UK CONSORTIUM ON TURBULENT REACTING FLOWS

Abstracts Booklet

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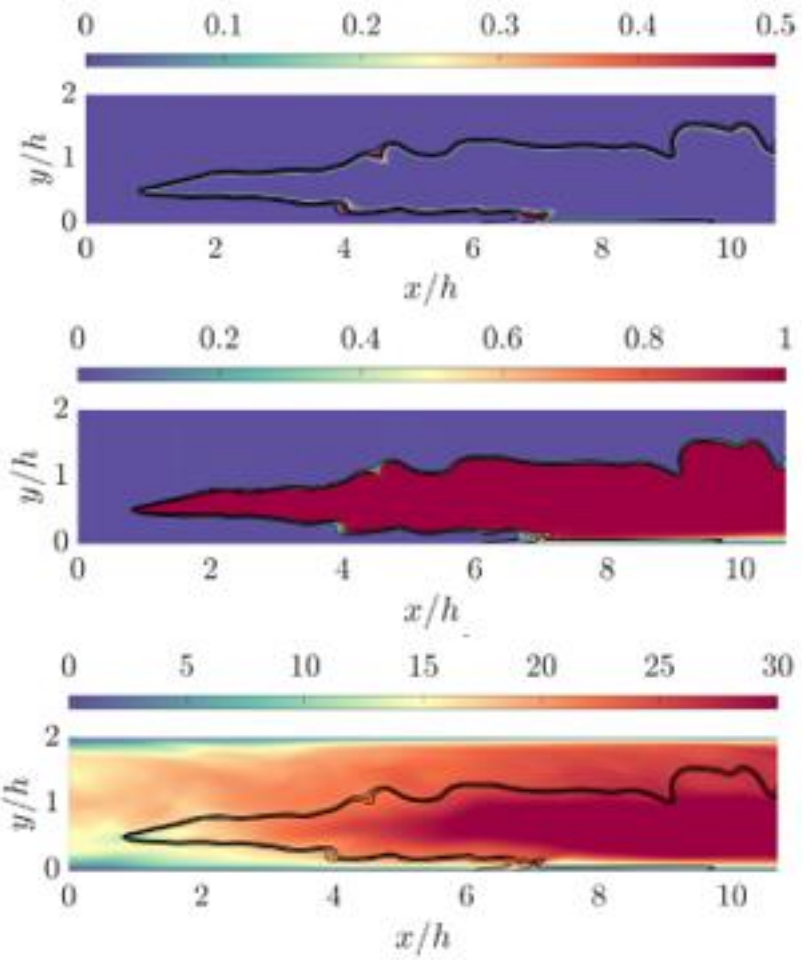

Multidimensional PDF modelling of turbulent premixed combustion

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Even today, where Large Eddy Simulations (LES) with fine computational grids are possible, subgrid models for premixed combustion are required because even at atmospheric pressure the laminar flame thickness is too small to be fully resolved. Premixed combustion is most often described by a single reaction progress variable c (c=0,1 in the fully unburnt/burnt regions, respectively). While presumed and transported probability density function approaches have met with considerable success in the case of non-premixed combustion, their application to perfectly premixed combustion with propagating, thin flame fronts has been more problematic. The classical Bray-Moss-Libby (BML) pdf method (representing the limit of infinitely thin reaction zones) with delta peaks at c=0,1 can calculate quantities which are not zero at c=0,1, excluding evaluation of the reaction source term. The often-used beta pdf for c is known to be inaccurate. Several variants of flamelet-based pdf's have been proposed, but met with numerical problems at the ends of the integration range c=0,1.

The talk will present analytical approximations to Arrhenius chemistry which however allow analytical solutions of the 1D steady laminar flame profile and the corresponding flamelet pdf. The integral of the pdf diverges logarithmically at c=0,1 but the valid pdf range does not cover the whole interval [0 … 1]. No delta peaks are needed even in the BML limit. An analytical model with 2D sinusoidally curved flame fronts and DNS data (using a single progress variable with Arrhenius source term and constant cp/lambda) show that the wrinkled flame subgrid pdf's for large filter widths resemble scaled 1D pdf's, where the scaling factor is an effect of subgrid wrinkling. It is shown that this effect can be approximated by filtering the 1D flame with an effective filter width smaller than the LES filter. It is shown how the analytical pdf approach can be applied to detailed chemistry flame profiles and how non-constant cp/lambda changes its form. A 2D pdf of reaction progress c and mixture fraction Z is derived for stratified combustion with thin flame fronts propagating through regions of varying mixture fraction. Finally, it is shown how multidimensional effects of flame fronts crossing through 3D filter volumes modify the 1D pdf. We also propose a model representing the effect of subgrid wrinkling based again on evaluations of DNS data.

References

Pfitzner M.: "A new analytic PDF for simulations of premixed turbulent combustion", Flow, Turbulence and Combustion, 106(4), pp. 1213-1239 (2021)

Pfitzner M., Klein M..: "A near-exact analytic solution of progress variable and pdf for single-step Arrhenius chemistry", Combust. Flame 226, 380-395 (2021)

Pfitzner M., Breda P.: "An analytic probability density function for partially premixed flames with detailed chemistry", Physics of Fluids 33/3, 035117, (2021)

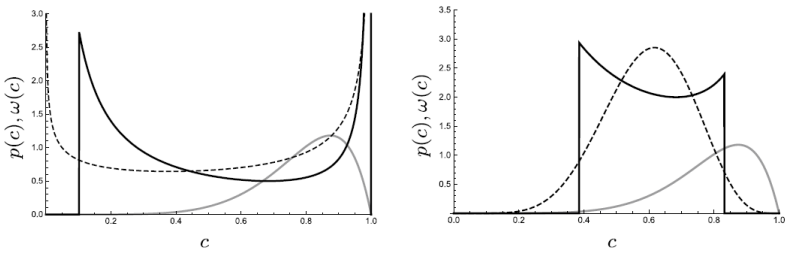

Fig. 9 Flamelet (black) and beta (dashed) pdf's with source term (gray); left: $\Delta = 2 * \delta_f$, right: $\Delta = 0.5 * \delta_f$

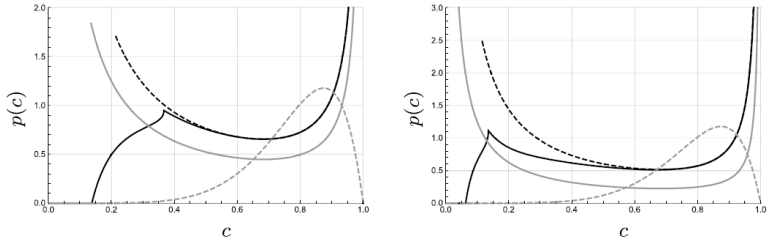

Fig. 13 Subgrid pdf for for $\Delta = 4, A = 1$ (left) and $\Delta = 8, A = 2$ (right), black: wrinkled flame pdf; gray: flat flame pdf, black dashed: flat flame pdf for filter Δ/Ξ; reaction rate (gray dashed) for comparison

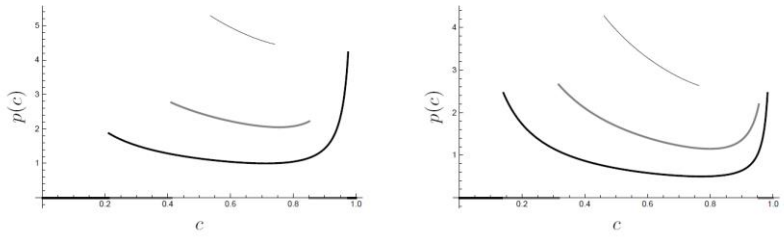

FIG. 19. $p(c)$ for $\overline{c} = 0.6$, $\Delta_x = 240\mu$ and $\phi = 1$ (Black), $\phi = 0.6$ (Gray),$\phi = 0.5$ (Black, thin); left: full c_p/λ, right:c_p/λ=$(c_p/\lambda)_u$

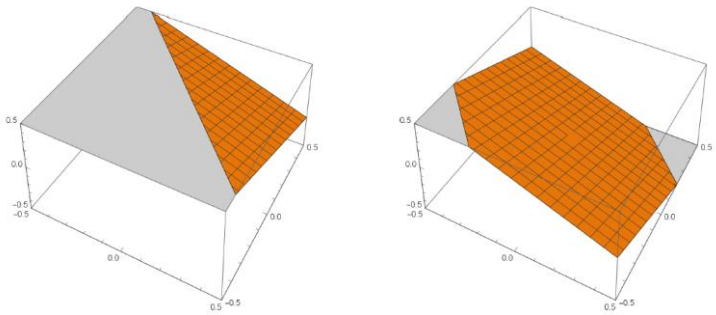

Fig. 2 Cuts of flat flame front through cubical filter volume

Large Eddy Simulation of Flame Dynamics in a Lean Technically Premixed Burner with Hydrogen Enrichment

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Combustion instability problems are most concerned with modern gas turbines, where swirl-stabilised combustors operated under lean, premixed conditions are often deployed for the benefits of enhanced stability and low NOx emissions. Most combustion instabilities are attributed to coupling mechanisms between unsteady heat release rate and acoustic pressure fluctuations, and still pose one of the most challenging problems in the combustion community [1].

