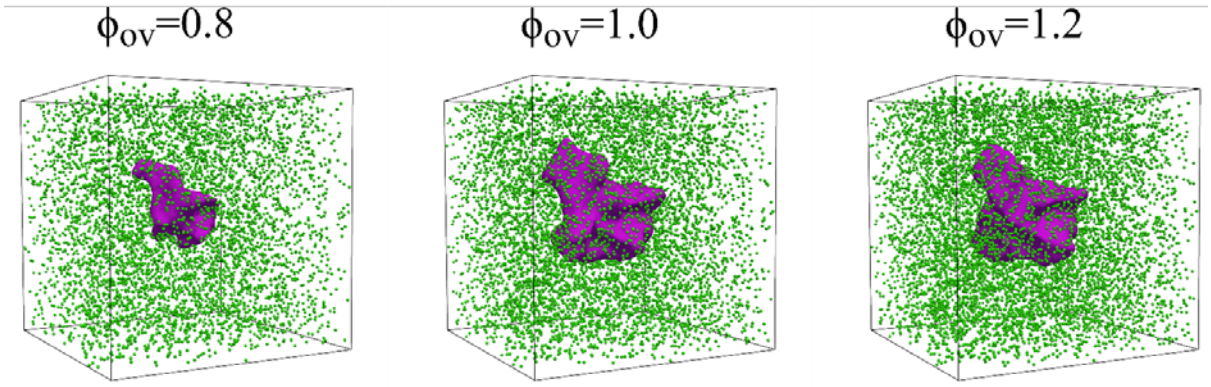
UK CONSORTIUM ON TURBULENT REACTING FLOWS

Abstracts Booklet
UKCTRF Meeting

Zoom

16th September 2020



Molecular dynamics simulation of nucleation in an aluminium-nanoparticles embedded n-decane/ethanol liquid mixture

H.T. Zhang[1,2], J. Xia[2], E. Smith[2], Z.H. Wang[1]

1. *State Key Laboratory of Clean Energy Utilization, Zhejiang University, China*
2. *Department of Mechanical and Aerospace Engineering, Brunel University, UK*

In order to understand nanoparticle effects on nucleation that initiates puffing and microexplosion, nucleation characteristics in a metastable n-decane/ethanol mixture with and without aluminium (Al) nanoparticles have been compared using molecular dynamics (MD) simulations. Firstly, vapor-liquid-equilibrium (VLE) MD results demonstrated that the TraPPE-UA force field is able to properly predict phase transition processes. The mean life time method is used in systems containing 10,000-100,000 molecules at the temperature T = 0.85, 0.9, 0.95T_c (critical temperature) to determine the dependence of nucleation rate J on the pressure and concentration of the binary system with/without nanoparticles. The results of the homogeneous nucleation simulation are compared with the classical nucleation theory (CNT). The effects of the nanoparticle size and concentration on heterogeneous nucleation characteristics are discussed. For cases in which the simulation domain contains only one metal nanoparticle, a density gradient was observed near the particle surface, which results in an increase in the nucleation rate and easier formation of bubbles further away from the particle surface, where the density is lower than that in the homogeneous nucleation case. Due to a larger van der Waals force between Al atoms, the aggregation of Al nanoparticles is observed in cases with multiple nanoparticles in the domain.

A study of turbulent coagulation with discretised population balance and DNS

Malamas Tsagkaridis[1], Stelios Rigopoulos[1], George Papadakis[2]

[1]*Department of Mechanical Engineering, Imperial College London, Exhibition Road, SW7 2AZ, London, UK*
[2]*Department of Aeronautics, Imperial College London, Exhibition Road, SW7 2AZ, London, UK*

Keywords: turbulent coagulation, planar jet, population balance, population balance equation
Contact: m.tsagkaridis18@imperial.ac.uk

Particle formation and growth are key processes in several applications, including soot formation, titania and silica formation, nanopowders, and atmospheric processes and in some of them, coagulation is the dominant mechanism. The aerosol dynamics can be described by the Population Balance Equation (PBE) and here a descretised/sectional method, which is free of a priori assumptions regarding the Particle Size Distribution (PSD), was used to solve the PBE. In most of the cases, particle formation and growth occur in turbulent flows where turbulence affects the aerosol dynamics. Direct numerical simulations (DNS) can be used to gain physical insight into such complex phenomena. The current study aims to study the effect of turbulence on coagulation. Reynolds decomposition of the PBE leads to unknown correlations (unclosed terms) due to the fluctuating terms and unknown correlations are also present when the transport equations of moments are Reynolds decomposed. These terms were calculated via DNS for the first time according to authors knowledge and the significance of those unknown correlations was investigated. DNS of three dimensional spatially developing planar turbulent jet were performed where the jet was laden with monodisperse nanoparticles and issued into a particle-free co-flow stream. The only mechanism that was considered was coagulation in the free molecular regime. Results showed that the unknown correlations were found to be a big percentage of the time averaged coagulation source term so the neglect of these terms can result in an error of 20% on the jet centreline which increases up to 40% close to the jet edges.

