UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS

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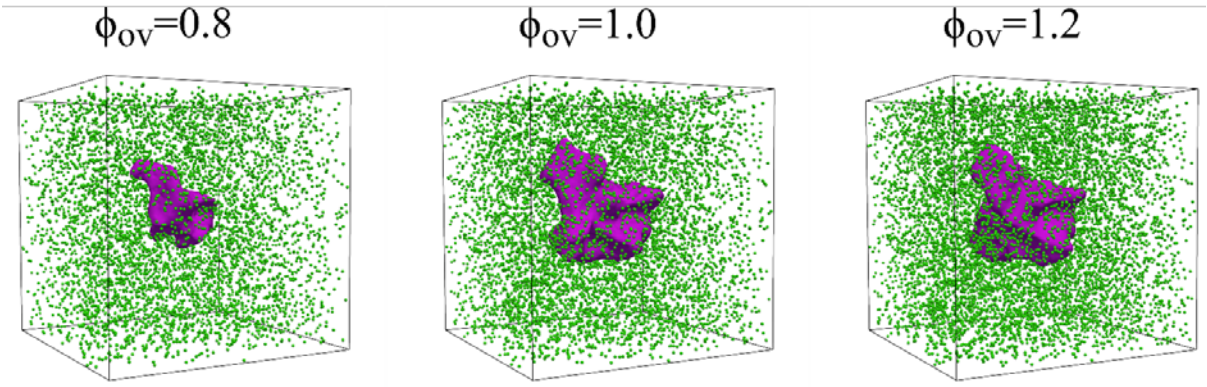
Abstracts Booklet

UKCTRF Meeting

Held on Zoom

30th & 31st March 2021



Evgeniy Shapiro, PhD

Ricardo

As Fluids Development Manager, Evgeniy is leading the team responsible for development and implementation of models and tools within Ricardo's Computational Fluid Dynamics suite incorporating real-time (WAVE-RT), 1D (WAVE) and 3D (VECTIS) products.

Prior to joining Ricardo in 2012, Evgeniy spent twelve years in academia (UCL, QMUL, Cranfield University) researching, developing, implementing, and teaching CFD models and methods across a diverse range of application areas ranging from automotive and aerospace to process systems and nano-technology. Currently Evgeniy's main focus is on combustion systems and thermal management modelling both in a technical lead capacity and through building and managing highly efficient Agile development teams. The key challenge of the former being adaptation and reduction of high-fidelity models to deliver run-times required for Virtual Product Development process. Development of accurate, efficient, and affordable solutions to complex CFD problems - who said you can only have two out of three?

Managing complexity in internal combustion engine modelling for virtual product development

Tightening emissions legislation drives OEMs to further optimise existing ICE powertrains in order to reduce tailpipe emissions while maintaining and improving engine efficiency. When considering already high levels of optimisation of existing powertrains and small deltas achievable with individual design modifications, the need for accurate simulation tools capable of delivering holistic analysis at whole vehicle simulation scale has never been higher. At the same time accurately capturing combustion phenomena still poses a remarkable challenge even at short time and length scales. Bridging the gap between state-of-the-art methods developed within the academic community aiming at full predictive capability and the turnaround times required for virtual product development prompts development of semi-predictive methods which can be calibrated on reduced data sets but once calibrated - can accurately respond to design modifications. In this talk we consider the place of 3D CFD ICE modelling within the envelop of the virtual product development and summarise the challenges facing attempts to achieve fully predictive modelling capability. We then illustrate tabulated and detailed kinetics-based methods which are actively developed within Ricardo VECTIS 3D CFD toolchain to address this gap and illustrate application of these for prechamber and SI natural gas combustion systems.

Analysis of turbulent coagulation in a jet with discretised population balance and DNS

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Keywords: Turbulent coagulation, jet, DNS, population balance, general dynamic equation, sectional method, nanoparticles, aerosols
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Abstract

The central objective of the present study is to investigate the turbulence-coagulation interaction via direct numerical simulation (DNS) coupled with the population balance equation (PBE). Coagulation is an important process in several environmental and engineering applications involving turbulent flow, including soot formation, gas-phase synthesis of nanoparticles and atmospheric processes, but its interaction with turbulence is not yet fully understood. Particle dynamics can be described by the PBE, whose Reynolds decomposition leads to unclosed terms involving correlations of number density fluctuations. In the present study, we employ a discretisation (sectional) method, which is free of a priori assumptions regarding the particle size distribution (PSD) to solve the PBE together with flow DNS. The behaviour and significance of the unknown correlations is investigated by performing DNS of a 3D spatially developing planar jet laden with monodisperse nanoparticles. Coagulation due to collisions in the free-molecule regime is considered in accordance with the kinetic theory of gases. The correlations of the turbulent fluctuations of the PSD are calculated at several points in the domain and found to be positive for most of the points examined. Negative correlations are also observed close to the jet break-up point. The correlation terms in the transport equation of the moments make a considerable contribution to the time-averaged coagulation source term and therefore neglecting these terms, as is common practice, can result in an error of 20% on the jet centreline and up to 40% close to the jet edges. Finally, the moments of the PSD were found to exhibit self-similar profiles in the cross-stream direction.

Codes used: PANTARHEI and CPMOD (inhouse codes)

Time usage on ARCHER (approx. kAU): 3000 kAUs

Turbulence-flame interaction in high Reynolds number methane and hydrogen turbulent jet flames

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A series of Direct Numerical Simulations (DNS) of turbulent methane and hydrogen jet flames has been performed to analyse the interaction of highly turbulent shear-driven velocity fields and combustion. The methane flame series include four cases at constant Karlovitz number and increasing jet Reynolds number up to 22400 [1,2], corresponding to an approximately constant turbulent intensity u' and increasing integral scale l. In addition, a turbulent hydrogen flame, with a Reynolds number of 11200 is considered.
The methane flames nominally belong to the thin reaction layer regime and display a flamelet-like behaviour characterized by reaction rates in progress-variable space matching the one-dimensional unstretched laminar flame [1]. However, for increasingly large integral scales, i.e., large Reynolds numbers, the reaction layer is increasingly thickened, even if the Karlovitz number is kept constant [2,3]. The combination of unperturbed reaction rates and inner layer thickening enhances the turbulent flame speed S_T, in addition to the increase due to the larger flame surface area at larger integral scales. Overall, S_T increases exponentially with the integral scale for l up to about 6 laminar flame thicknesses, while the scaling becomes a power-law for larger values of l; in addition, the ratio of turbulent flame speed to area attains a power-law scaling $l^{0.2}$. To understand the effect of flame on turbulence, the evolution of the characteristic scales of turbulence across the flame is investigated. It is found that the decay of turbulence in the flame brush happens differently for increasing integral scale and Reynolds numbers. In particular, the decrease of the Reynolds number across the flame, or equivalently the ratio between the integral and the Kolmogorov scales, is mostly related to an increase of the Kolmogorov scale at low Reynolds number, while it is linked mostly to a decrease of the integral scale for high Reynolds number.
The hydrogen flame included in the analysis is strongly affected by thermo-diffusive instabilities, linked to the non-unity Lewis number of hydrogen, which cause local flame extinction, temperature overshoots in the burned gas, and an enhanced S_T. The increase of S_T in turbulent flames due to thermo-diffusive effects is larger than that observed in laminar unstable flames [4], suggesting a synergistic coupling of turbulence and thermo-diffusive instabilities, in contrast with the idea that turbulence might mitigate intrinsic combustion instabilities.

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[4] Berger, Kleinheinz, Attili, Pitsch. Proc Comb Inst, 37, 2019

Code(s) used: NGA/CIAO

Time usage on ARCHER (approx. kAU): NA

Billy McGregor

Portfolio Manager *in the e-Infrastructure theme at EPSRC*

Responsibilities include: ExCALIBUR programme/ Tier-2 services/ HEC Consortia/ ARCHER2 calls including Access to HPC, Pioneers and DECI.