Recently, lean premixed hydrogen-enriched flames have been studied extensively with swirl burner configurations. The specific objective of this work is to study the effect of hydrogen enrichment on a series of CH4/H2/Air flames in terms of flame topology, velocity field and combustion dynamic characteristics. The flames are investigated experimentally by Chterev et al.~ [2] based on the PRECCINSTA design. To reproduce the self-excited limit-cycle oscillations, a fully compressible LES- pdf method [3] is employed, where the solution to the temporal evolution of joint sgs-pdf equations is obtained by the stochastic field approach. The flow dynamics, flame topology and combustion instabilities are investigated numerically and compared with experimental measurements. The results revealed that as the concentration of hydrogen increases, the flame is shortened in the axial direction and more confined in the cross-sectional direction, which is consistent with experimental observations. The self-excited limit-cycle oscillations for both considered cases were successfully reproduced, with the predicted peak frequencies of the chamber pressure spectra in good agreement with the measured values. The feedback loop of the oscillations in the combustion is successfully captured and analysed with the temporal evolution of axial velocity and heat release presented.

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[3] D. Fredrich, W. P. Jones, and A. J. Marquis, “Thermo-acoustic instabilities in the PRECCIN-STA combustor investigated using a compressible LES-pdf approach,” Flow, Turbulence and Combustion (2020).

Code(s) used: BOFFIN

Time usage on ARCHER (approx. CUs): 5,000 CUs

Fuel Adaptability of an Advanced Vortex-tube Combustor: LES with *sgs-pdf* Approach

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The combustion characteristics of five representative gaseous fuels were studied to investigate the fuel adaptability in an advanced vortex-tube combustor (LSVC). The flammable limit, pressure fluctuation, and flame topology of different fuels were studied under various global equivalence ratios. Results show that the lean stability limit of the five fuels arises at a global equivalence ratio φ_g less than 0.15 with a uniform flame `front´. In addition, except for the intense thermal-acoustic coupling condition, the amplitude of the pressure fluctuation is always below 1000 Pa, indicating a super-steady combustion process. The non-premixed flame structure guarantees a high species concentration in the vicinity of the reaction zone. The vortex flow structure can decrease the local flow velocity and promote laminarization, whose synergistic action with the species and enthalpy distributions can promote the intensity of the combustion process. The intensified combustion is beneficial and increases the density gradients, which increase the Richardson number, R_i^*, yielding a highly-steady combustion procedure. Besides, the flame dynamics can also affect the stabilization, which relates closely to the amplitude of the pressure fluctuations for different fuels and can be quantified by the Rayleigh number, $Ra(x)$. Ultimately, the generalized criterion of stabilization can be defined by the combination of R_i^* and $Ra(x)$. The large R_i^* and small $Ra(x)$ are required for the highly steady combustion procedure.

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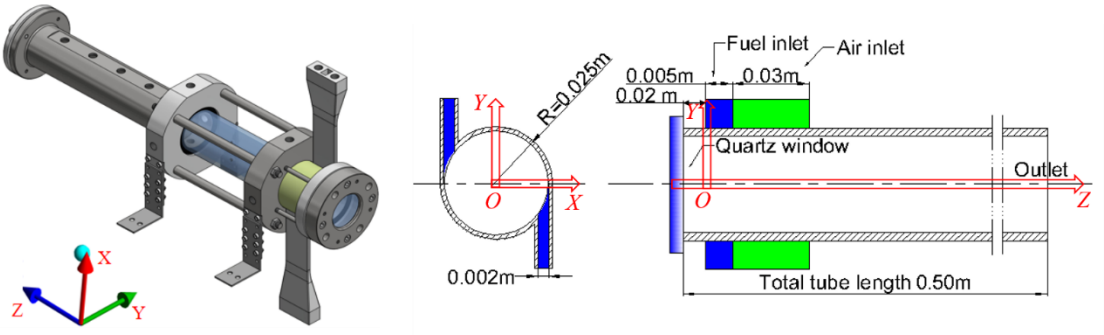
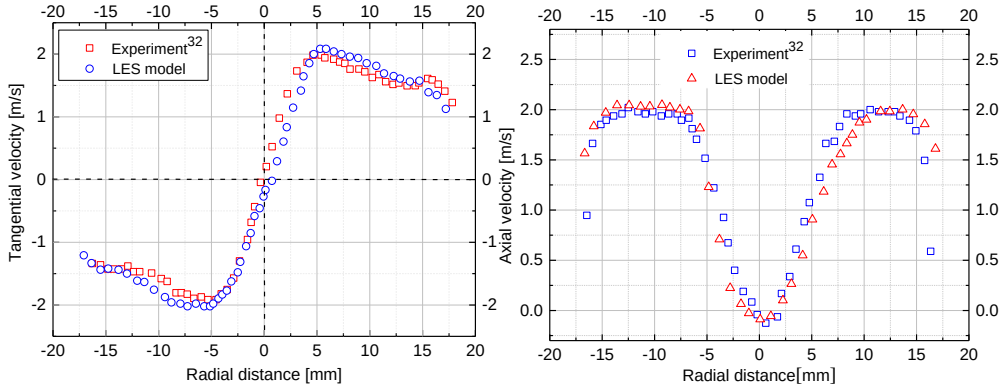
Code(s) used: BOFFIN-LESc

Time usage on ARCHER (approx. CUs): 4857.5



(a) Combustor configuration (b) 2-D cutaway view

Fig. 1 Schematic of the LSVC.



(a) Tangential velocity (b) Axial velocity

Figure. 2 Comparison of LES results and measurements in the vortex-tube combustor under the cold condition at z =160 mm. (a) Tangential velocity, (b)Axial velocity.

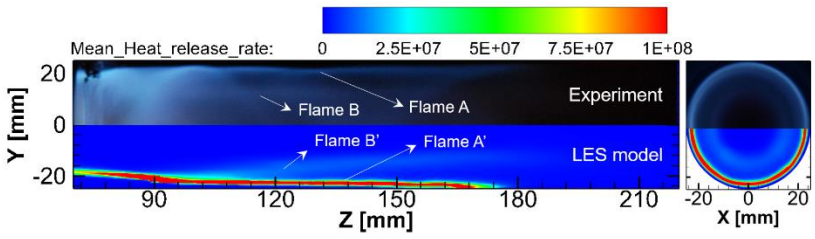


Figure. 3 Flame topology: LES and experiment in the vortex-tube combustor at φ_g = 0.8 and q_f = 12.0 L/min.

Reacting Flow DNS with Adaptive Mesh Refinement using the HAMISH Code

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A new Direct Numerical Simulation (DNS) code HAMISH with Adaptive Mesh Refinement (AMR) has been developed to simulate compressible reacting flow. The focus is on problems where high gradients of temperature, density and species mass fraction are localised in space. The code uses an unstructured Cartesian mesh in conjunction with an octree data structure indexed using a Morton space-filling curve, allowing for efficient adaptive refinement and de-refinement. The spatial discretisation scheme uses fourth-order polynomial reconstruction together with third-order adaptive explicit Runge-Kutta time-stepping. The code is fully parallelised with dynamic domain decomposition and automatic load-balancing over an arbitrary number of processors. Testing to date has included simulations of (a) 1-D planar laminar premixed flames; (b) fully developed laminar channel flow; (c) 2-D expanding flames under quiescent laminar condition; (d) 3-D non-reacting Taylor-Green vortex flows; (e) 3-D premixed turbulent flame propagation under isotropic homogeneous decaying turbulence. Results from these test cases indicate that the code is capable of producing accurate solutions in a computationally efficient manner.