Influences of configuration on flame propagation in turbulent droplet-laden mixtures

Gulcan Ozel-Erol[1], Nilanjan Chakraborty[1]

[1]*School of Engineering, Newcastle University, Newcastle-Upon-Tyne, NE17RU, UK*

Turbulent combustion of droplet-laden mixtures is of interest in many engineering applications including automotive engines, gas turbines, and industrial furnaces. Complex interactions between processes such as evaporation, mixing, combustion, and turbulence require a detailed understanding of underlying physics considering the wide range of applications of turbulent combustion of spray. In this study, flame propagation into droplet-laden mixtures has been analysed for two different flame configurations: (i) unsteady spherically expanding flames, and (ii) statistically stationary rod-stabilised V-flames. The effects of flame configuration on the reaction zone structure, mixture composition within the flame, flame surface area and overall burning rate for the aforementioned spray flame configurations have been analysed using three-dimensional DNS with a modified single-step Arrhenius-type chemistry [1] for prescribed values of overall equivalence ratio (i.e. considering fuel in both liquid and gaseous phases) and initially mono-sized droplet diameters. The simulations have been performed for different initially mono-sized droplet diameters a_d (i.e. a_d/δ_{st} =0.04, 0.05 and 0.06 where δ_{st} is the thermal flame thickness of the laminar stoichiometric premixed flame) for an overall equivalence ratio of unity (i.e. $\phi_{ov} = 1.0$). The V-flame is subjected to a moderate level of inlet turbulence (i.e. $u'_{inlet}/S_{b,st} = 2.0$ with $S_{b,st}$ is the unstrained laminar burning velocity of the stoichiometric mixture), with a mean inlet velocity of $u_{mean}/S_{b,st}$ =5.0, whereas spherically expanding flames are considered for different initial turbulence intensities (i.e. $u'/S_{b,st} =$ 4.0 and 8.0) without any mean flow. It has been found that combustion takes place predominantly under fuel-lean mode and the probability of finding fuel-lean burning increases with increasing droplet diameter. This fuel-lean nature of the gaseous phase combustion even for globally stoichiometric (i.e. $\phi_{ov} = 1.0$) spray flames is found to be qualitatively similar for the flame configuration, but in both cases, the reaction zone structure and flame propagation are influenced by the droplet size, turbulence intensity, and number density of liquid droplets [2,3]. The presence of droplets has been found to give rise to dimples on the reaction progress variable isosurface as shown in Fig. 1, but the influences of droplet–induced flame wrinkling on flame curvature distributions in the V-flame configuration weakens in the downstream direction due to a decrease in the frequency of flame-droplet interaction. The mean values of consumption speed are found to decrease with increasing droplet diameter because of the greater likelihood of fuel-lean combustion in large droplet cases. By contrast, the mean density-weighted displacement speed remains comparable for all the droplet sizes for the V-flame configuration. Recent DNS analyses in statistically planar flames [2] and spherically expanding flames [3] under both laminar and weakly turbulent conditions revealed significant differences in flame curvature, density-weighted displacement speed and consumption speed in response to droplet diameter, whereas the effects of droplet diameter are relatively weaker in V-flames than in spherically expanding flames. For the spherically expanding flames with a globally stoichiometric equivalence ratio [3], the mean values of density-weighted displacement speed were found to exhibit a mild increase with the increasing droplet diameter, whereas the mean values of consumption speed showed a decreasing trend with the increasing droplet diameter. The statistically planar and spherically expanding flames interact with droplets at all stages of their propagation into the unburned gas [2,3] but in turbulent V-spray flames, the droplets

evaporate in the mean flow direction. Therefore, the frequency of flame-droplet interaction decreases and the mean value of ϕ_g increases in the downstream direction.

References

1. Ozel-Erol, G., Hasslberger, J., Klein, M., Chakraborty, N., 2020. Int. J. Multiphase Flow, (accepted).
2. Wacks, D., Chakraborty, N., Mastorakos, E., 2016. Flow, Turbul. Combust. 96, 573–607.
3. Ozel Erol, G., Hasslberger, J., Klein, M., Chakraborty, N., 2019. Combust. Sci. Technol.,https://doi.org/10.1080/00102202.2019.1678373.