Presenting on ExCALIBUR: a jointly funded programme led by the Met Office, UKAEA and UK Research and Innovation to deliver research and innovative algorithmic development to harness the power of exascale HPC.

Presenting on the current landscape of UK funded exascale software projects, the progress of the ExCALIBUR programme to date and the future opportunities that will become available to the UKCTRF communities. If there are any questions before or after the presentation or anyone would like to discuss further the current or future opportunities of the ExCALIBUR programme, please feel free to email Billy.mcgregor@epsrc.ukri.org.

Large-eddy simulation of under-expanded cryogenic hydrogen jet flames

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Abstract

In this work, a large-scale large eddy simulations is carried out to compute the ignited turbulent hydrogen jet released from a high-pressure reservoir with cryogenic temperature. The simulation is conducted using rhoReactingFOAM, which is a compressible reacting flow solver with the frame of open-source computational fluid dynamics (CFD) code OpenFOAM. One-equation eddy-viscosity subgrid scale (SGS) model [1] is applied for modelling the SGS stress tensor. Combustion is treated by the Eddy Dissipation Concept (EDC) model [2] with detailed hydrogen-air chemistry[3].

For the hydrogen jet, the total pressure is 200 bar and the total temperature is 80 K. The effects of spatial locations of the hot spots for ignition are considered. The development of the transient flame kernel from the ignition spots is analysed. The resulting combustion patterns involving either jet flame or turbulent deflagration, due to the complex interactions between turbulence, fuel-air mixing at cryogenic temperature, and chemical reactions, are revealed in this work.

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Code(s) used: rhoReactingFOAM based on OpenFOAM

Time usage on ARCHER (approx. kAU): 8000 kAUs

Study of turbulent precipitation in a T-mixer with DNS and DPB

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2: Dept. of Aeronautics, Imperial College London, U.K.

In this study, a coupled DNS-PBE solver (Tang, et al. 2020) is employed in simulating an unseeded continuous nanoparticle precipitation experiment (Schwarzer & Peukert, 2004) where Barium Sulphate ($BaSO_4$) particles are precipitated from mixing Barium Chloride ($BaCl_2$) and Sulphate acid (H_2SO_4) in a T-mixer. The particle size distribution (PSD) at the exit is compared with the measurements with good agreement (Fig.1). Thanks to the high spatial and temporal resolution of the supersaturation and species concentration fields, detailed kinetics and PSD information are retrieved that allows understanding on turbulent precipitation process through different aspects.

Kinetics intermittency, conditional statistics, correlation maps, time and length scales are studied to investigate the interplay of turbulence and precipitation. In the studied case, both nucleation and growth are highly comparable to the mixing timescales (i.e. Damköhler numbers of both mechanism are close to unity), indicating the process is neither mixing- nor kinetic-controlled. Length scales of nucleation site are also measured and compared with Kolmogorov scale to show the importance of resolving nucleation burst thickness. In particular, the study on the time and length scales lead to modelling implications on micro-mixing models, where the inherent assumptions (e.g. scale separation, timescales, etc.) in some models could lead to incorrectly interpreted rate determining aspects.

In addition, concerning the contribution from nucleation and growth, zones of different rate determining mechanism has been identified. Good matching is found between the dominant mechanism map and supersaturation contour (Fig.2) despite of the reduced correlation with between supersaturation and growth consumption at high supersaturation due to lack of growth site (Fig.3). Since the formation of the PSD is a result of the competing mechanisms, the role of mixing is on determining the distribution of each dominant zone.

References

Schwarzer, Hans-Christoph & Peukert, Wolfgang 2004 Combined experimental/numerical study on the precipitation of nanoparticles.*AIChE Journal* **50** (12), 3234–3247.

Tang, Hin Yan, Rigopoulos, Stelios & Papadakis, George 2020 A methodology for coupling DNS and discretised population balance for modelling turbulent precipitation.*International Journal of Heat and Fluid Flow* **86**, 108689.

Code(s) used: Pantarhei

Time usage on ARCHER (approx. kAU): 8,000

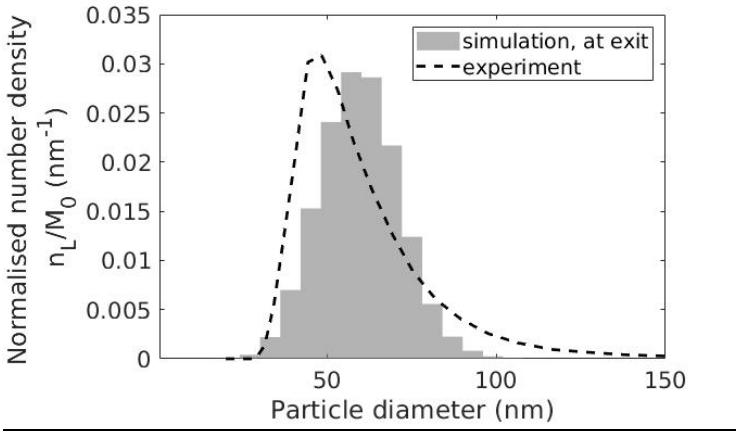

Figure 1 Exit PSD, compared with measurement by Schwarzer & Peukert (2004)

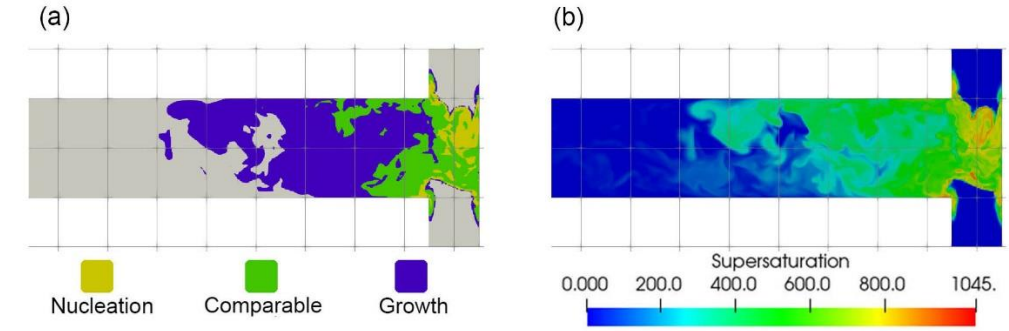

Figure 2 Dominant zone map (a), and its mapping with the supersaturation field (b)

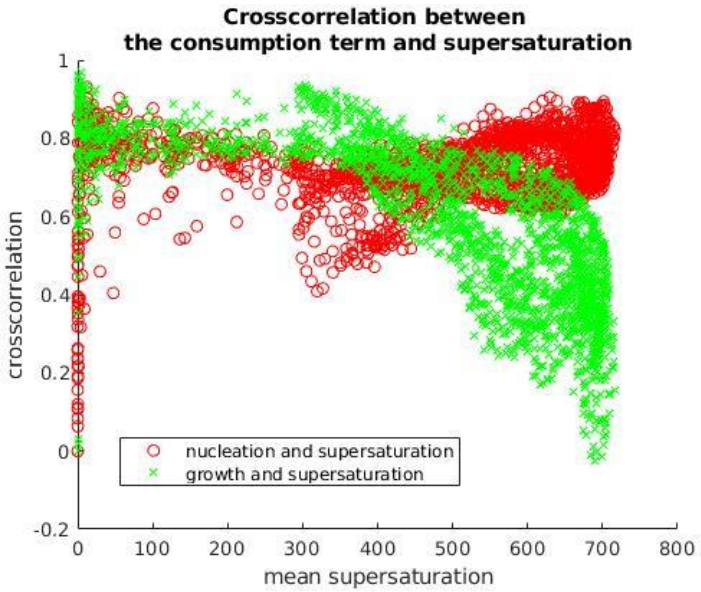

Figure 3 Crosscorrelation between the source terms and supersaturation

Numerical Modelling of Fire Spread on Wood Cribs: Parametric Analysis and Impact on Fire Modes

Xu Dai, Stephen Welch

Edinburgh Fire Research Centre, The University of Edinburgh

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. This 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" shows good promise in representing the evolution of the heat release rate due to fire spread, gas phase temperature, and burn-away, though this modelling strategy is computationally demanding (i.e. 170 hrs running time with 16 processors, 2.8 m diameter × 0.315 m height wood crib).