Anisotropy Invariant Mapping of a Turbulent Boundary Layer by Deep Learning

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Anisotropy invariant map (AIM) of a zero-pressure gradient (ZPG) turbulent boundary layer is constructed for a 93%, 88%, and 33% horizon multi-step prediction of untrained data by nonlinear autoregressive neural network (NAR). Neural network setup parameters and hyperparameters are presented for a best-fit scenario given secondary sourced direct numerical simulation data. It is shown that NAR, trained via an ensembled 'committee of machines' approach, tends to predict close-to-mean AIM profiles as a result of nearly stationary data. Comparison with Reynolds stress model (RSM) simulated results indicates greater computational efficiency and reliability of NAR for AIM generation. Predicted invariant data is translated to a Barycentric and colour contour domain for different useful depictions of turbulence anisotropy.

Code(s) used: N/A

Time usage on ARCHER (approx. CUs): 0

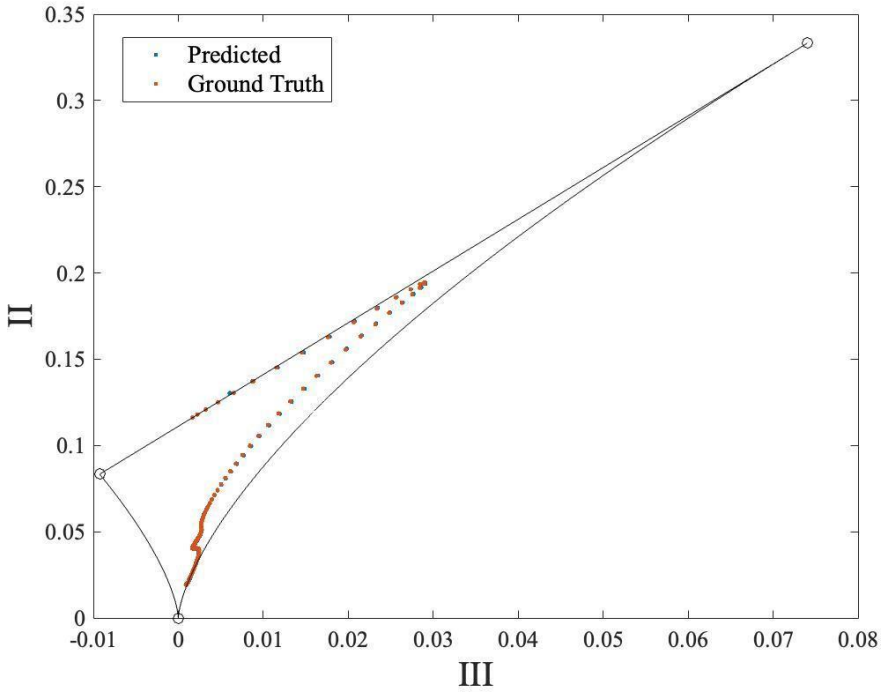

Figure 1. Single-Step Prediction for Re_θ = 4060

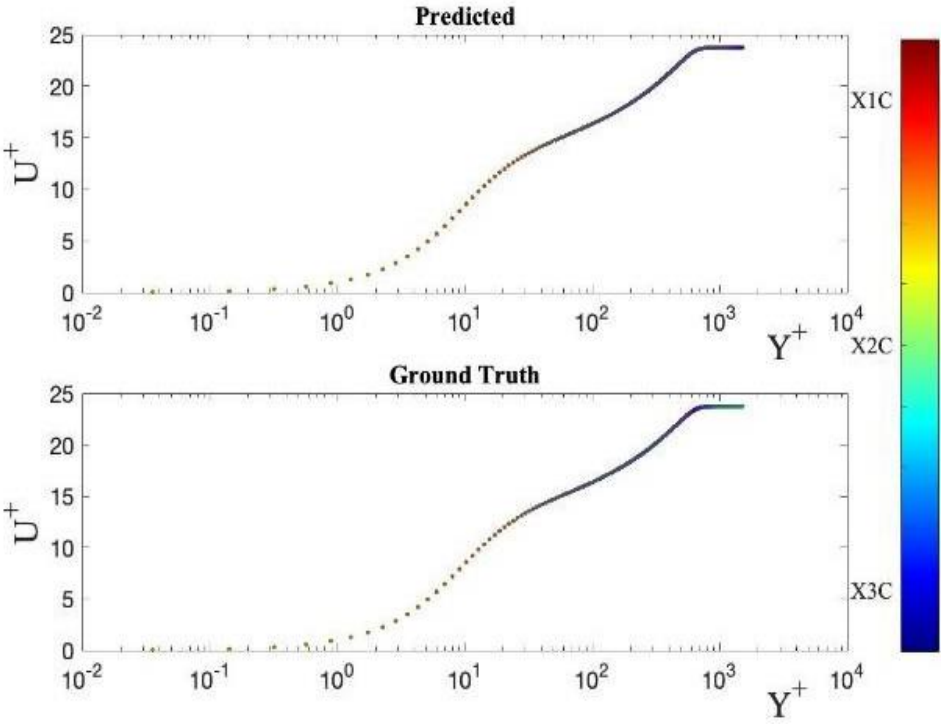

Figure 6. Colour Contour Visualization of 33% Horizon Mean Re_θ

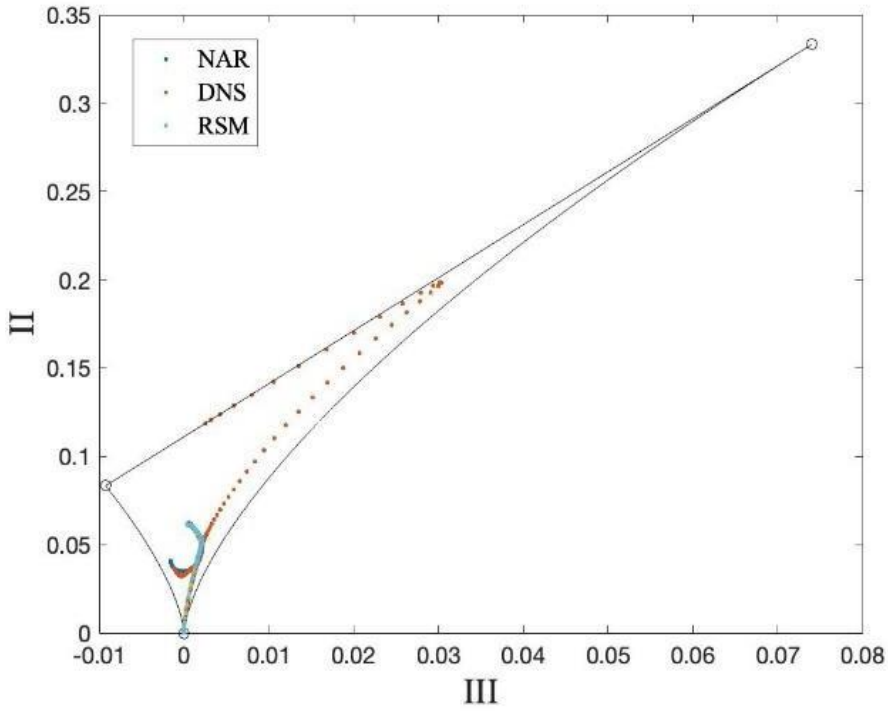

Figure 7. Reynolds Stress Model Comparison

Flame Self-Interaction and Flow Topology in Turbulent Homogeneous-Mixture n-heptane MILD Combustion