Code(s) used: SENGA+

Time usage on ARCHER (approx. kAU): 20,000 kAU

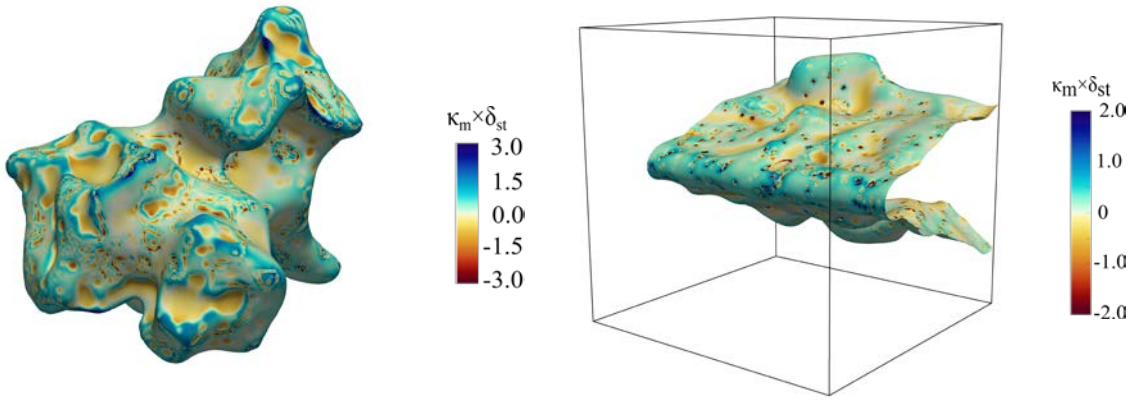


Fig. 1: Instantaneous views of c =0.5 isosurface coloured with normalised curvature $\kappa_m \times \delta_{st}$values for statistically spherically expanding flame with initial $u'/S_{b,st} = 4.0$ and also for the V-shaped spray flames with $u_{mean}/S_{b,st}$ =5.0 and inlet turbulence intensity of $u'_{inlet}/S_{b,st} = 2.0$ for $\phi_{ov} = 1.0$ with initial droplet diameter a_d/δ_{th} =0.06.

Minimum Ignition Energy Transition in Biogas Mixtures, and Droplet-Laden Turbulent Flows

V.S. Papapostolou[1,*], Gulcan Ozel Erol[1] C. Turquand d'Auzay[1,2], N. Chakraborty[1]

[1]School of Engineering, Newcastle University, NE1 7RU, UK
[2]Ricardo Ltd., Shoreham Technical Centre, Shoreham-by-Sea, BN43 5FG, UK

The minimum ignition energy (MIE) requirements for ensuring successful thermal runaway and self-sustained flame propagation have been analysed for forced ignition of (a) homogeneous stoichiometric biogas-air mixtures, and (b) uniformly dispersed mono-sized n-heptane droplet-laden mixtures, using three-dimensional Direct Numerical Simulations (DNS) for both configurations. A wide range of initial turbulence intensities and CO_2 dilutions have been investigated for (a), whilst the effects of droplet diameter, overall (i.e. liquid and gaseous phases) equivalence ratio, and initial turbulence intensity have been investigated for (b). The stochasticity of the ignition event has been analysed by using different realisations of statistically similar turbulent flow fields for the energy inputs corresponding to the MIE and successful outcomes are obtained more than once, justifying the accuracy of the MIE values identified.

The variations of the normalised MIE (MIE normalised by the value for the quiescent laminar condition) with normalised turbulence intensity for both configurations are found to be qualitatively similar to those obtained for the undiluted homogeneous premixed CH_4-air mixture [1-3]. For both configurations, the MIE values increase with increasing rms turbulent velocity, and they increase more steeply beyond a critical turbulence intensity than in the case of smaller turbulence intensities.

For configuration (a) the biogas is represented by a CH_4 + CO_2 mixture and a two-step chemical mechanism has been used. The MIE increases with increasing CO_2 content in the biogas due to the detrimental effect of the CO_2 dilution on the burning and heat release rates and the critical turbulence intensity has been found to decrease with increasing CO_2 dilution. The normalised MIE increases with increasing rms turbulent velocity following a power-law and the power-law exponent has been found not to vary much with the level of CO_2 dilution and is similar to values reported both experimentally [1,2] and computationally [3] for undiluted mixtures.

For configuration (b) the MIE requirement increases with increasing initial droplet diameter and with decreasing overall equivalence ratio [4]. The MIE requirements for droplet-laden mixtures have been found to be greater than the corresponding value for homogeneous mixtures with same nominal values of initial turbulence intensity and equivalence ratio. This behaviour arises due to the deposited energy being partially utilised to supply the latent heat of evaporation and also due to the predominantly fuel-lean composition of the gaseous flammable mixture. This tendency of obtaining fuel-lean mixture strengthens with increasing (decreasing) initial droplet diameter (overall equivalence ratio).

Keywords: Minimum ignition energy, Direct Numerical Simulations, Biogas, turbulence intensity, droplet diameter, overall equivalence ratio

References

1. Shy, S.S., Liu, C.C., Shih, W.: Ignition transition in turbulent premixed combustion. Combust. Flame. 157 (2), 341–350 (2010).
2. Cardin, C., Renou, B., Cabot, G., Boukhalfa, A.M.: Experimental analysis of laser-induced spark ignition of lean turbulent premixed flames: new insight into ignition transition. Combust. Flame. 160 (8), 1414–1427 (2013).
3. Turquand d'Auzay, C., Papapostolou, V., Ahmed, S.F., Chakraborty, N.: On the minimum ignition energy and its transition in the localised forced ignition of turbulent homogeneous mixtures. Combust. Flame.201, 104–117 (2019).
4. Papapostolou, V., Ozel-Erol, G., Turquand d'Auzay, C., Chakraborty, N.: A Numerical Investigation of the Minimum Ignition Energy Requirement for Forced Ignition of Turbulent Droplet-laden Mixtures. Combust. Sc. Technology. (2020).