The results for an extensive sensitivity study for a selected test case (LB7) provide useful insights into the robustness of the model. High sensitivities of the fire spread are shown to: heat of combustion, ignition temperature, heat release rate per unit area (HRRPUA) and soot yield; the effects of changes in thermal inertia and emissivity of the wood are more modest. In terms of design parameters, decreasing the compartment ceiling height, increasing the opening downstand depth and the fuel load densities, all raise the incidental radiant heat flux on the top horizontal surface of the fuel bed, driving more rapid fire spread and ultimately giving rise to fire mode transitions: from an idealised travelling fire, to a growing fire, and even to a fully-developed fire, i.e. flashover. In addition, detailed studies of the effects of crosswinds showed strong impacts above 2-4 m/s, i.e. force 3 winds and upwards.

Despite the observed high sensitivity to uncertain input parameters (and required variation of ignition temperature by 60°C for a different stick arrangement), the calibrated model is of potential value for extending experimental datasets and interpreting phenomena underpinning fire spread. Application of the calibrated model in "scaling up" to full-scale compartment scenarios is of great interest and is currently being explored in simulations on ARCHER2.

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/).

References

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Code(s) used: Fire Dynamics Simulator (FDS), NIST, USA

Time usage on ARCHER (approx. kAU): 10,500kAU 19/20, 7,000kAU current

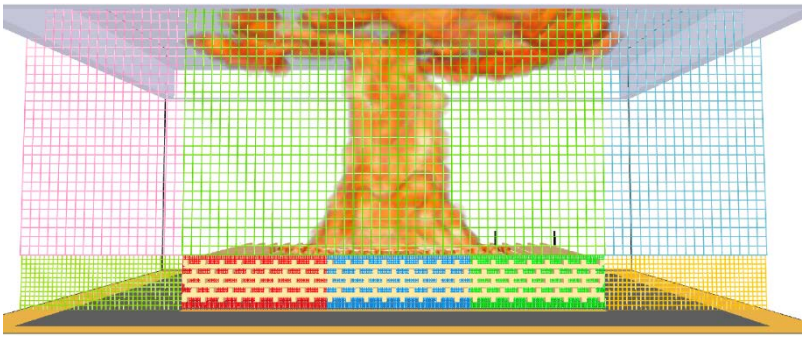

Figure 1. FDS numerical grid for crib fire experiment LB7 [2]: 15 mm × 15 mm × 17.5 mm per cell for wood sticks in the solid phase, 60 mm × 60 mm × 70 mm and 30 mm × 30 mm × 35 mm cell size in the gas phase, total number of cells ~1.3 million.

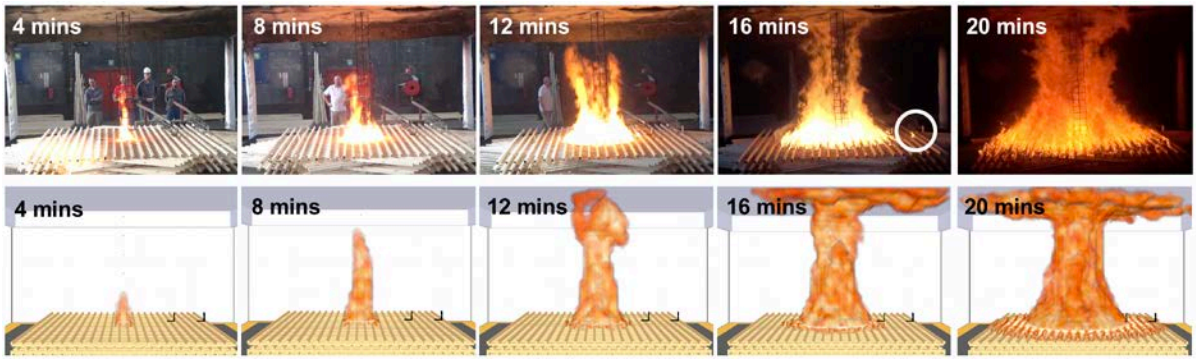

Figure 2. FDS simulated fire spread comparison with LB7 test [2], at 4, 8, 12, 16 & 20 mins.

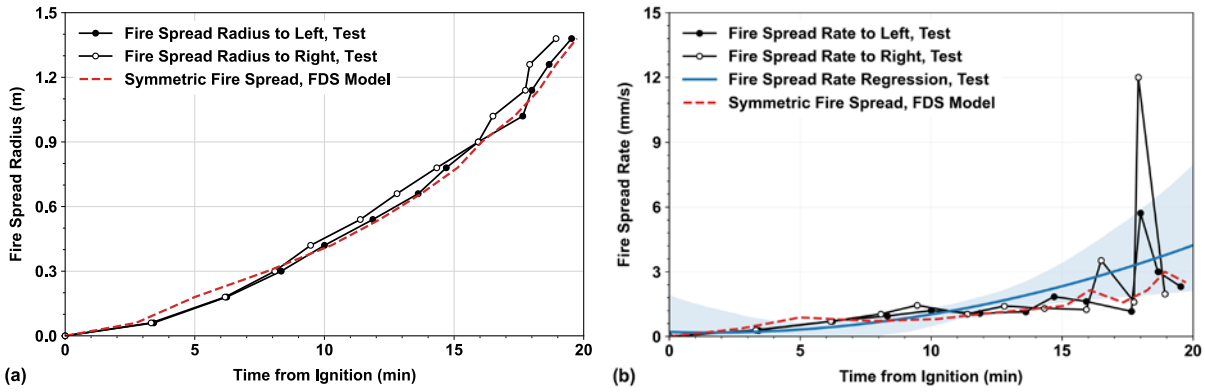

Figure 3. Comparison between LB7 test and FDS model, (a) Fire spread radius from wood crib centre to edge, and (b) Fire spread rate from wood crib centre to edge.

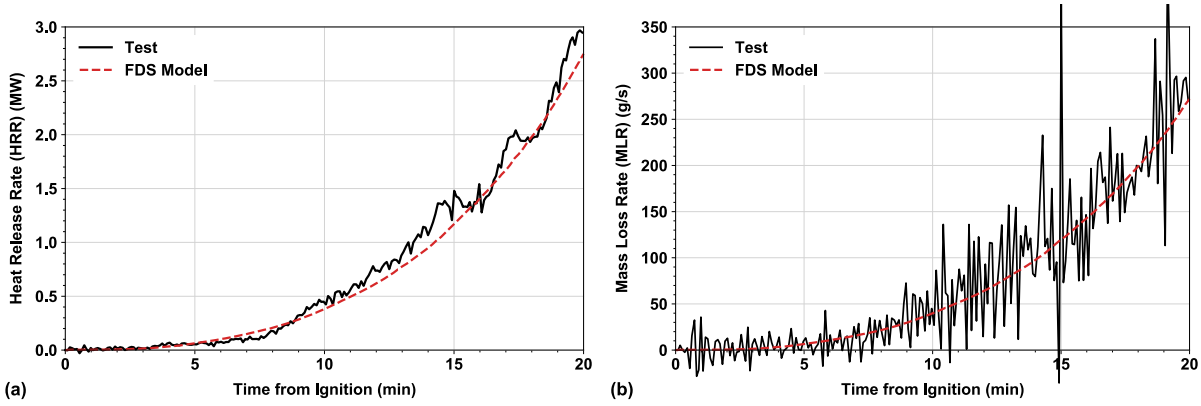

Figure 4. Comparison between LB7 test and FDS model, (a) Heat release rate, and (b) Mass loss rate.