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Moderate or Intense Low-oxygen Dilution (MILD) combustion has been demonstrated to have the potential to achieve both high energy efficiency and ultra-low emissions. This study adopts the critical point theory to investigate the effect of turbulence intensity and dilution level on Flame-Self Interactions (FSI) and Flow Topology in the turbulent, homogeneous mixture, n-heptane MILD combustion processes using Direct Numerical Simulations (DNS) with a reduced chemical mechanism. The local flame geometry has also been categorised using the mean and Gauss curvatures. In this analysis, a DNS dataset of EGR type, turbulent, homogeneous mixture, n-heptane MILD combustion cases at two dilution levels, and two turbulent intensities has been considered. The process for creating the initial scalar and turbulence fields was described in detail by Minamoto et al. [1]. The turbulence levels used in this study are comparable to those reported by Oldenhof et al. [2]. The unburned gas temperature of T_r = 1100 K is also comparable to that used in the experimental investigation by Ye et al. [3]. Figure 1 shows the instantaneous views of the progress variable iso-surfaces and contours of *c* for all cases. These *c* iso-surfaces represent the reaction progress variable value corresponding to the maximum heat release for the equivalent unstretched laminar premixed flame used for initialising each simulation, and thus it can be considered to represent the flame surface. The figure shows a considerable amount of flame self-interactions at these *c* iso-surfaces. It can also be seen that increasing the turbulence intensity gives rise to noticeably more wrinkled *c* iso-surfaces while increasing dilution in the *c* iso-surfaces covering a smaller portion of the domain. The distributed nature of the flame in MILD combustion is evident in the contours of the progress variable and is consistent with experimental observations. Figure 2 shows the temperature variation for one case (low turbulence-low dilution). It can be seen from Fig. 2 that only a modest increase in temperature exists in this case. This is consistent with experimental observations. Figure 2 also shows the contours of flow topologies in the midplane for the same case. It can be seen from the figure that the flow topologies associated with non-zero values of dilatation rate are rare in MILD combustion, which is a consequence of the weak dilatation rate because of weak thermal expansion due to the modest temperature rise. In this study, it was found that increasing the turbulence intensity has led to enhanced FSI frequency and resulted in the range of mean curvature values while increasing the dilution factor caused a reduction in the frequency of FSI events towards the burned gas side but produced higher ranges of mean and Gauss curvatures.

References

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Code(s) used: SENGA+

Time usage on ARCHER (approx. CUs): 8000

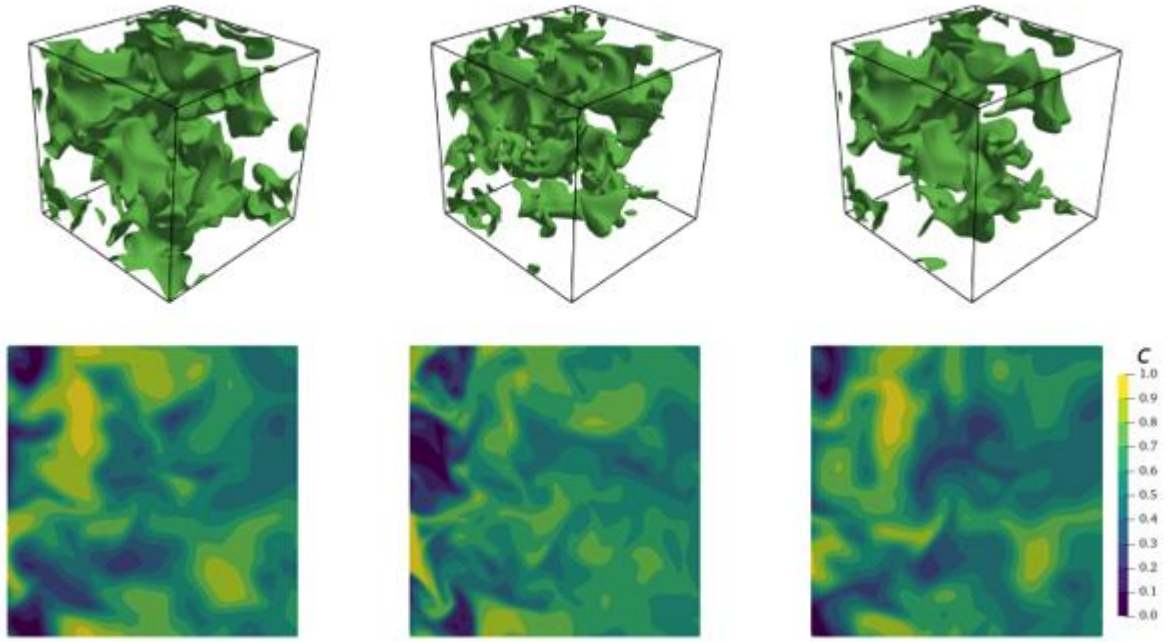

Figure 1: The iso-surfaces of the progress variable at the location of maximum heat release for the equivalent laminar flames (1st row) and contours of the progress variable in the midplane (2nd row) for the MILD combustion setup at various initial turbulence intensities and dilution levels (1st column low turbulence-low dilution, 2nd column high turbulence-low dilution, 3rd column low turbulence-high dilution).

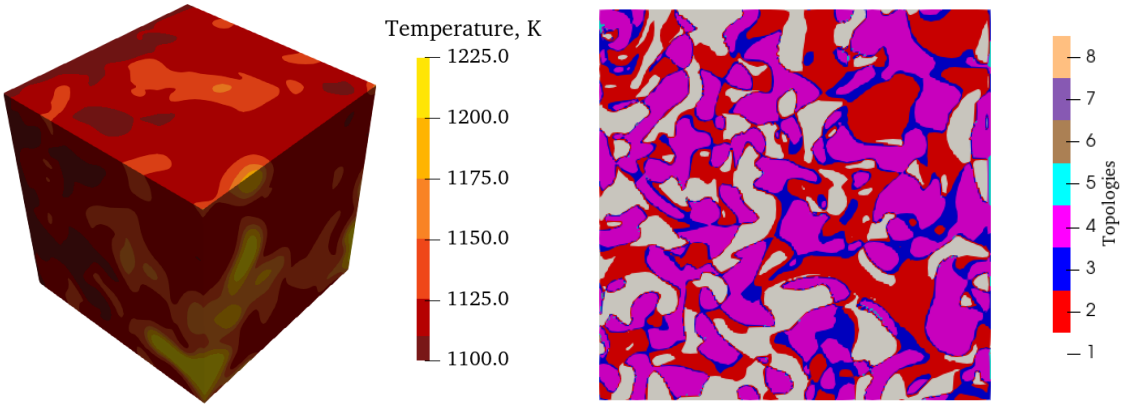

Figure 2: The temperature distribution and flow topologies for the MILD case at low turbulence- low dilution levels.

The effect of heat release on the recirculation zone structure in bluff body stabilised turbulent premixed swirling flames

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The recirculation zone created through vortex breakdown mechanisms in swirling flows plays a vital role for aerodynamic stabilisation of turbulent flames in practical combustion systems. This zone interacts with the wake of an upstream bluff body and leads to a complex flow behaviour that depends on the blockage ratio and swirl number. The vortex breakdown bubble merges with the wake at large swirl number or blockage ratio. Although these behaviours were studied well for isothermal flows, the effects of heat release on these structures and flow patterns are not understood sufficiently. In this study, the influences of heat release on this flow structure and their physical mechanisms are explored through a series of large eddy simulations of bluff body stabilised swirling premixed flames. Detailed analyses of the results show that the bubble moves upstream leading to its stronger interaction with the wake in combusting flows which can affect the thermo-acoustic characteristics of the combustor. Comparisons of simulation results with measurements are observed to be good.

DPK would like to thank EPSRC, Rolls-Royce and Cambridge Trust for financial support and UKCTRF for providing access to HPC services. UCL authors would like to thank UKRI for financial support through grants EP/T009314/1 and MR/T019735/1.