Code(s) used: SENGA+
Time usage on ARCHER (approx. kAU): 60,000 kAU

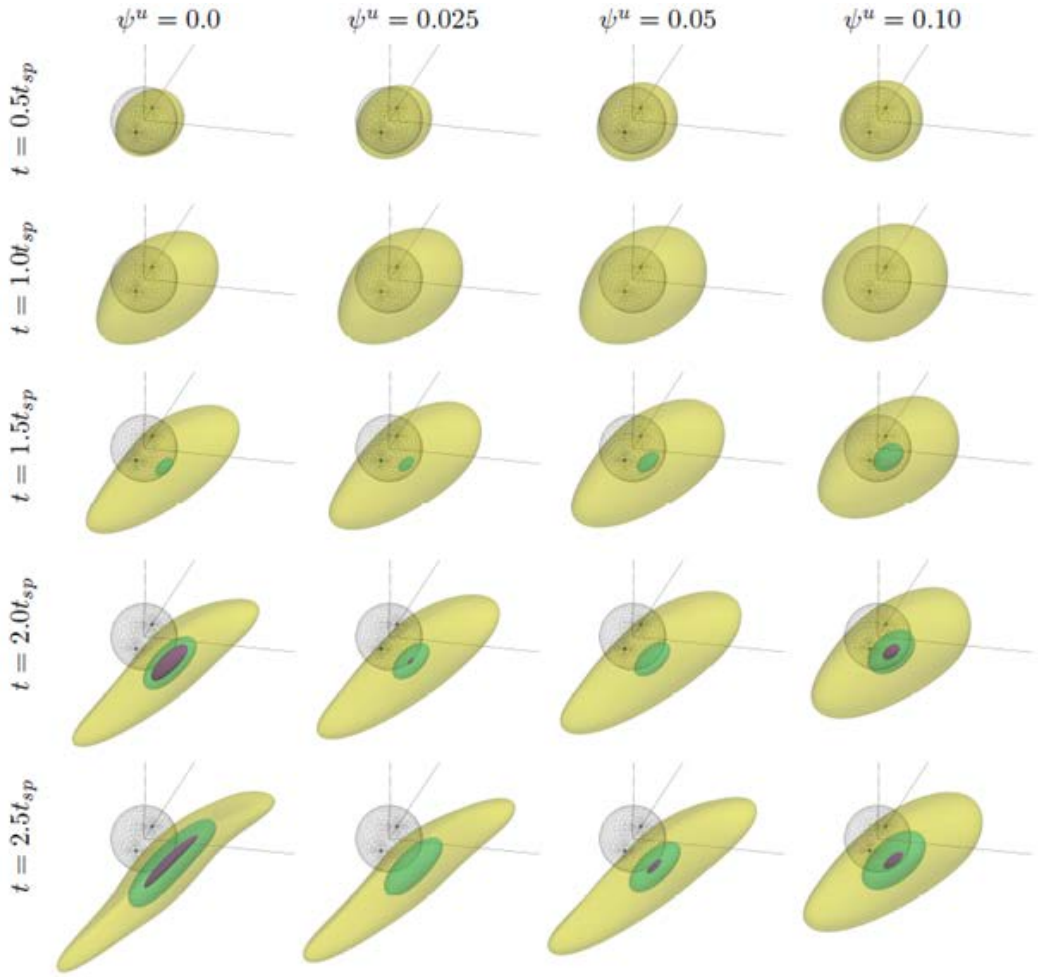


Figure 1. Isosurfaces of normalised temperature, $T_{norm} = \left(\hat{T} - T_0\right)/\left(T_{ad}^{\psi^u} - T_0\right) = 0.1$ (yellow), 0.5 (light green) and 1.0 (purple) with the energy deposition region indicated by the wireframe sphere, obtained for the ignition energy just sufficient for ensuring thermal runaway for $u'/s_l^{\psi^u} \approx 10.50$ at $\psi^u = 0.0, 0.025, 0.05$ and 0.10 (left to right) and for $t/t_{sp} = 0.5, 1.0, 1.5, 2.0$ and 2.5 (top to bottom). The overall simulation time is $t = 10t_{sp}$, where t_{sp} is the time over which energy was deposited by the external ignitor, T_0 is the unburned gas temperature, and ψ^u indicates the mole fraction of CO_2 in the respective homogeneous reactant mixture and $s_l^{\psi^u}$ and $T_{ad}^{\psi^u}$ are the corresponding unstrained laminar burning velocity and adiabatic flame temperature, respectively.

Analysis of hydrogen flame flashback in swirling annular flows

James Bailey, Edward Richardson
University of Southampton

Low emission combustion systems commonly premix fuel and oxidiser upstream of the combustion chamber in a fuel injector or premixer that imparts high levels of swirl into the flow. Avoidance of flashback into the fuel injection is essential for safe and efficient utilisation of hydrogen, a fuel which is prone to flashback. This investigation uses three dimensional direct numerical simulation with detailed chemistry to analyse the mechanisms of flashback in swirling and non-swirling annular channel flows. Swirl produces secondary flow structures that are not present in the axial-flow annular boundary layers and these impact the flame topology and its upstream propagation. The swirl also sets up a radial pressure gradient that tends to promote upstream motion of the flame surface along the inner wall of the annulus. Attempts to model the flashback speed in swirling annular flows will be discussed.

