Annual Report for EPSRC High End Computing Consortia

Reporting Period: November 2019 – October 2020

HEC Consortia: UK Consortium on Turbulent Reacting Flows (UKCTRF)

Consortia Chair: Prof. Nilanjan Chakraborty

Allocation and Usage profiles during the reporting period

EPSRC to complete when template has been submitted.

Summary (max. 2 pages):

Background

The current incarnation of UK Consortium on Turbulent Reacting Flows (UKCTRF) was launched on the 8th of January 2019 upon the successful outcome of EP/R029369/1: Addressing Challenges Through Effective Utilisation of High Performance Computing - a case for the UK Consortium on Turbulent Reacting Flows (involving 15 UK institutions, 1 Principal Investigator and 34 Co-Investigators), which was submitted to the Engineering and Physical Sciences Research Council (EPSRC) in response to the High End Computing (HEC) call. The new expanded UK Consortium on Turbulent Reacting Flows will further utilise the developments of High-Performance Computing (HPC) to offer improved fundamental understanding and modelling of turbulent reacting flows, which are pivotal in the effective usage of energy resources, development of reliable fire safety measures, and manipulation of the combustion processes to ensure environmental friendliness. These challenges are multi-faceted and will require collaboration across a wide range of scientific areas. The UKCTRF brings together 43 experts (PI, 6 Co-Investigators, and 36 members) across 19 UK institutions, experienced in using HPC to enable concerted collaborative Computational Fluid Dynamics (CFD)-related fundamental and applied research on turbulent reacting flows to reduce duplication, and tackle challenges grander than individual attempts. Since its inception in 2014, the UKCTRF has achieved significant scientific and industrial impact with over 500 journal and conference papers which utilised ARCHER. The President of the Combustion Institute (PCI), Prof. J.F. Driscoll, has stated in his support letter that the publications of the UKCTRF members are among the best which help develop the minds of young researchers and the support letter from Rolls Royce states that as a result of the UKCTRF significant progress was made in the prediction of combustion phenomena with the help of HPC. During the tenure of the current funding period, the consortium's goals are to: (i) further utilise HPC resources to conduct world-leading turbulent reacting flow research involving Reynolds Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS); (ii) extract fundamental physical insights from simulations to develop high-fidelity modelling methodologies to study turbulent reacting flows relevant to power production, transportation and fire safety engineering; and (iii) ensure a forward-looking software development strategy to develop computationally efficient algorithms, and effectively exploit current and future developments of HPC hardware. The proposed research will build on the foundations of the previous incarnation of UKCTRF (EP/K025163/1, which ran between 2014-2019) and Flagship Software development (EP/P022286/1) grants and will address universal challenges of energy efficiency, sustainability and high-fidelity fire safety. The progress in HPC will enable this new incarnation of UKCTRF to reinforce existing strengths, but also address the following timely intellectual and industry-driven challenges: (i) simulation and modelling of multi-phase reacting flows (e.g. droplet and pulverised coal/biomass combustion); (ii) combustion analysis of biogas and low calorific fuels derived from coal gasification; (iii) flame-wall interaction; and (iv) combustion at elevated pressures, which have only recently become accessible due to the advancement of HPC.

Workshops and New Opportunities

The 2nd annual progress review meeting of the current incarnation of UKCTRF, and the meeting between the management team and the Impact Advisory Panel (IAP) members, was supposed to take place on 16th -17th September 2020 at Daresbury Laboratory. This meeting was postponed because of the pandemic. Although the annual meeting was postponed in 2020 because of the pandemic, we held a virtual meeting based on the research carried out by PhD student users on the 6th of September 2020 (https://www.ukctrf.com/index.php/past-events-2020/). In this event 12 PhD student users delivered 10 minutes-long presentations over Zoom and it was a highly successful event. The management team members of the UKCTRF took this opportunity to meet virtually discussed about the future meetings of the UKCTRF and the travel funding. It was decided the postponed meeting of 2020 will take place on the 30th and 31st of March 2021 in a completely virtual format. One keynote speaker from industry (Dr.E. Shapiro from Ricardo) and another academic of significant international repute (Prof. B. Greenberg from the University of Technion, Israel) have already been invited for keynote lectures (45 min). Every member research group who received computational time allocation in 2019-2020 will be invited to present their work in the online meeting (15 min presentation) but the number of presentations per group will be limited to two due to the time constraint. The Impact Advisory

Panel (IAP) members will be invited to attend this meeting and it is planned that a meeting between the management team members of the UKCTRF and academic and industrial members of IAP regarding the progress of the research activities of this consortium and its future course of action. In order to showcase the diverse range of ongoing research within the consortium, the annual progress review meetings in 2021 (to be held at Brunel University in September 2021 if in person meeting is possible.) and 2022 (to be held at Newcastle University) will be treated as international conferences with workshops on simulation and modelling of turbulent reacting flows.

