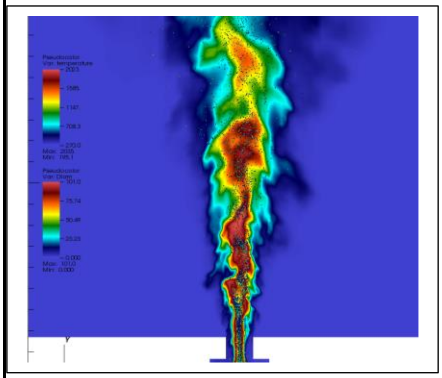
1. Project Title: Large Eddy Simulation of Multi-phase combustion systems

2. Title of Case Study: Large Eddy Simulation of a Methanol Spray Flame with a Stochastic Model

3. Summary of Case Study:

Two-phase combustion systems with liquid fuels are widely used in many engineering applications including, for example IC engines, gas turbines and industrial furnaces. If improved low emissions and more efficient low CO_2 designs are to be achieved then there is a clear need for accurate methods of predicting their properties. The accurate simulation of liquid fuel spray flames remains a challenging task owing to their multi-scale nature. In the present work Large Eddy Simulation (LES) is applied to the study of a methanol/air turbulent spray flame representative of that occurring in practical combustion devices. The burner considered is is a canonical turbulent spray flame where the liquid fuel is delivered into the burner housing using a commercial ultrasonic atomizer (Sono-Tek). The fuel is methanol and the experimental results of Karpetis and Gomez are available for validation purposes. In LES the large scale motions are computed directly whilst the influences of those with scales smaller that the computational grid size are modelled. The sub-grid-scale (sgs) stresses are represented by a dynamic version of the Smagorinsky model and sgs turbulence/chemistry interactions are described by a modelled evolution equation for the joint sgs probability density function (pdf) for enthalpy and all the species mass fractions needed to describe reaction. The LES equations are solved using the in-house parallel code Boffin-LES in which a stochastic fields method is used to solve the sgs-pdf equation. A Lagrangian probalistic droplet tracking approach is adopted for the spray droplets and chemical reaction is described by a 14 reaction step, 18 chemical species systematically reduced mechanism. The predictive capabilities of the method are demonstrated in terms of the gas and droplet velocity components, gas temperature and spray properties such as droplet number density, arithmetic mean diameter and pdf of droplet size. In addition the key features of the particle-laden flame including the occurrence of external group combustion and the seperation of flame structures into separate combusting islands are well represented. gas temperature and spray properties such as droplet number density, arithmetic mean diameter and probability density function (pdf) of droplet size. Furthermore, the key features of the particle-laden flame including the occurrence of external group combustion and the switch of flame structures into separate combusting islands are well represented. The method devised is applicable to gas-turbines and internal combustion engines and the results shed important light on spray-flame phenomena.



Instantaneous temperature field with droplets

4. Key outputs:

The results of the work were presented at the 35th International Symposium on Combustion, San Francisco, USA 2014. The published paper, [1] was selected as "the distinguished paper in the Spray and Droplet Combustion Colloquium".

[1] W. P. Jones, A. J. Marquis, D. Noh, Proceedings of the Combustion Institute[*]. ***35*** *(2015) 1685-1691*

[*]Impact Factor: 3.688

5. Names of key academics and any collaborators:

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6. Sources of significant sponsorship (if applicable):

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