COUPLING DIRECT NUMERICAL SIMULATION WITH POPULATION BALANCE MODELLING FOR PREDICTING TURBULENT PARTICLE PRECIPITATION IN A T-MIXER

H.Y. TANG[1], G. PAPADAKIS[2], S. RIGOPOULOS[1*]

1: Dept. of Mechanical Engineering, Imperial College London, U.K.
2: Dept. of Aeronautics, Imperial College London, U.K.
* Corresponding author: s.rigopoulos@imperial.ac.uk

In this study we develop a methodology for predicting the particle size distribution (PSD) in particulate process, a process used for producing particulate materials, using population balance modelling and direct numerical simulation. This DNS-PBE approach is implemented by coupling two in-house codes, CPMOD (Rigopoulos & Jones, 2003) and Pantarhei (Paul, et al.,2017). It can be applied to any particulate process as long as the kinetics is known. To demonstrate the applicability, it is employed in simulating an unseeded continuous nanoparticle precipitation experiment (Schwarzer & Peukert, 2004). Barium Sulphate ($BaSO_4$) particles are precipitated from mixing Barium Chloride ($BaCl_2$) and Sulphate acid (H_2SO_4) in a T-mixer. The setup is illustrated in Figure 1.

The flow field and the transport of scalar quantities including the species concentration and PSD are calculated with DNS. Population balance source term due to the contribution of precipitation mechanisms are added as source terms. A method of computing the reaction source term is proposed to ensure consistency with the population balance source term. The model for the precipitation kinetics was taken from literature (Mersmann, 2001).

Thanks to the high spatial and temporal resolution of the supersaturation and species concentration fields, the local kinetics has been successfully captured with the coupled solver. In the context of turbulent precipitation in a T-mixer, it is found that the proportion of consumption in each precipitation mechanism depends on the mixing intensity. Most particle formation occurs in the impingement zone at spots with high supersaturation whereas the mixing channel even out the spatial differences. This leads to different locally dominating mechanism in the reactor. Due to the local effects, four particle formation states and their characteristics on the PSD in the formation zone are identified. Figure 2 illustrates the resultant PSD obtained at the outlet and the result agree with measurements.

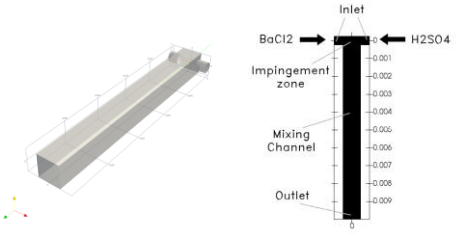


Figure 1. Illustration of the T-mixer

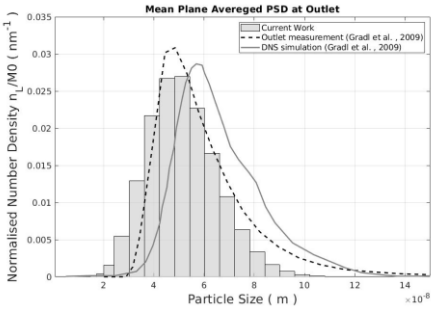


Figure 2. Plane averaged PSD at the outlet, comparing with measurements

REFERENCES

Mersmannm, A., 2001. Crystallization Technology Handbook. 2 ed. New York: Marcel Dekker.

Paul, I., Papadakis, G. & Vassilicos, J., 2017. Genesis and evolution of velocity gradients in near-field spatially developing turbulence. *Journal of Fluid Mechanics*, Volume 815, pp. 295-332

Rigopoulos, S. & Jones, A., 2003. Finite-element scheme for solution of the dynamic population balance equation. *AlChE J.,* 49(5), pp. 1127-1139.

Schwarzer, H. & Peukert, W., 2004. Combined experimental / numerical study on the precipitation of nanoparticles. *AIChE J.*, Volume 50, pp. 3234-3247.

ACKONWLEDGEMENT

This work used the ARCHER UK National Supercomputer Service (http://www.archer.ac.uk) and was supported by the UK Consortium on Turbulent Reacting Flows [EP/K026801/1].

Stratified flame simulations under forced scalar turbulence

Peter Brearley[1], Umair Ahmed[1], Nilanjan Chakraborty[1]
[1]*School of Engineering, Newcastle University, Newcastle upon Tyne, NE17 RU, UK.*