Lean blowoff of swirl kerosene spray flames using LES-CMC

J. M. Foale[1], A. Giusti[2], E. Mastorakos[1]

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[2]*Dept. of Mech. Engineering, Imperial College London*

This work has endeavoured to simulate this first blowoff curve of a heavy hydrocarbon fuel using several points of the experimental Jet-A kerosene blowoff curve from the work of Allison et al. [1]. The objectives are: (i) to analyse the physical phenomena contributing to the blowoff of the flame, such as local extinction and fuel starvation, (ii) to study species behaviour during the blowoff transient and (iii) verify the capability of LES-CMC to predict the blowoff of heavy hydrocarbon spray flames. The flames are modelled at three fuel mass flow rates in a lab-scale swirl bluff body-stabilised burner used previously for experiments and simulations of blowoff using both gaseous [2] and liquid [3-5] fuels. A detailed high-temperature chemical mechanism for kerosene is used, known as HyChem [5]. During the blowoff simulations, local extinctions are identified by regions of low OH and temperature and high fuel and formaldehyde (CH2O) mass fractions. Pyrolysis products like benzene and ethylene are observed to decrease during the transient due to reduced fuel pyrolysis. Fuel starvation in combination with local extinctions cause the flames to blowoff. The simulations capture the blowoff events within 20% of the experimental values, indicating the maturity of the LES-CMC approach in its ability to accurately predict blowoff of heavy hydrocarbon fuel flames.

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Code(s) used: OpenFOAM 2.3.1 with Conditional Moment Closure (CMC) combustion model

Time usage on ARCHER (approx. kAU): 12,000

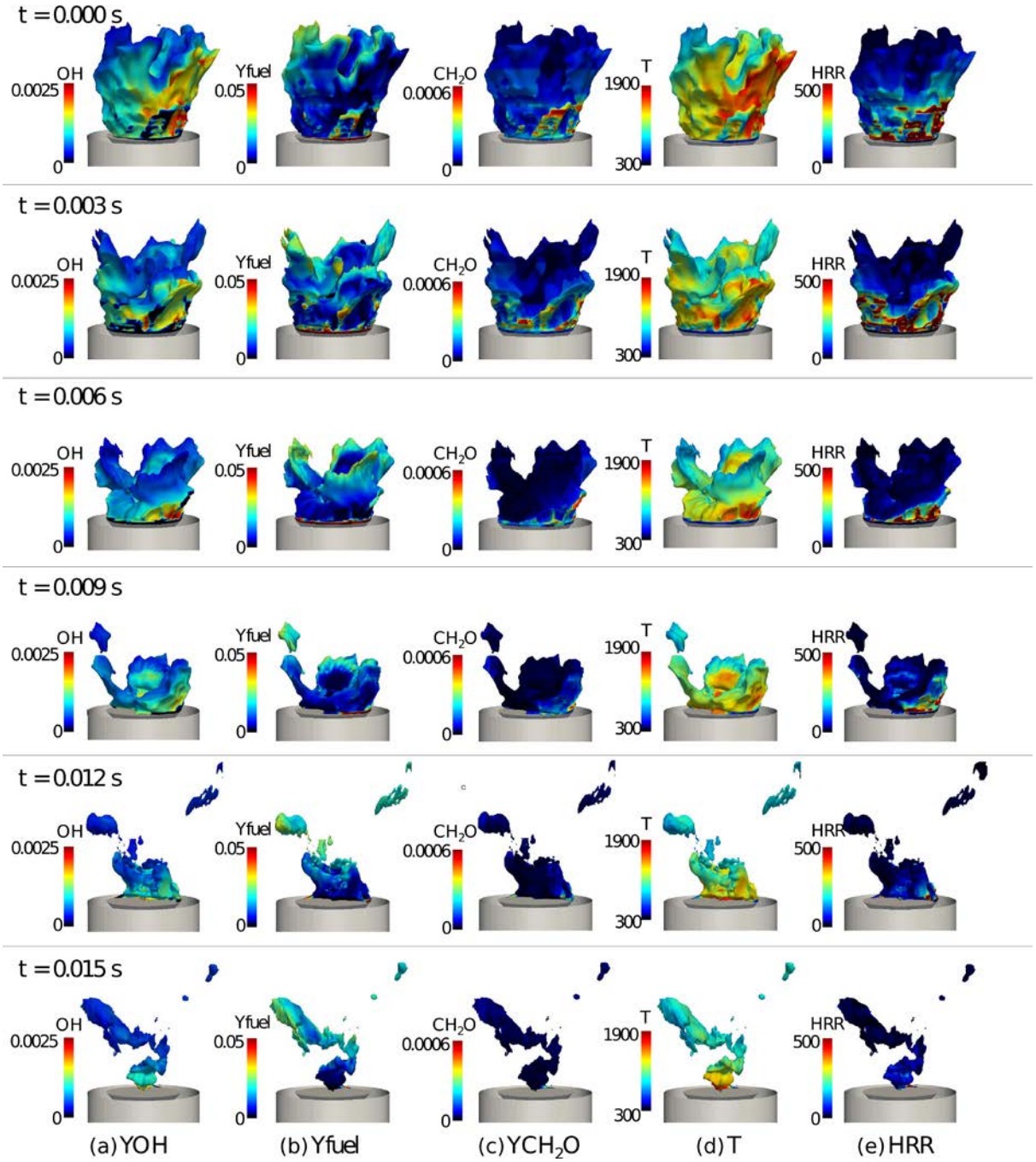

Figure 1: Stoichiometric mixture fraction instantaneous isocontours of (a) OH mass fraction, (b) fuel mass fraction, (c) formaldehyde (CH_2O) mass fraction, (d) temperature (K), and (e) heat release rate (MW/m^3) at six instances during the blowoff event, time increasing from top to bottom.

Investigation of the effects of body forces on flame-turbulence interactions in turbulent premixed combustion

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The presence of body forces such as buoyancy and external pressure gradients are expected to have a strong influence on turbulent premixed flames due to the large changes in density between the unburned and fully burned gases [1,2]. The present work utilises Direct Numerical Simulations (DNS) of three-dimensional statistically planar turbulent premixed flames to study the influence of body forces on evolutions of vorticity, enstrophy, turbulent kinetic energy, turbulent scalar flux and Flame Surface Density (FSD) within the flame brush. The body force and external pressure gradient effects are accounted for by introducing a source term in the momentum conservation equation in the mean direction of flame propagation. Simulations under decaying turbulence have been used to analyse flame-turbulence interaction for different turbulence intensities (u'/S_L = 3.0, 5.0, 7.5 and 10.0 where u' is the root-mean-square velocity fluctuation and S_L is the unstretched laminar burning velocity) under different strengths of normalised body force (g^* = -3.12, -1.56, 0.0, 1.56 and 3.12 where $g^* = 1/Fr^2$ with Fr being a Froude number based on S_L and Zel'dovich flame thickness δ_Z). A positive (negative) value of g^* signifies an unstable (stable) configuration. It is found that for a given set of turbulence parameters, flame wrinkling increases with an increase in body force magnitude in the unstable configuration, which can be substantiated from Fig. 1. This is also reflected in the increased values of normalized turbulent flame speed and flame surface area for an increase in g^*, as can be seen from Fig. 2. The enstrophy has been found to decay significantly from the unburned to the burned gas side of the flame brush for high turbulence intensities, and this trend becomes particularly prominent in the cases with positive g^* values. The magnitudes of the turbulent kinetic energy and its dissipation rate are found to decrease as the magnitude of g^* increases (i.e., from -3.12 to 3.12). Furthermore, high positive values of g^* promote gradient-type transport of scalar flux and this tendency weakens in the stable configuration where the counter-gradient type transport is promoted. The statistical behaviors of the different terms in the transport equations for enstrophy, turbulent kinetic energy, turbulent scalar flux and the FSD and their closures in the context of Reynolds Averaged Navier-Stokes simulations will be analysed in detail. It has been found that the behaviour of the vorticity components is anisotropic within the flame brush which can be attributed to the contribution of the baroclinic torque term. It has also been demonstrated that the effects of body force on the FSD and the terms of its transport equation weakens with increasing turbulence intensity due to the diminishing relative strength of body force in comparison to the inertial force.

