Case Study 1

1. Title of Case Study: Numerical prediction of local and global extinction in non-premixed swirl flames using LES/CMC

2. Grant Reference Number: EP/K025791/1

3. One sentence summary:

Local and global extinction in non-premixed swirl flames have been investigated using LES/CMC to further validate the capability of this method to capture the finite-rate chemistry effects leading to blow-off.

4. One paragraph summary:

The prediction of local extinctions and their development into a global blow-off is a very challenging target for current generation combustion models, as this requires a proper representation of turbulence-chemistry interactions and dynamic behaviour of the local flame structure. In this research, the capability of the LES/CMC approach to capture local extinction and blow-off in non-premixed swirl flames is investigated. Both gaseous non-premixed flames and spray flames are considered at conditions progressively close to blow-off. Results demonstrate a promising capability of LES/CMC to capture local and global extinction in swirl flames.

5. Key outputs in bullet points:

- Validation of the LES/CMC approach to capture local extinction and blow-off
- The local extinction can be captured quantitatively by LES/CMC
- LES/CMC showed a promising maturity in capturing the blow-off of swirl flames
- LES/CMC can predict the blow-off curve of gaseous non-premixed flames with a deviation from experiments within 25%

6. Main body text

Swirl flames are of great interest for many combustion systems, ranging from industrial furnaces to aero-engines. At adverse conditions, finite rate chemistry effects become important leading to the presence of local extinctions and eventually blow-off, and these phenomena that have recently been studied at Cambridge in laboratory-scale flames with different configurations and fuels [1],[5]. Both non-premixed gaseous flames and spray flames have been investigated, developing an extended database for model validation in conditions close to and at blow-off.

The numerical prediction of local extinction and blow-off in turbulent flames is very challenging since requires a proper representation of the finite-rate chemistry effects, and all the processes affecting the local behaviour of the flame. Our approach consists in the use of Large Eddy Simulation (LES) and the Conditional Moment Closure (CMC) combustion model, which allows us to solve the time evolution of the local flame structure. All the fundamental physical processes affecting the flame evolution are included in the formulation, with terms representing turbulent transport, mixing at the molecular level, and interactions with spray. To properly capture finite-rate chemistry effects, detailed chemical mechanisms have to be used together with very refined numerical grids. The consequent huge computational cost makes the availability of HPC resources a key factor to continue this fundamental piece of research, and the authors greatly acknowledge UKCTRF and Archer for providing these computational resources.

Several achievements have been reached in the last three years of research. In the context of non-premixed gaseous flames, LES/CMC has shown some success in predicting both local extinctions and the global blow-off [2] with the prediction of the experimental blow-off curve within 25% of the experimental blow-off velocity [2],[5], as shown in Fig. 1. The prediction of the full blow-off curve with combustion CFD is a very novel result that would not have been possible without access to supercomputers.

Based on the CMC code used for the gaseous flame computations just described, the spray LES/CMC package was developed. Some of the spray computations were done in an internal cluster with the sponsor's own LES code and further extensive validation was done in Archer with a different LES code (openFOAM). In spray flames, the LES/CMC approach has been shown to be able to capture local extinctions both qualitatively and quantitatively [3]. A blow-off case of an ethanol spray flame has also been investigated [4], pointing out the strong coupling between the fuel evaporation and the development of local extinctions into a global blow-off. Figure 2 shows an example of blow-off transient of a spray flame.

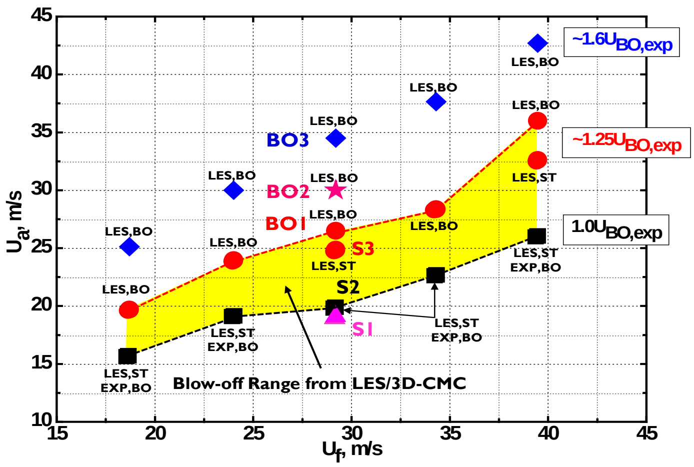

Figure 1: Air bulk velocity at blow-off as a function of the fuel jet velocity from experiments [2] and LES/3D-CMC. LES, BO: blow-off in LES; LES,ST: stable flames in LES; EXP, BO: blow-off in experiments.

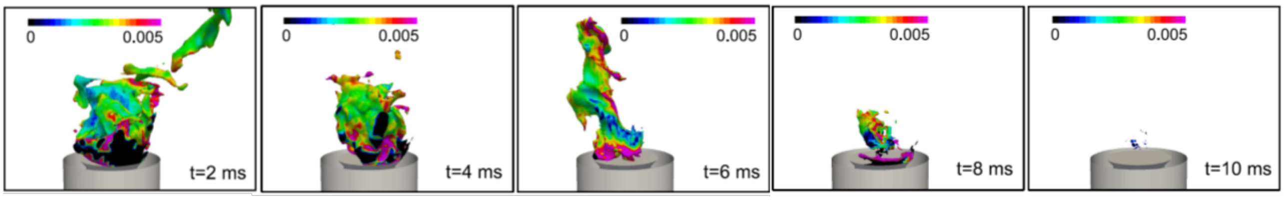

Figure 2: blow-off transient of an ethanol spray flame visualized though iso-surfaces of the stoichiometric mixture fraction coloured with OH mass fraction [4].

In conclusion, because the prediction of finite-rate kinetics effects, such as those present in extinction phenomena, requires both a very detailed description of the turbulence (as with LES), and a very thorough description of the chemistry, the ensuing computations are very expensive. Massively parallel computations are absolutely necessary. The present results show that such computations provide unique insights into the extinction process, and also offer its quantitative prediction. This development can potentially be used at the design stage of new low-emission devices by industry, thus saving time and cost from the development process.

References

[1] R. Yuan. Measurements in Swirl-stabilised Spray Flames at Blow-off. PhD thesis, University of Cambridge, 2015.

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[5] D.E. Cavaliere, J. Kariuki, E. Mastorakos, Flow Turbul. Combust., 91(2):347-372, 2013.

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8. Sources of significant sponsorship (if applicable): Rolls-Royce Group and EPSRC

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