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

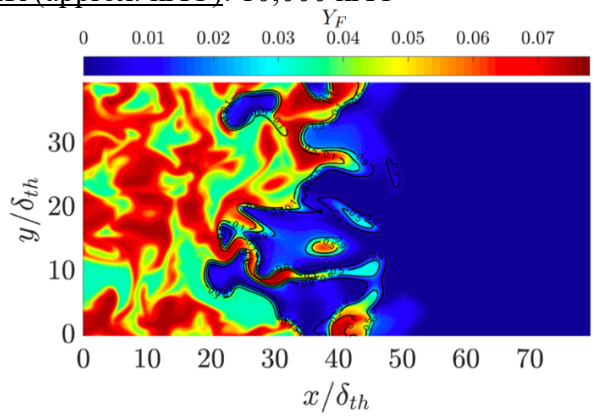
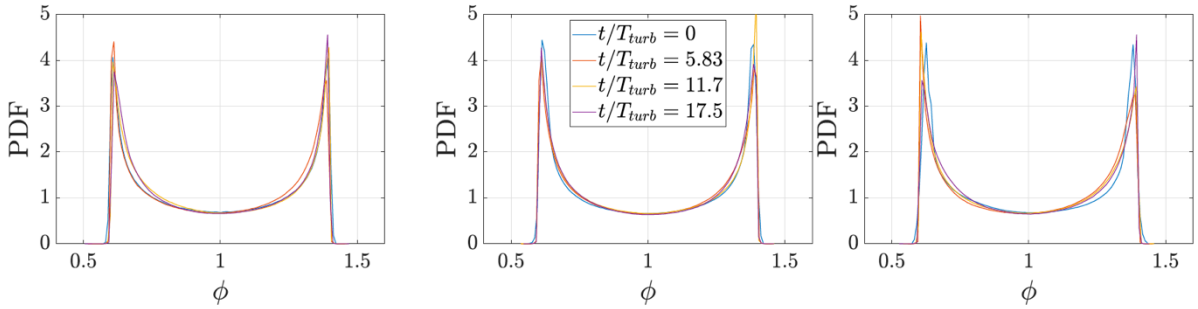
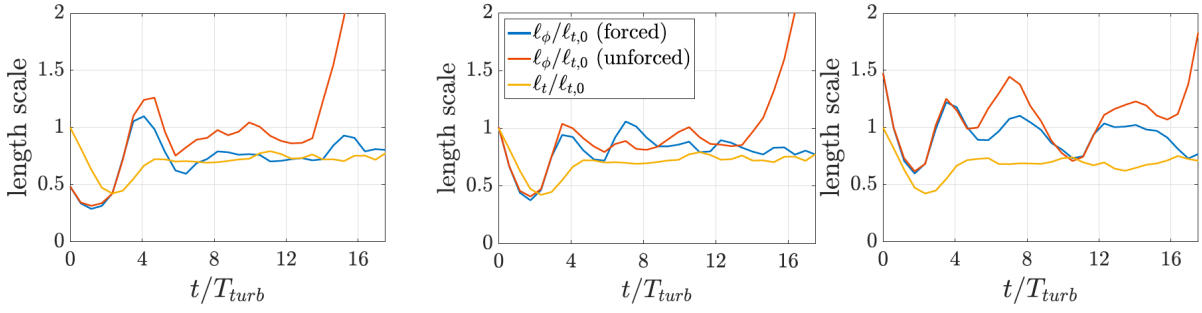


Figure 1: Coloured contours of the fuel mass fraction with contours of the reaction progress variable superimposed for a reacting case with initial $\ell_\phi/\ell = 1.5$. Both the turbulence intensity $u'/S_L = 5.0$ and scalar standard deviation $\phi' = 0.285$ are maintained by Lundgren forcing and 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 $\ell_\phi/\ell = 0.5, 1.0, 1.5$.

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

Arun Ravi Varma[1], Umair Ahmed[1], Nilanjan Chakraborty[1]

[1]*School of Engineering, Newcastle University, Newcastle-Upon-Tyne, NE17RU, UK*

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 flame wrinkling, turbulent scalar flux, Flame Surface Density (FSD) and its evolution 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 $g^* = 1/\sqrt{Fr}$ 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. Furthermore, high positive values of g^* promote gradient-type transport and this tendency weakens in the stable configuration where the counter-gradient type transport is promoted. Even though the wrinkling factor increases with the strengthening of body force in the unstable configuration, the decrease in the resolved FSD supersedes this and causes the generalized FSD to decrease. Since the inverse of the maximum resolved FSD is a measure of the turbulent flame brush thickness, a decrease in the resolved FSD indicates a broadening of the flame brush with the strengthening of body force in the unstable configuration. The statistical behaviors of the different terms in the FSD transport equation and their closures in the context of Reynolds Averaged Navier-Stokes simulations have also been analysed in detail. It has 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.

References

1. Chomiak, J., Nisbet, J. R., Combust. Flame, 102, 371-386 (1995).
2. Veynante, D. , Poinsot, T., J. Fluid Mech., vol. 353, pp. 83-114, 1997.