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Code(s) used: SENGA+
Time usage on ARCHER (approx. kAU): 6,000 kAU

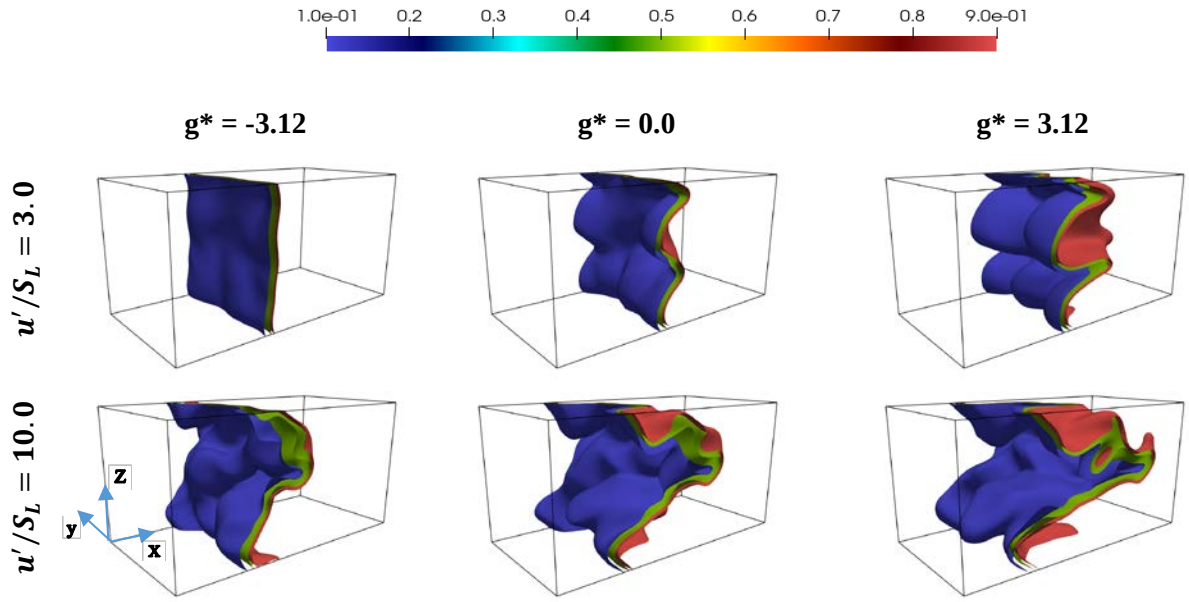

Figure 1. Isosurfaces of reaction progress variable c for g^* = -3.12 (first column), 0.0 (second column) and 3.12 (third column) for u'/S_L = 3.0 (first row) and 10.0 (second row)

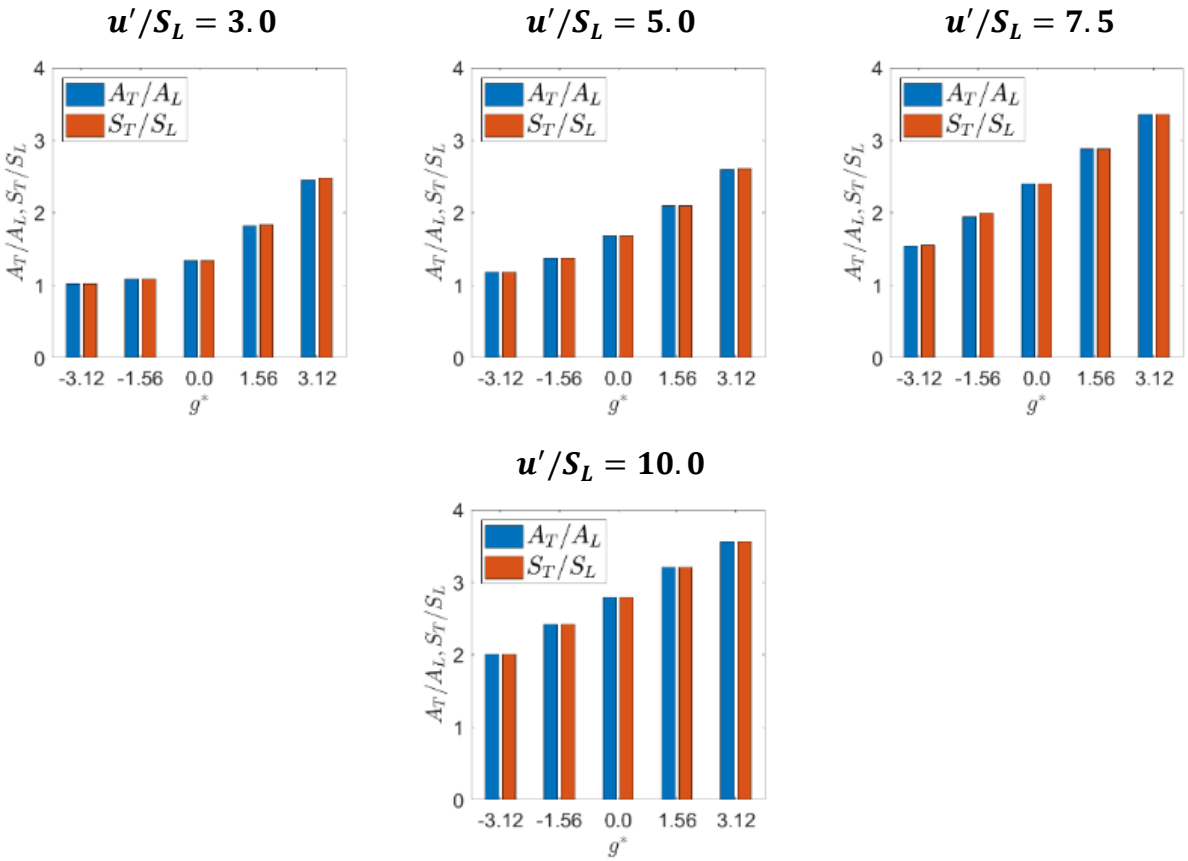

Figure 2. Variations of normalised flame surface area A_T/A_L and turbulent burning velocity S_T/S_L with g^* for all sets of turbulence parameters considered for the study using decaying turbulence approach. The sub-scripts T and L are used for turbulent and laminar conditions, respectively.

A skeletal mechanism for n-heptane MILD combustion

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[b]*Department of Mechanical Engineering, University of California Berkeley, CA 94720, USA*

The Computer Assisted Reduction Mechanism (CARM) approach is employed to develop a skeletal mechanism for n-heptane MILD combustion with an aim to make this mechanism useable in turbulent reacting flow simulations. This mechanism involves 36 species and 205 reactions. The new mechanism is validated for ignition delay times and laminar flame speeds over a range of conditions of interest for MILD combustion using available experimental data and those computed using a comprehensive mechanism. The agreement is observed to be excellent for the skeletal mechanism. The use and performance of the skeletal mechanism for turbulent MILD combustion simulation is also tested and validated by performing Unsteady Reynolds Averaged Navier- Stokes (URANS) simulations with finite-rate chemistry based combustion model. The computed statistics of temperature and OH number density agree quite well with measurements for highly diluted combustion cases.

