for high-fidelity engineering simulations which can contribute to design of next generation energy-efficient and environment friendly devices. However, high quality temporally and spatially resolved three-dimensional data is required to develop models for Large Eddy Simulations (LES), which is either difficult to generate or impossible to obtain by experimental means. This limitation can be avoided by utilising the advancement of high-performance computing to carry out Direct Numerical Simulations (DNS) of the carrier phase without recourse to turbulence modelling, where Lagrangian droplets are treated as sub-grid point sources. The turbulent flame propagation, where fuel is supplied in the form of mono-dispersed droplets, is found to differ significantly from equivalent (i.e. same overall equivalence ratio) premixed turbulent flames: droplet cases burn under leaner conditions and exhibit thicker reaction zone than the corresponding single-phase premixed flame. Moreover, both premixed and non-premixed modes are active in these flames. DNS is also employed to investigate the autoignition of mono-dispersed droplets in the presence of a gaseous fuel such as methane, a configuration relevant to gas-fuelled and pilot-ignited engines. Although this is an increasingly important area for natural gas utilization due to the lower NOx, CO2 and soot emissions, there has been only limited work regarding the dual-fuel combustion mode focusing mainly on global quantities. DNS was used to elucidate the behaviour observed in experiments while revealing key features that would help in defining the optimum operation conditions. It was found that the amount of the liquid fuel dictates the pilot fuel autoignition time and the gaseous flame ignition mechanism. Furthermore, the presence of a gaseous fuel mixing layer within the droplet-laden region, such as in direct injection of methane, leads to increased ignition delay times, but also to better fuel oxidation. The DNS data is used to assess the accuracy of existing models and develop new combustion models, hence providing useful tools for optimising of the efficiency and emission control in IC engines and gas engines and hazard control in industrial fires.

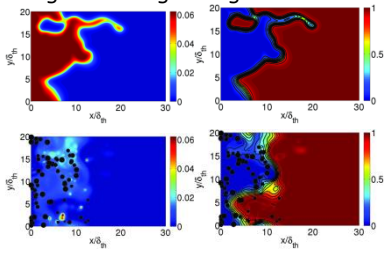

Fig. 1. Instantaneous fields for a stoichiometric turbulent premixed flame (top row) and a droplet case (bottom row) with initial diameter 10% of stoichiometric laminar flame thickness for droplet equivalence ratio $\phi_d = 1.0$ (left to right) fuel mass fraction Y_F and fraction of chemical reaction completion c (i.e. 0=unburned gas and 1.0= fully burned products). Black lines show $c = 0.1$ to 0.9 contours (from left to right) in steps of 0.1.

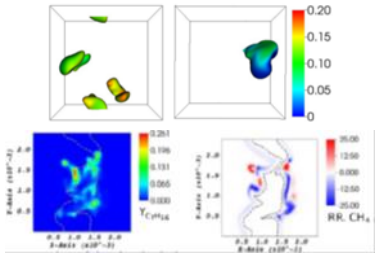

Fig. 2. (Top) Pilot fuel autoignition in premixed methane-air environment: ignition centres T=1250 K. Droplet heat release 0.55 (left) and 0.16 (right) of total heat release. Coloured by mixture fraction. (Bottom) Interaction of the droplet-laden region with methane mixing layer (dual fuel non-premixed combustion): Mass fraction of evaporated n-heptane (left) and methane reaction rate (right).

4. Key outputs: Knowledge: The project has contributed greatly to the fundamental physical understanding and modelling of turbulent flame-droplet interactions, which has already enriched the literature of droplet combustion and improved the knowledge-base of the research team. It has furthermore the potential to provide the industry with the required insights to facilitate engine design and operation thereby improving efficiency and reducing emissions. Finally, it has strengthened the collaboration between the research teams of Cambridge and Newcastle Universities, which is beneficial for their on-going and future research activities.

Developing leaders and skilled people: The research has allowed especially the early-career researchers (e.g. PhD students and PDRAs) to develop expertise in advanced thermo-chemistry, Computational Fluid Dynamics (CFD), most specifically multi-phase reacting flow DNS, and to gain extensive experience in the use of HPC facilities for research purposes: much-sought-after skills for future academic or industrial research.

Dissemination: Some results have already been publicised at a number of recent national and international conferences and through conference proceedings (e.g. 7th European Combustion Meeting and 9th Mediterranean Combustion Symposium). Further results will be disseminated at conferences and through peer-reviewed journals (e.g. Combustion and Flame). The DNS database created by the project will be made available to other interested researchers upon request. Results have been communicated to Rolls-Royce and Siemens for quick assimilation of newly developed methodologies in the industrial framework.

Societal and economic impact: The improved physical understanding and models, developed during the course of this project, have the potential to play a key role in industrial CFD calculations leading to improvements in engine design and efficiency, better hazard control and reduced pollutant and greenhouse gas emissions, thus benefiting both the UK economy and the environment.

5. Names of key academics and any collaborators: Ms. E. Demosthenous, Prof. E. Mastorakos, Prof. R.S. Cant, (University of Cambridge); Prof. N. Chakraborty, Dr. D.H. Wacks (Newcastle University)

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