Code(s) used: SENGA+

Time usage on ARCHER (approx. kAU): 6,000 kAU

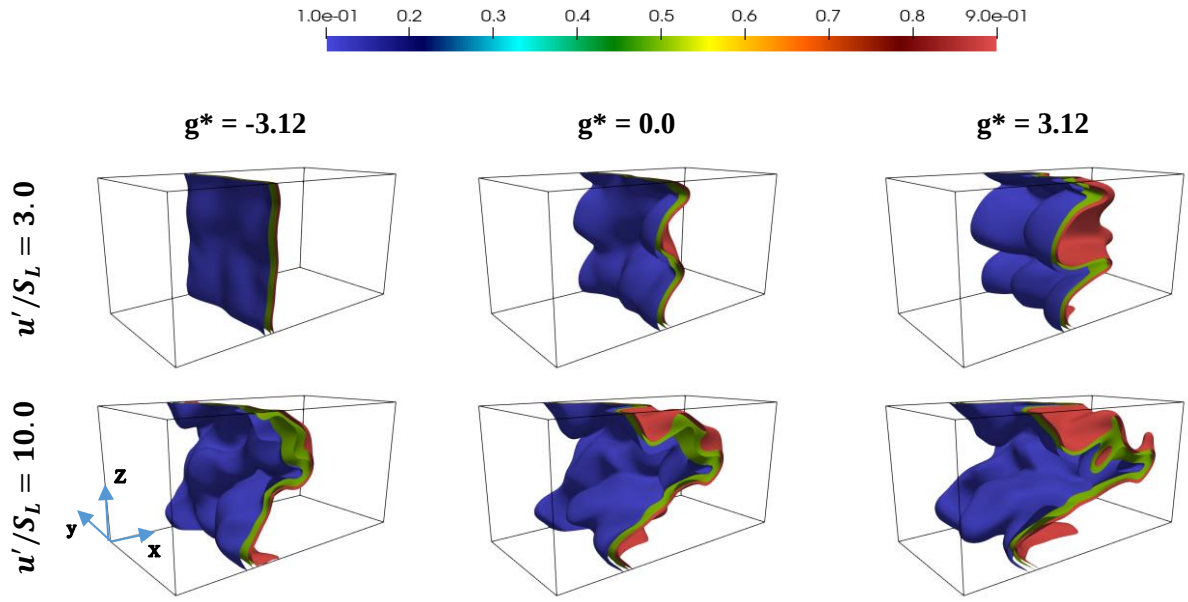


Figure 1. Isosurfaces of reaction progress variable c for g^* = -3.12 (first column), 0.0 (second column) and 3.12 (third column) for u'/S_L = 3.0 (first row) and 10.0 (second row)

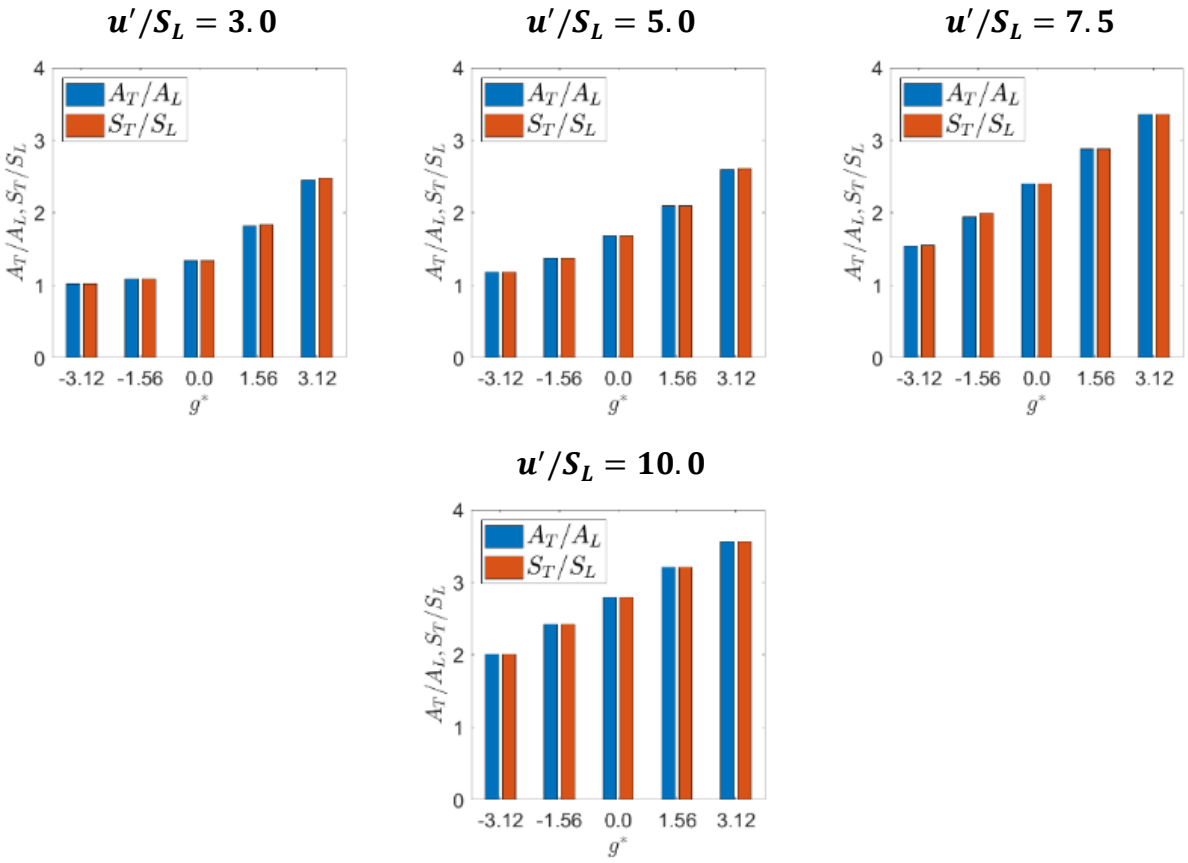


Figure 2. Variations of normalised flame surface area A_T/A_L and turbulent burning velocity S_T/S_L with g^* for all sets of turbulence parameters considered for the study using decaying turbulence approach. The sub-scripts T and L are used for turbulent and laminar conditions, respectively.