Code(s) used: OpenFOAM 7

Time usage on ARCHER (approx. CUs): 2200

Evaluations of turbulent burning velocity and wall heat flux using integral energy equation for premixed flame-wall interaction in turbulent boundary layers

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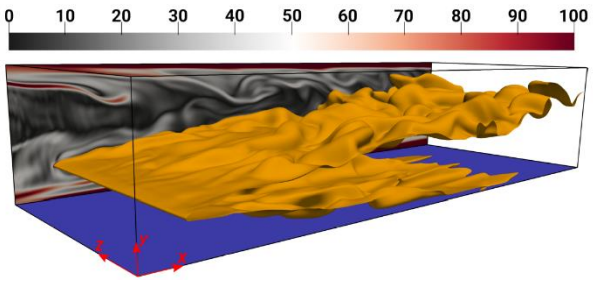
An integral form of the energy conservation equation has been derived from the first principle for low Mach number conditions for turbulent premixed flame-wall interaction (FWI) in turbulent boundary layers under a quasi-stationary state. The validity of this equation has been assessed using three-dimensional Direct Numerical Simulation (DNS) data of statistically stationary oblique quenching of turbulent premixed V-shaped flame by an inert isothermal wall in a channel flow configuration. Figure 1 exemplarily shows the reaction progress variable $c = 0.5$ iso-surface and contours of instantaneous normalised vorticity magnitude in the x-y plane. The distributions of instantaneous reaction progress variable, non-dimensional temperature, and streamwise velocity component in the central midplane are shown in Fig. 2. The significant decay in the vorticity magnitude is observed with an increase in temperature across the flame front. The flame quenches due to the heat loss to the wall. The results obtained from DNS data reveal that the wall heat flux and the heat release rate integrated across the turbulent boundary layer in the wall-normal direction remain the major contributors in the energy integral equation and the difference between these contributions is balanced by the term arising from thermal advection. Due to the flame quenching, the heat release rate contribution in the energy integral equation decreases with increasing distance from the leading edge of the boundary layer. The wall heat flux magnitude increases with increasing distance from the leading edge of the boundary layer. Integrating the energy integral equation along the streamwise direction for the whole width of the wall reveals a close relationship between the mean Nusselt number and turbulent burning velocity and they are independent of each other. Therefore, once one of these quantities is estimated, the other one can be found provided the variations of the Favre mean values of streamwise velocity component and sensible enthalpy in the wall-normal direction are known. This suggests that experimental measurement of wall heat flux enables the evaluation of turbulent burning velocity in the case of premixed flame-wall interaction in turbulent boundary layers. It has been found that a revised Flame Surface Density (FSD) based mean reaction rate closure FSD to account for near-wall behaviour can be utilised to evaluate the mean Nusselt number within the turbulent boundary layer in the case of premixed flame-wall interaction.

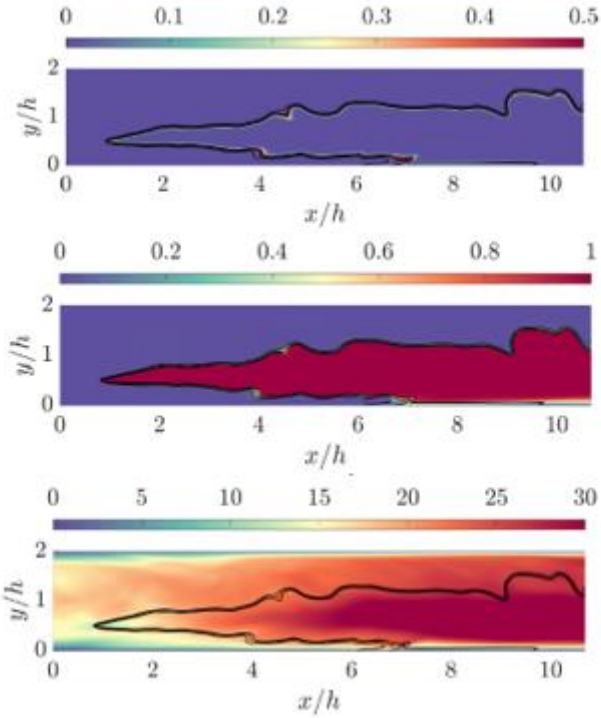
Code(s) used: SENGA$^+$

Time usage on ARCHER (approx. CUs): 30,000

* Corresponding author



Figures 1: V-flame with isothermal wall boundary conditions. The iso-surface coloured in yellow represents c = 0.5. The instantaneous normalised vorticity magnitude is shown on the x-y plane. The blue surface denotes the bottom wall.



Figures 2: (a) Instantaneous behaviour of the non-dimensional reaction rate of the progress variable c (top), (b) non-dimensional temperature $\theta = (T - T_u)/(T_{ad} - T_u)$ (middle), (c) and the non-dimensional axial velocity (bottom) along with the c = 0.1, 0.5 and 0.9 isolines (black lines) in the V-flame OWQ configuration.

A priori Direct Numerical Simulation Analysis of the Closure of Cross-Scalar Dissipation Rate of Reaction Progress Variable and Mixture Fraction in Turbulent Stratified Flames

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The cross-scalar dissipation rate of reaction progress variable and mixture fraction $\widetilde{\varepsilon_{c\xi}}$ plays an important role in the prediction of the mean reaction rate in industrial calculations of stratified combustion. In this work, the evolution equation for $\widetilde{\varepsilon_{c\xi}}$ has been derived and analysed using a Direct Numerical Simulation (DNS) database of statistically planar turbulent stratified flames with a globally stochiometric mixture. A parametric analysis has been performed in terms of initial root-mean-square velocity fluctuation normalised by the laminar burning velocity of the stoichiometric mixture $u'/S_{b(\phi=1)}$ and the scalar integral length scale normalised by velocity integral length scale ℓ_ϕ/ℓ. The explicitly Reynolds averaged DNS data suggests that the linear relaxation (LR) model for $\widetilde{\varepsilon_{c\xi}}$ is inadequate for most cases, but its performance appears to improve with increasing ℓ_ϕ/ℓ and $u'/S_{b(\phi=1)}$. The budget of the unclosed terms in the $\widetilde{\varepsilon_{c\xi}}$ transport equation has been analysed in detail. It has been found that the terms arising from the density variation, scalar-turbulence interaction, chemical reaction rate and molecular dissipation rate play leading order roles in the $\widetilde{\varepsilon_{c\xi}}$ transport. These observations have been justified by a scaling analysis, which has also been used to identify the dominant components of the leading order terms for developing closures involving the aforementioned leading order terms of the cross-scalar dissipation rate $\widetilde{\varepsilon_{c\xi}}$ transport equation. The performances of newly proposed models for the unclosed terms have been assessed with respect to the corresponding terms extracted from DNS data, and the newly proposed closures have been found to yield satisfactory predictions for the unclosed terms in the $\widetilde{\varepsilon_{c\xi}}$ transport equation.