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Code(s) used: OpenFOAM

Time usage on ARCHER (approx. kAU): 235

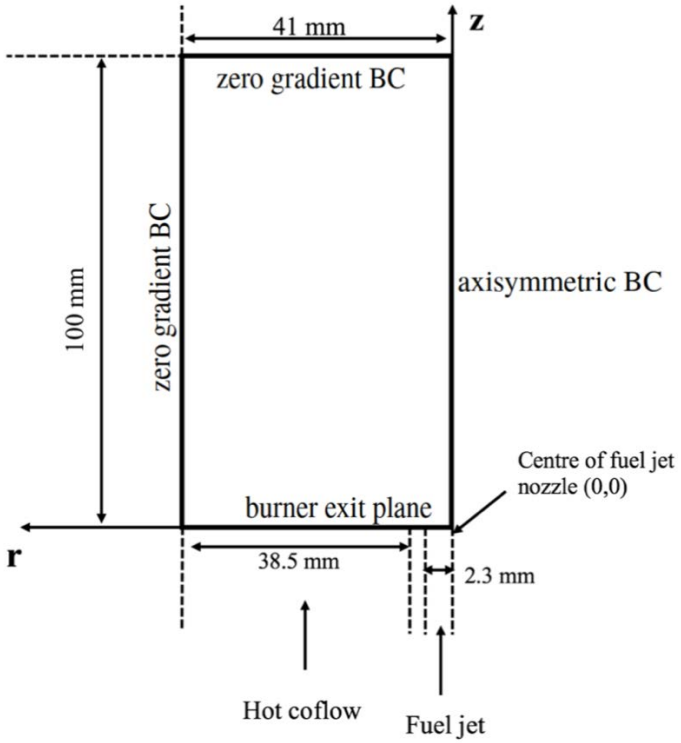

Figure 1:Two-dimensional schematic of the Jet in Hot Coflow burner and the computational domain used along with boundary conditions employed.

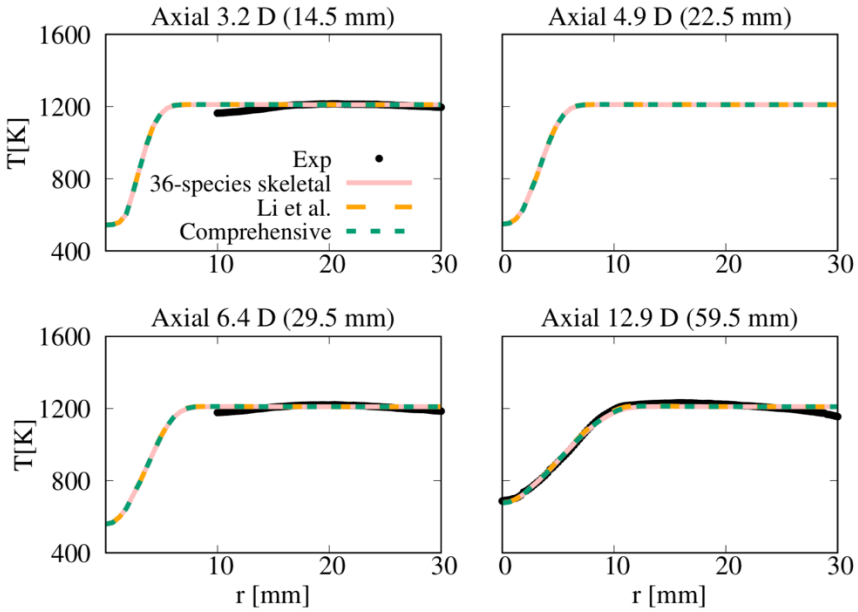

Figure 2: Mean experimental and numerical temperature profiles at four axial locations. Coflow oxygen level of 3 %.

Stratified flame simulations under forced scalar turbulence

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Abstract

In stratified mixture combustion, fuel and oxidiser are in the process of mixing during the combustion process but the variations of equivalence ratio remain within the flammability limit. To study the effects of mixture inhomogeneity on flame dynamics using Direct Numerical Simulations (DNS), it is desirable to sustain the unburned mixture inhomogeneity for a prolonged period of time. However, the presence of a strong turbulent velocity field causes rapid mixing, which makes isolating the effects of mixture inhomogeneity on flame dynamics a challenging task. Similar to turbulent velocity forcing, it is possible to sustain the scalar variance in a turbulent flow field using a scalar forcing methodology. Most efforts of scalar forcing to have taken inspiration from successful velocity forcing schemes by adding a linear forcing term to the conservation equation of the scalar, which is required to be forced. The result is Gaussian scalar PDFs which have no theoretical upper and lower limit. In stratified combustion, the equivalence ratio field can assume a range of different PDFs, and some of them exhibit strict bounds. In a non-reacting configuration, Daniel et al. (2018) demonstrated a forcing term capable of producing a wide range of PDFs, including a bi-modal distribution, which has natural scalar bounds. Thus, it is desirable to have a scalar forcing mechanism which will maintain mixture inhomogeneity in the unburned gas for the whole duration of simulation time enabling the analysis of scalar variance on stratified mixture combustion in isolation.

In this work, the scalar forcing methodology developed by Daniel et al. (2018) has been adapted and implemented into three-dimensional DNS of turbulent stratified flames with an initially bi-modal equivalence ratio distribution in the unburned gas. The newly developed forcing scheme following Daniel et al. (2018) maintains a bimodal distribution with a specified value of scalar variance. The initial root-mean-square of the turbulent velocity fluctuation u' is maintained using physical space Lundgren forcing. The resultant effect yields a turbulent statistically stationary stratified reacting flow field with a specified unburned gas equivalence ratio variance that maintains the effects of mixture inhomogeneity alongside a large sample size for converged statistics. Coloured contours of the fuel mass fraction with reaction progress variable contours overlayed are shown in Fig. 1 for a sample case.

A successfully forced scalar field should share many of the same qualities (e.g. scalar length scale evolution) as an unforced scalar field, and should not interfere with the flow physics. This has been assessed by considering non-reacting simulations in a triply-periodic cube with a bimodal distribution of equivalence ratio with three different initial scalar length scales normalised by the velocity length scale $\ell_\phi/\ell = 0.5, 1.0, 1.5$ both with and without Lundgren forcing. Figure 2 shows the evolution of the PDFs of the equivalence ratio ϕ for the non-reacting, Lundgren forced cases. Moreover, the temporal evolution of the integral scalar length scale is shown in Fig. 3 for different values of ℓ_ϕ/ℓ with Lungren forcing. Figures 2 and 3 show the bi-modal distribution is maintained and the forced scalar integral length scale evolution shows a close resemblance to that of the evolution in the case of the corresponding unforced simulations, until the unforced scalar sharply rises due to complete premixing.

References

Daniel, D., Livescu, D., and Ryu, J. (2018). Reaction analogy based forcing for incompressible scalar turbulence, Physical Review Fluids 3, 094602.