Surface properties of soot particles

Kimberly Bowal

Cambridge University

In this work, we employ advanced molecular modelling techniques to provide a detailed numerical evaluation of soot particle surface properties. The temperature-dependent behaviour of surface roughness and number densities of reactive sites are evaluated for particles from 1-5 nm in diameter. The percentage of carbon atoms and zig-zag sites on the particle surface are found to be independent of molecular composition, while molecule heterogeneity influences the accessible hydrogen atoms and free-edge sites. These relationships allow the prediction of surface composition for a given particle diameter. The surface densities of carbon and hydrogen atoms are explained by the morphological changes and molecule size contributions for solid-like and liquid-like configurations. Small molecules contribute significantly to the particle surface properties at low temperatures, regardless of the proportion of molecule sizes. This quantitative evaluation of the accessibility of reactive sites provides important information for understanding soot particle growth and oxidation.

The role of strain and mixture fraction variance in the prediction of local extinctions in LES of partially premixed combustion

Alessandro Soli, Dr Ivan Langella, Dr Zhi X. Chen
Loughborough University, TU Delft, University of Cambridge

The mechanisms behind the onset of extinction holes in stratified jet flames are investigated in this work using LES with unstrained flamelets and presumed PDF modelling. The Sidney/Sandia flame with inhomogeneous inlets is studied for this purpose using both Eulerian and Lagrangian approaches at bulk velocities corresponding to 70% and 90% of the experimental blow-off value. At 70% blow-off rate large eddies aligned with the flame surface are responsible for casting packets of cold, inhomogeneous reactants onto the stoichiometric line, while locally inducing high levels of resolved strain. The mixture inhomogeneity is represented in the LES by the mixture fraction variance and plays a crucial role for the formation of an extinction. At 90% blow-off rate local extinctions are mostly strain-induced and the role of mixture fraction variance is observed to be of minor importance, whose reasons are investigated in the present study.

Simulating the acoustic responses of burners

Jialin Su, Dong Yang, Aimee S. Morgans

Department of Mechanical Engineering, Imperial College London

The acoustic characteristics of burners play a critical role in the combustion stability for combustors. Of particular interest is the acoustically induced hydrodynamic fluctuations downstream of the burner. To gain the first insight into the underlying physics, high-resolution compressible large eddy simulations (LES) were performed for the isothermal air flow of a fictional representative bluff-body burner subject to acoustic perturbations from the upstream side of the burner. The LES results provide the validation for a vortex-sheet based semi-analytical model [1] for prediction of the acoustic properties of axisymmetric bluff-body burners. By resolving more than 80% of the turbulence, the LES data support an in-depth analysis of the periodic unsteady flow field downstream of the burner. In addition, a passive scalar, which can represent, for example, the mixture fraction, was introduced in the simulations such that its transportation in the acoustically perturbed flow field can be examined. For more realistic combustors, we also performed incompressible reacting LES calculations for premixed flames produced with axial-swirl burners.

References

[1] Jialin Su, Dong Yang and Aimee S. Morgans, Modelling of sound-vortex interaction for the flow through an annular aperture, *Journal of Sound and Vibration* (submitted).

Acknowledgements

The authors would like to gratefully acknowledge the Engineering and Physical Sciences Research Council (EPSRC) grant (code EP/P003036/1) CHAMBER (2017–2019) and the ERC Consolidator Grant AFIRMATIVE (2018–2023) for supporting the current research.

Code(s) used: OpenFOAM (version 6.0)

Time usage on ARCHER: approx. 14000 kAUs

Soot emissions prediction in aero-engine combustors using Incompletely Stirred Reactor Network modelling

S. Gkantonas[1], A. Giusti[2] and E. Mastorakos[1]

[1]*Department of Engineering, University of Cambridge, UK* [2]*Department of Mech. Engineering, Imperial College London, UK*

The simulation of soot from swirl flames is a problem of relevance for the development of low-emission combustors for gas turbines. Apart from global quantities related to soot mass, future regulations also call for the control of particle number. Therefore, theoretical models for soot from combustion devices must include various nucleation, growth, and oxidation mechanisms and aerosol physics in order to predict the soot particle number distribu-tion. In this talk, a new approach that simplifies calculations and facilitates parametric analyses with very complex soot models will be introduced. The method is based on Incompletely Stirred Reactor (ISR) theory, which is here extended to a reactor network formulation. An ISR is a volume that is inho-mogeneous in terms of mixture fraction, but conditional averages are homo-geneous. Then a network (ISRN) is deployed to cover the whole combustor and capture separately soot production and oxidation regions, that exhibit different degrees of micromixing and residence times. The ISRN approach is demonstrated on two ethylene lab-scale Rich-Quench-Lean combustors and a kerosene single sector combustor operating at pilot-only mode. It is found that reasonable accuracy in soot emission predictions is produced at a significantly reduced computational cost.