Code(s) used: SENGA+

Time usage on ARCHER (approx. CUs): 5000 CUs

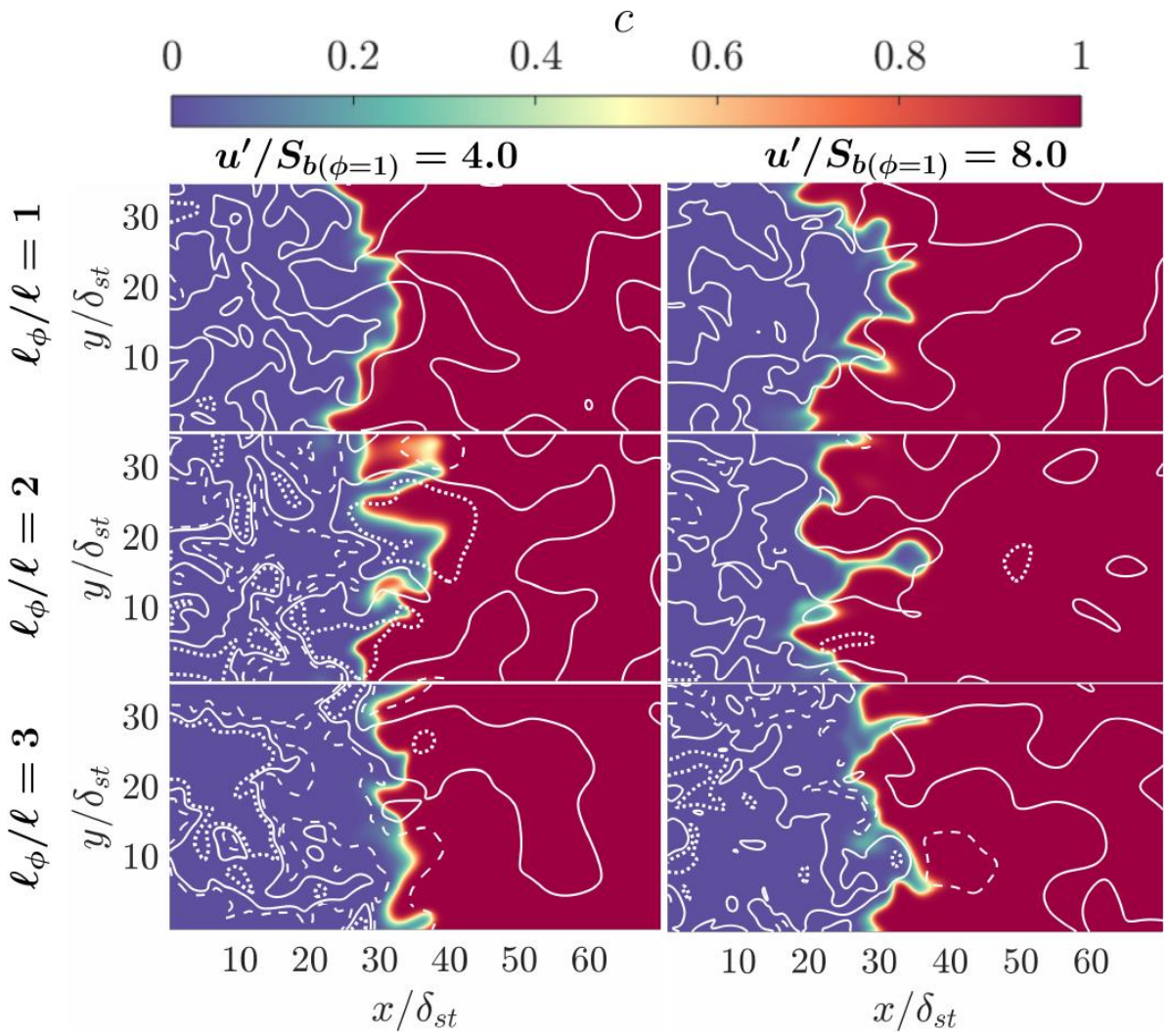

Figure 1: Distributions of reaction progress variable c in the central x-y plane with the contours of $\xi/\xi_{st} = 0.8$ (dashed white line), 1.0 (solid white line) and 1.2 (dotted white line) superimposed for different initial values of ℓ_ϕ/ℓ and $u'/S_{b(\phi=1)}$.

Modelling and simulation of soot formation and evolution in turbulent flames

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Soot emission is a major concern for thermal engines, furnaces and all combustion-based processes. Soot particles are dangerous for human health when they are in too high concentration, and their emission level is subjected to more and more constraining regulations. To fulfill these obligations, manufacturers are engaged in the development of low-soot burners, acting on the fuel formulation, the injection system and the operating conditions. The production and evolution of soot particles result however from a number of complex and interacting non-linear phenomena, which put in difficulty trial-and-error methods. High-fidelity numerical simulation is then essential for the prediction of soot in real systems and the design of the next generation of low-soot burners.

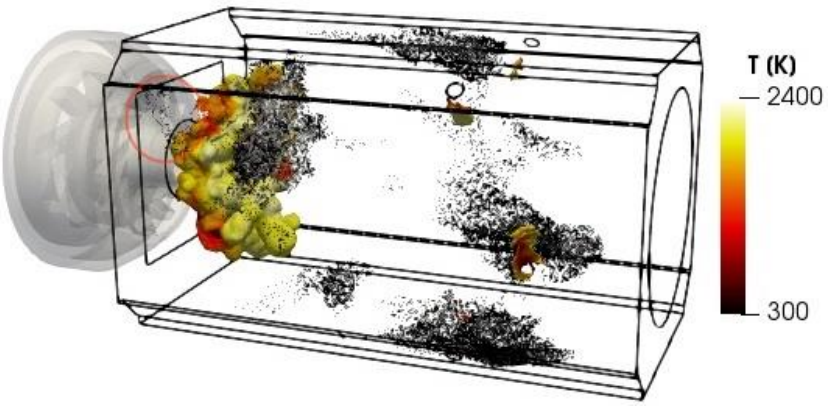
CERFACS has recently developed a complete model for the soot formation, transport and oxidation in turbulent flames and complex geometries [1]. The approach is based on a Lagrangian description of the soot particles, coupled to a semi-detailed chemical mechanism based on the Analytically Reduced Chemistry (ARC) concept. This approach allows to include soot precursors in the flame calculation which are known to be the key element of soot formation. Particular efforts have been put on the Lagrangian Soot Tracking (LST) algorithm to maintain high parallel computing efficiency. With this approach, the description of the particle size distribution comes with almost no additional cost, and any particle property, such as morphology for example, can be easily included.

In this presentation, the modelling approach followed to predict soot within the Large Eddy Simulation (LES) framework implemented in the in-house, massively parallel code AVBP (www.cerfacs.fr/avbp7x) will be described. Both physical phenomena and numerical aspects of the model will be detailed and illustrated in academic cases. The performance and accuracy of the approach will finally be assessed on practical configurations, also allowing to identify limitations and paths for improvement.

References

[1] L. Gallen, *Prediction of soot particles in Gas Turbine Combustors using Large Eddy Simulation*, PhD 2020.

[2] M. Stohr, K. Geigle, R. Hadef, I. Boxx, C. Carter, M. Grader, and P. Gerlinger, *Time-resolved study of transient soot formation in an aero-engine model combustor at elevated pressure*, Proc. Combus. Inst., vol. 37, no. 4, pp. 5421{5428, 2019.



Visualisation of soot particles (black dots) and the flame (heat release rate isosurface, colored with temperature) in the configuration of DLR [2]

Electrostatic fields for the control of evaporating fuel droplets in a charged electrospray

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The current socio-economic shift towards electrification of the transport sector provides new opportunities for the development of advanced aeronautical propulsion technologies. In today's contemporary design space, the flow field inside an aircraft engine is inevitably defined by the geometry of the solid walls confining the fluid flow, e.g., the architecture of the combustion chamber and fuel injectors, along with the corresponding mass flow rates. The present work explores the potential use of electrostatic fields as an additional measure for fluid control to overcome this limitation. In particular, electrostatic fields are envisioned as a means for modulating the trajectories of electrically charged fuel droplets, independently of any physical boundaries. Such mechanism would allow increased control over the evaporation process, i.e., the location of the fuel vapour release, with a successive impact on the fuel-air premixing quality, the flame behaviour, and the formation of pollutants. Broadly similar technologies involving the control of charged particles or liquids using electrostatic fields have previously been investigated in the field of electrohydrodynamics (EHD). Some of these technologies are already well established in industry relevant applications such as electrostatic precipitation [1], powder coating [2] and ink-jet printing [3]. We propose the hypothetical concept of an electrospray in cross-flow (ESICF). Such ESICF combines the use of an external electrostatic field together with an electrospray of charged fuel droplets [4] injected perpendicular into a bulk flow of air. Within this framework, the specific objectives of the present work are:

(i) To modulate the droplet trajectories of the ESICF using a range of external electrostatic potential differences and bulk flow velocities. These conditions are to be varied parametrically to evaluate the effect of the electrostatic forces imposed on the droplets versus the inherent drag forces induced by the bulk flow. (ii) To increase the effective time available for droplet evaporation over a finite-length mixing region. This is accomplished by applying an external electrostatic field, which acts in the opposite direction to the bulk flow. The resulting higher relative velocity between the droplets and the bulk flow may also lead to enhanced evaporation rates and fuel-air mixing. In general, it is to be demonstrated that this strategy can provide control over the location of the fuel vapour release – a concept introduced here as '*targeted evaporation*'. Subsequent effects on the combustion process, i.e., the flame dynamics and the formation of pollutants, will be further investigated in future work.

[1] T. Yamamoto, H. R. Velkoff, J. Fluid Mech. 108 (1981) 1–18.
[2] A. G. Bailey, J. Electrostat. 45 (1998) 85–120.
[3] P. Galliker et al., Nat. Commun. 3 (2012).
[4] T. Ahmed et al., Combust. Flame (2021)

Code(s) used: OpenFOAM

Time usage on ARCHER (approx. CUs): 600

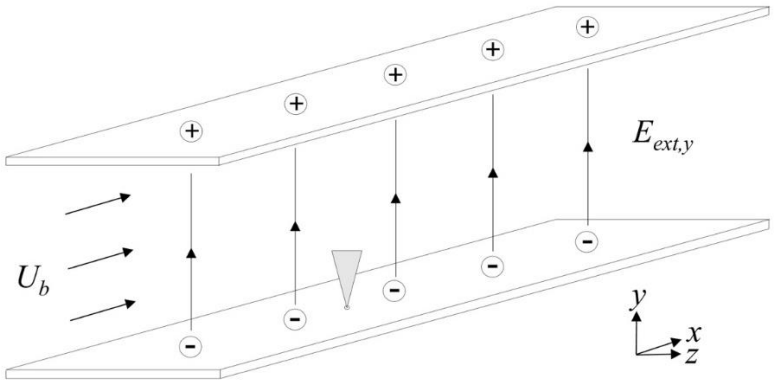

Figure 1: Schematic of the simulated ESICF configuration indicating a (vertical) external electrostatic field in the *y*-direction.