Code(s) used: SENGA+

Time usage on ARCHER (approx. kAU): 10,000 kAU

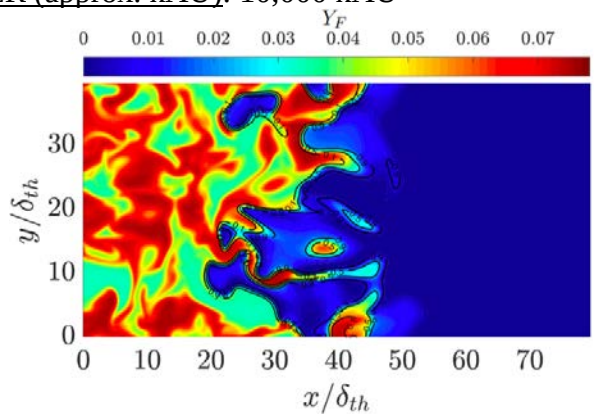
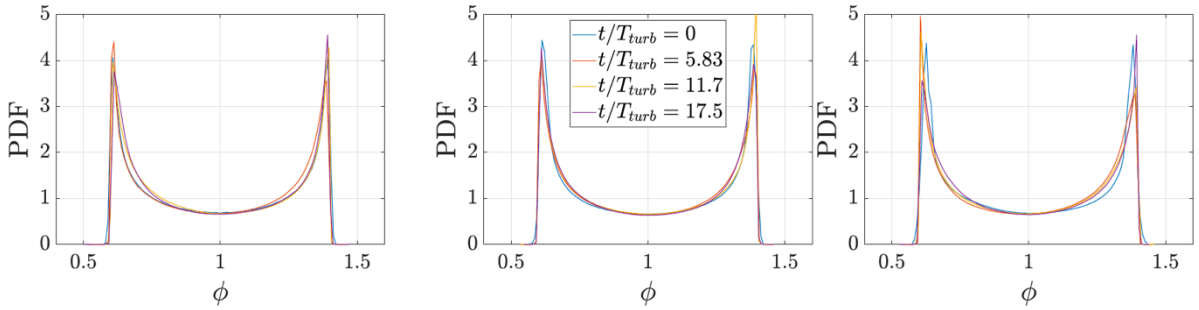
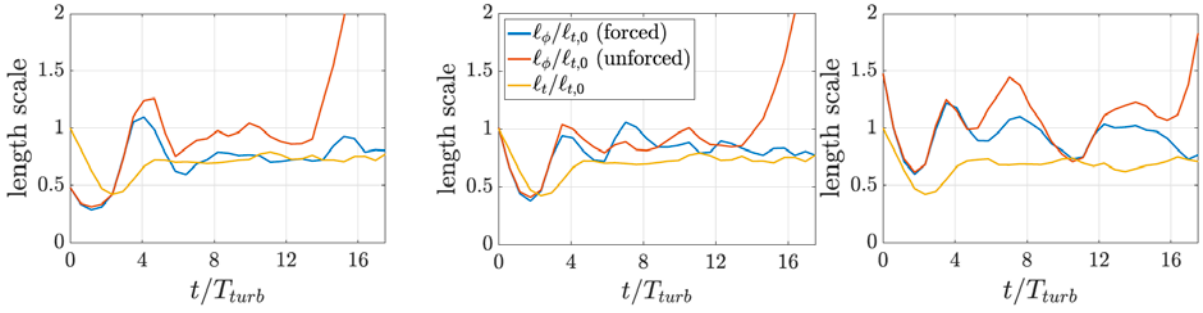


Figure 1: Coloured contours of the fuel mass fraction with contours of the reaction progress variable superimposed for a reacting case with initial $\ell_\phi/\ell = 1.5$. Both the turbulence intensity $u'/S_L = 5.0$ and scalar standard deviation $\phi' = 0.285$ are maintained by Lundgren forcing and scalar forcing respectively.



(a) $\ell_\phi/\ell = 0.50$ (b) $\ell_\phi/\ell = 1.00$ (c) $\ell_\phi/\ell = 1.50$

Figure 2: Evolution of the PDF of the equivalence ratio ϕ for the non-reacting, triply periodic, Lundgren forced cases for different normalised scalar integral scales $\ell_\phi/\ell = 0.5, 1.0, 1.5$. T_{turb} is the eddy turn over time.



(a) $\ell_\phi/\ell = 0.50$ (b) $\ell_\phi/\ell = 1.00$ (c) $\ell_\phi/\ell = 1.50$

Figure 3: Temporal evolution of the normalised turbulence length $\ell_t/\ell_{t,0}$, and the normalised unforced and forced scalar length scale $\ell_\phi/\ell_{t,0}$ for the non-reacting, triply periodic, Lundgren forced cases for $\ell_\phi/\ell = 0.5, 1.0, 1.5$.

Prof J. Barry Greenberg

Emeritus Professor at the Faculty of Aerospace Engineering in the Technion, Israel Institute of Technology

J. Barry Greenberg is an Emeritus Professor at the Faculty of Aerospace Engineering in the Technion, Israel Institute of Technology, Haifa, Israel. He received his PhD in 1974 from the University of Leeds in the field of combustion theory, and joined the Technion in January, 1975. His main fields of interest include spray combustion, reactive flows, fluid mechanics, fire safety and numerical methods. He was a member of the Editorial Board of Combustion and Flame (2001-2006) and the American Institute of Aeronautics and Astronautics Propellants and Combustion Technical Committee (2001-2016), a Co-Chair of the 33rd and 34th International Combustion Symposium Colloquia on “Spray and Droplet Combustion” and is a member of (the British) EPSRC peer-review college since 2006. In addition, he is a Member of the Editorial Board, International Journal of Spray Combustion and Dynamics, since 2012.

Abstract for talk on “Some Recent Results in Water-in-Fuel Emulsion Spray Combustion Theory”

International protocols have set stringent standards governing the restricted emission of damaging pollutants to the atmosphere. One of many ideas under consideration to attempt to meet these standards is the use of water-in-fuel emulsions. Understanding combustion of water-in-fuel emulsion (hereinafter referred to as WIFE) droplets and/or sprays involves considering processes occurring within the droplet and their impact on the immediate vicinity outside the droplet. In fact, it is such processes that are responsible for the benefits that the droplets potentially possess, which may be advantageously exploited under appropriate operating conditions. In particular, the possible occurrence of micro-explosions of WIFE droplets can serve as a source of secondary atomization providing more rapid evaporation, that enables better mixing, resulting in a more uniform mixture of fuel vapor with the oxidizer. The water provides a sufficiently significant heat sink for temperature reduction that, if correctly controlled, lowers the onset of cracking of liquid phase hydrocarbons within the droplet and thereby reduces the formation of particulate matter. In the talk, some recent mathematical analyses of WIFE spray flames will be outlined. Both premixed and diffusion spray flames will be considered. The impact of micro-explosions on (a) the stability of the premixed flames will presented, and (b) the limits of sustainability of diffusion flames will be discussed.

Pulsating flame spread over liquid fuel pool – a numerical study

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Abstract

Fire spread over liquid fuel pool is of great interest to fire safety due to its complicated nature. Although it has been studied nearly for a century, there still exist knowledge gaps, especially for the pulsating behaviour. In this study a fully coupled three dimensional numerical formulation is proposed to numerically study the pulsating behaviour. The fire dynamics of gas phase is directly solved using a compressible solver with a one-step finite rate chemical kinetics and a mixture-averaged diffusion model, and the flow motions of liquid phase are solved using an incompressible solver with variable fluid properties. The solvers are coupled at the phase interface by a conjugate heat transfer model and a diffusion-based evaporation model. The proposed formulation is used to study the pulsating behaviour of fire spread over a laboratory-scale n-propanol pool. The effects of initial pool temperature and pool depth are also investigated. It is revealed that the convective motions and heat transfer along the pool surface play an important role in the pulsating fire spread.

Code(s) used: rhoReactingFOAM based on OpenFOAM
Time usage on ARCHER (approx. kAU): 4000 kAUs

Study of thermoacoustic instabilities in premixed hydrogen-enriched swirling flames using LES

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Large eddy simulations (LES) of premixed hydrogen-enriched swirling flames were performed to investigate the flame topology and combustion instabilities with different hydrogen concentrations. A compressible LES approach is utilised to account for the self-excited combustion dynamics. Non-reflective outlet boundary condition is utilised to minimise flow distortion and numerical reflection at the exit. A transported probability density function (pdf) approach is adopted to account for sub-grid scale (sgs) turbulence-chemistry interaction, and the solution to the joint sgs-pdf evolution equation of the scalars is obtained by the stochastic field method. The flame topology, flow field and acoustic features under different operating conditions are investigated and the effect of hydrogen enrichment on these properties are discussed.

Ignition and kernel to flame transition in a non-premixed biogas-air planar turbulent jet

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Ricardo Ltd., Shoreham Technical Centre, Shoreham-by-Sea, BN43 5FG, UK

Localised forced ignition (spark, laser) of flammable mixture is a topic of fundamental importance in combustion science, from safety standard to the design of efficient and reliable internal combustion engines, but also for the relight of gas turbine at altitude. The ignition of turbulent flammable mixtures is not only influenced by the minimum ignition energy or the critical flame radius, but it also is strongly dependent on the local properties of the energy deposition region and of the overall flow field [1–3].

Furthermore, "biogas" (mixture of CO_2 and CH_4) and has been identified as a carbon neutral fuel [4] and is also widely accepted as a sustainable fuel that can be used either as a complement or a replacement of natural gas in applications such as power generation or within the transport sector [5,6]. However, to date, limited effort has been directed to the understanding of its ignition, and the uncertain combustion behaviours arising from the various amount of methane and CO_2 on the ignition process are yet to be analysed in detail. In particular, the ignition of biogas in inhomogeneous mixtures and in the presence of shear has not been studied.