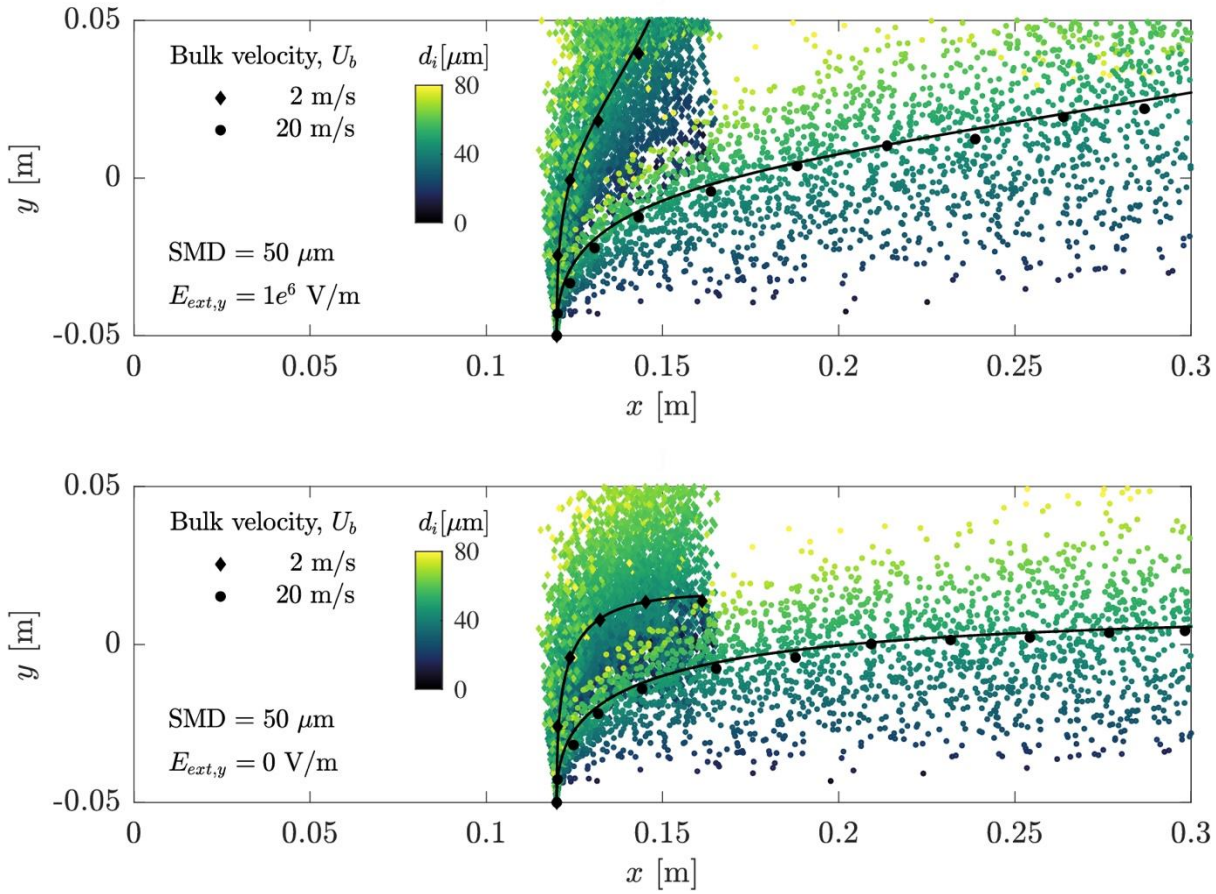

Figure 2: Instantaneous droplet size and spatial distributions (2D projection) obtained from LES including evaporation for different bulk flow velocities. Top: external electrostatic field in the *y*-direction. Bottom: no electric forces. Black symbols indicate the respective bin averages. Solid lines represent the corresponding 2D-model predictions.

Numerical Modelling of Fire Spread on Wood Cribs: the Role of the Char and Enhanced Grid Sensitivity Studies

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The temperature heterogeneity due to fire in large open-plan office compartments, of relevance to structural fire design, is closely associated with fire spread behaviour, and has been tackled historically through experimental investigations using timber cribs. Our previously reported study explores the ability of Computational Fluid Dynamics (CFD) models, specifically the Fire Dynamics Simulator (FDS) 6.6.0 [1], to reproduce the results of full-scale tests involving fire spread over timber cribs on continuous fuel-beds with nominal fuel load density 511 MJ/m^2 which matches typical office buildings [2]. The "stick-by-stick" model with "simple pyrolysis" showed good promise in representing the evolution of the heat release rate due to fire spread, gas phase temperature, and burn-away.

Two important aspects of the simulations have now been studied in more detail: the role of wood char in the combustion, and further grid resolution studies inside the crib structure itself. For the former it is recognised that as combustion proceeds the timber is progressively converted to glowing char, which of course burns in a different manner – with a heat of combustion value typically much higher than that of the virgin fuel. Explicit representation of the charring phase was established in a new set of simulations (Figure 1), with further parametric studies for the sensitivities to the new model parameters, including the choice between single and double plateau models and char thermal properties. This required some recalibration of the existing model, which was achieved with still excellent matches to the macroscopic fire spread parameters (Figure 2) and some improvement to the temperature comparisons. Mesh sensitivity studies found support for the earlier results via simulations with 0.75cm cell size within the crib structure.
Application of the calibrated model in "scaling up" to full-scale compartment scenarios is of great interest and is still underway in more computationally demanding simulations (8.3M cells, 7200s test, 125 nodes x c. 50 48hr jobs each, on ARCHER2) of the series of 3 travelling fire tests performed at University of Ulster under the TRAFIR project.

Code(s) used: Fire Dynamics Simulator (FDS), NIST, USA
Time usage on ARCHER/2 (approx. kAU/CU): 7,000kAU Nov-20; 3,500 CU Jun-21 (+ 5,000 CU Nov-21)

Acknowledgement
This work was carried out as part of the TRAFIR project, funding from the Research Fund for Coal and Steel (grant N°754198). Other partners are ArcelorMittal Belval & Differdange, Liège Univ., RISE Sweden and the Univ. of Ulster. This work also used the resources provided by the Edinburgh Compute and Data Facility (ECDF) (http://www.ecdf.ed.ac.uk/). Contributions from Chang Liu via dissertation for MSc in Structural and Fire Safety Engineering and Peter Charley via MEng thesis in Civil & Environmental Engineering.

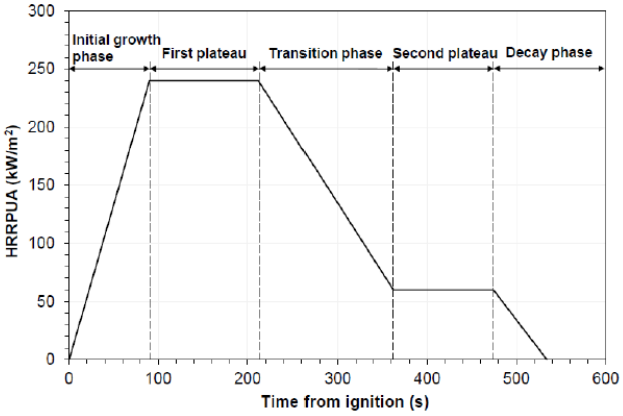

Figure 1. HRRPUA ramp framework for FDS modelling with explicit treatment of char.

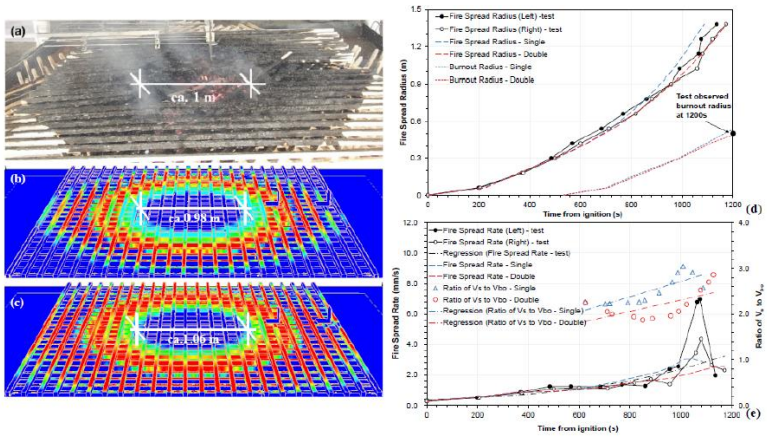

Figure 2. Predicted fire spread and burn-out with recalibrated model including char representation.

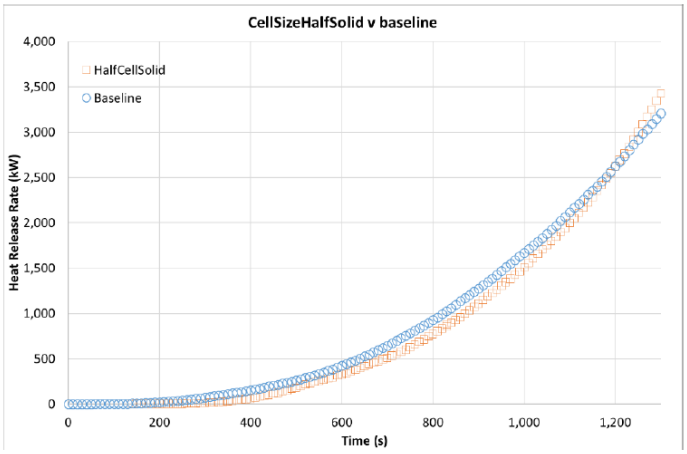

Figure 3. Evolution of HRR for baseline case with 1.5cm cells within fuel bed (total 2.2M cells) and finely resolved mesh with 0.7cm cells in fuel bed (total 7.2M cells).

Spectral behaviour of the heat release rate in swirl-stabilised and bluff body flames

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Pressure fluctuations produced by the unsteady heat release rate (HRR) can result in direct combustion noise or can feedback into the combustor resulting in destructive resonance. Predicting this broadband noise and self-excited thermoacoustic oscillation is challenging and its mitigation is important. The power spectral density of the pressure fluctuations, which is a measurable quantity in experiments, is related to the product of local spectral densities of a Green's function and fluctuating HRR (ψ_q), integrated over flame volume appropriately [1]. The quantity ψ_q is challenging to measure but easy to obtain from large eddy simulation (LES) results. The behaviour of ψ_q for a wide range of thermochemical and turbulence conditions is investigated. Three combustors operating at atmospheric conditions with CH_4-air mixtures are studied: the dual-swirl burner developed by DLR, the PRECCINSTA single-swirl burner and a premixed bluff body burner. These cases are simulated using the LES-FlaRe (Flamelets revised for physical consistencies) model for sub-grid scale combustion. The dependence of ψ_q on spatial location and flame configuration and its relation to volume-integrated HRR spectra are studied. It is observed that ψ_q can be modelled using velocity and scalar spectra which will be shown in the oral presentation.

Code(s) used: OpenFOAM v7
Time usage on ARCHER (approx. CUs): 19,375.00

[1] Currently at Peking University.

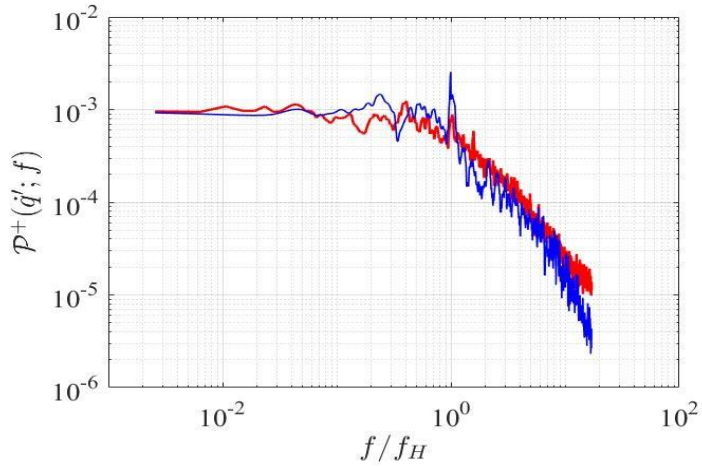

Figure 1: Local heat release spectrum for flame C (swirl-stabilised) from LES results (—) and modelled spectrum based on isothermal flow (—).

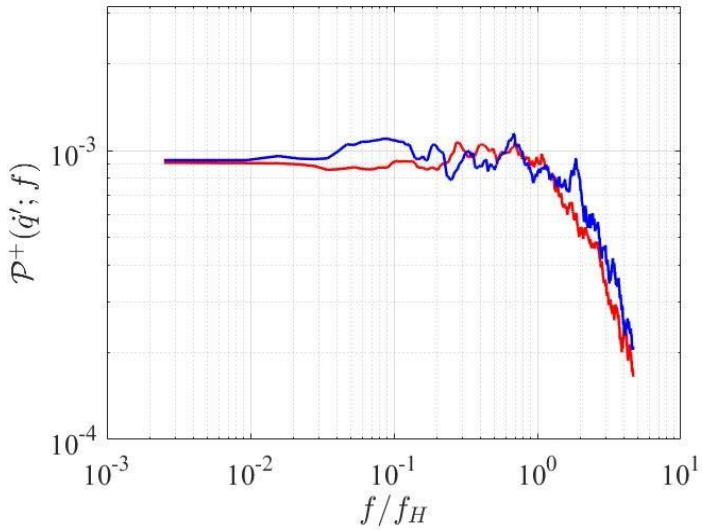

Figure 2: Local heat release spectrum for bluff body flame from LES results (—) and modelled spectrum based on isothermal flow (—).

Large eddy simulation of aerosol synthesis of silica nanoparticles in turbulent flame

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Aerosol synthesis of nanoparticles in flames is one of the main methods for the manufacturing of nanoparticles and received increased attention over the last few decades. Large eddy simulation of aerosol synthesis of silica nanoparticles in turbulent methane jet flame is presented here. Silica nanoparticles are formed through the vapour-precursor (hexamethyldisiloxane) oxidation and several aerosol processes like nucleation, condensation, coagulation, and sintering. The pdf-stochastic field method was employed to capture the turbulence-chemistry interaction in the context of LES, while a monodisperse model was used to describe the evolution of particle number, area, and volume concentrations (Kruis et al, 1993). The chemistry was represented by the GRI 1.2 reaction mechanism with 31 gas species and 175 reactions. Three extra species and 2 reactions were introduced to the chemical mechanism to represent the precursor decomposition. The results are compared with the detailed experimental data of Camenzind et. al. (2008). Specifically, the flame temperature, the silica volume fraction, the number concentration of primary particles, and the primary particle diameters were measured for several locations along the jet centreline. Preliminary results showed that while the flame temperature is captured relatively well, there is still large discrepancy between the modelled and experimental silica volume fraction and particle number concentration. Specifically, the model overpredicts the formation rate of new particles, thus the predicted silica volume fractions were found to be one order of magnitude larger than the experimental values. This could be caused because of uncertainties in the validity of the instantaneous-nucleation assumption or the precursor-decomposition kinetics. Nevertheless, the performance of the model is reasonable considering the modelling complexities associated with aerosol synthesis of nanoparticles. This study is an important step towards predicting aerosol synthesis of nanoparticles in turbulent flame since it is one of the very few simulations where detailed comparisons with experimental data are presented.

References

Kruis, F. E., Kusters, K. A., Pratsinis, S. E., & Scarlett, B. (1993). A simple model for the evolution of the characteristics of aggregate particles undergoing coagulation and sintering. *Aerosol science and technology*, *19*(4), 514-526.

Camenzind, A., Schulz, H., Teleki, A., Beaucage, G., Narayanan, T., & Pratsinis, S. E. (2008). Nanostructure evolution: from aggregated to spherical SiO2 particles made in diffusion flames.

Code(s) used: BOFFIN

Time usage on ARCHER (approx. CUs): N/A

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