Building on previous numerical studies of biogas/air ignition [1-3] and on experimental ignition of round methane/air jet measurements [7], Direct Numerical Simulations (DNS) have been carried out to investigate the ignition of a biogas planar jet. A two-step mechanism involving incomplete oxidation of CH_4 to CO and H_2O has been used [2]. This two-step mechanism captures the variation of the unstrained laminar flame speed with equivalence ratio and CO_2 dilution with sufficient accuracy when compared with detailed chemistry results. The study focuses on the three stages of flame evolution, i.e., (i) flame kernel growth, (ii) downstream flame expansion and radial propagation, and (iii) potential upstream flame propagation which relies on edge flame propagation. The flame expansion spans different combustion modes, from premixed to non-premixed in the presence of edge flames.

It will be shown that an increase in CO_2 content may lead to more favourable regions for the flame development closer to the jet nozzle. The different flame development stages reported experimentally have also been observed irrespective of the CO_2 dilution level. The flame structure arising from the kernel growth appears tribrachial in which a triple point propagates along the stoichiometric mixture fraction iso-surface. The stabilisation of the flame was found to primarily rely on the propensity of the triple point to locally propagate faster than the streamwise flow velocity. The CO_2 dilution was also found to increase the flame lift-off length relatively long after the energy deposition has ended by decreasing by reducing the laminar flame speed and the heat release rate.

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[2] C. Turquand d'Auzay, et al., Combust. Sci. Technol. 191 (5-6) (2019) 868–897
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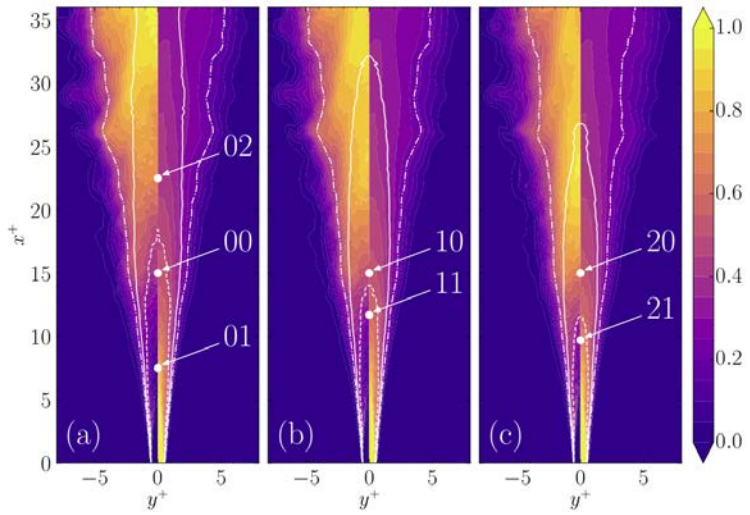

Figure 1: *(left panel)* Flammability factor ($\mathcal{F}$) and *(right panel)* mean mixture fraction ($\tilde{\xi}$) for different biogas compositions (a) $\psi_f = 0.0$, (b) $\psi_f = 0.1$ and (c) $\psi_f = 0.2$ - *(plain line)* $\tilde{\xi}_{\mathrm{st}}$, *(dashed line)* $\tilde{\xi}_r$ and *(dash-dotted line)* $\tilde{\xi}_l$ - The white dot denotes the energy deposition location

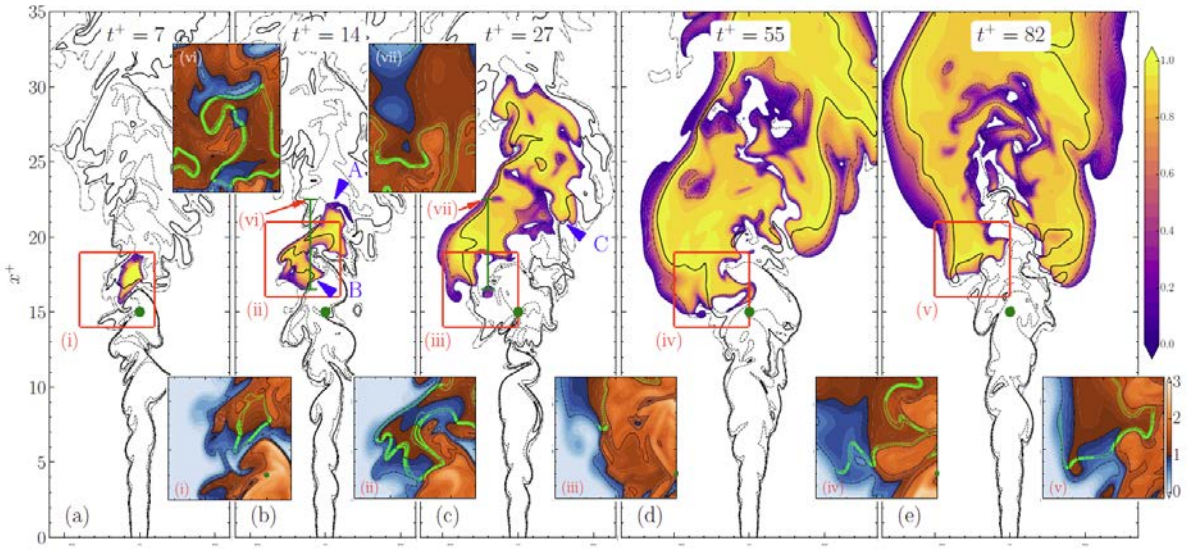

Figure 2: (a)-(e) Time evolution of T in the mid-x^+y^+ plane for case 0*a* overlaid with *(plain line)* ξ_{st}, *(dashed line)* ξ_r and *(dash-dotted line)* ξ_l - The green dots denote the energy deposition - insets (i)-(v) and (vi)-(vii) show the ξ/ξ_{st} field overlaid with *(green lines)* corresponding to 10%, 40% and 70% of $\dot{\omega}^0_{T,\mathrm{max}}$ (CH_4/air stoichiometric adiabatic unstrained laminar flame maximum heat release) in the x^+y^+ and x^+z^+ planes respectively

Numerical Simulation of Flame-Flame Interaction and Thermoacoustic Instability

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Department of Mechanical Engineering, Imperial College London

Thermoacoustic instabilities arise from the coupling between unsteady heat release and pressure oscillations, which can result in a positive feedback loop. In the worst case, such self-amplifying oscillations can result in structural failure of the engine or flashback of the flame.

Annular combustor thermoacoustics are significantly more complex than canonical cases of a single heat source in a cylindrical chamber, that has already been studied extensively [1]. One particular reason is the presence of multiple individual burners that influence neighbouring flames during an acoustic mode. In order to investigate this further, a duel flame burner inspired from recent experiments [2] was simulated using 3D-LES and a modified Artificially Thickened Flame (ATF) model. The simulations captured the distribution of flame curvature reasonably well when compared with experiments.

The different scalar structures and flow topologies were identified using the invariants of the corresponding tensor [3]. Conditioning the flow topologies on scalar structures was then used to probe effects of the flow on the flame. Dilatation was identified as one underlying driving force. The duel flame increased dilatation and was seen to discourage certain flame topologies, leading to a preference of concave scalar structures. The opening of the duel flames also facilitated the survival of focal, compressive topologies within the reaction zone which is not commonly observed in single flames.

Following on from this study is a collaboration with our experimental partners in studying a fully 3D annular combustor with multiple fuel injectors. The combustor is known to exhibit thermoacoustic instability at certain operating points. This work is currently under-way with the use of LES and AMR (Adaptive Mesh Refinement) being employed to maintain computational tractability. The overarching goal is to obtain a DMD (Dynamic Mode Decomposition) analysis during a period of instability.

References

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Code(s) used: CompReal

Time usage on ARCHER (approx. kAU): ~5000KAUs