The biennial International colloquium on dynamics of explosions and reactive systems (ICDERS), the Society of Industrial and Applied Mathematics: Numerical Combustion conference (SIAMNC), and the Mediterranean Combustion Symposium (MCS) are the premier conferences in the field of combustion. Papers presented at these meetings are of the highest quality, and the interactions with peers during the symposium are intellectually stimulating. UKCTRF members in the past have been successful in getting papers accepted for special issues of journals like Combustion Science and Technology, Combustion Theory and Modelling, Flow, Turbulence and Combustion in a very competitive environment, especially as the publications in these journals carry high impact factors. To help members to maximise the impact of disseminating their results, partial funding for attending one of the ICDERS, SIAMNC and MCS conferences has be provided, at a rate of £500-1000 per Research group depending on the conference and its format and location.

The proposal entitled "Collaborative Computational Project on Reacting Turbulent Flows (CCP-ReacT)" from the UKCTRF community in response to EPSRC's Collaborative Computational Project (CCP) Networks call in 2019 was not successful to secure funding. However, many of the challenges of the UKCTRF and UKTC (i.e. UK Turbulence Consortium) are similar, and thus, the consortium chairs of UKTC and UKCTRF are in discussion so that the UKCTRF members can take advantage of the training activities of CCP-Turb and both communities can join forces to take advantages of the funding opportunities of ExCALIBUR programme so that the codes for both communities remain ready to take advantages of Exascale computing.

Issues and Problems

The consortium has now reached a level where the demand for computational time is much greater than the amount awarded to the consortium. Almost 100% of computational time for last three allocation period was utilised, for the latest allocation cycle which started from July 2020, we have received requests for computer time for a total of 350,000kAUs within the application deadline decided by the UKCTRF management team, whereas we only had 241,051 kAUs to allocate. In order to allocate computational time to all applicants, the management team had to award reduced computational time to the applicants, which will adversely affect productivity. Computational time usage will be very closely monitored by the management team of UKCTRF, and if there is no significant usage within a period of two months, then that time will be reallocated to other deserving users. The disruption at the beginning of the year for ARCHER to ARCHER2 transition adversely affected the consortium users. The access to the computational time in Tier-2 facilities for the UKCTRF users was not timely provided. The UKCTRF users got access to ARCHER at the beginning of March 2020 and therefore the users did not have access to ARCHER for sufficiently long period to utilise the full allocation. EPSRC allowed the remaining amount to be rolled over to July-December 2020 allocation period but the disruptions posed by the on-going pandemic, queue time and downtime of ARCHER adversely affected the utilisation of the computational time in the last allocation cycle.

Several countries (e.g., China, Japan, USA, Germany, France, etc.), including those which did not traditionally have a track record of computational research (e.g. China, India, Saudi Arabia), are investing heavily in high-performance computing infrastructure. In this scenario, the investment in ARCHER2 (which is expected place the UK around 15th position in the Top 500 list) is not only timely but also essential for maintaining the UK's world-leading status in turbulent reacting flow research. Furthermore, a vision for exascale computing capability based in the UK in the near future is urgently necessary for the UKCTRF community to remain globally competitive. Our recent input into UKRI's e-Infrastructure roadmap pushed for the UK to establish a clear strategy for exascale computing at the earliest opportunity. It is worth noting that the advancements in computational power will enable reactive flow simulations, which are typical of engineering applications and laboratory-scale experiments. Thus, one-off simulations in short term (or medium term) are expected to be routine in medium term (or long term). Furthermore, it will enable UK researchers to aim for multi-scale multi-physics simulations in the future, which are currently inaccessible because of computational limitations.

Support from CoSeC (0.5FTE) for UKCTRF software development regarding an adaptive mesh refinement based DNS code HAMISH has not been up to the level expected by the developers of this code at the University of Cambridge and Newcastle University. It has been found that the code variant developed at Daresbury Laboratory was not useful for the UKCTRF community, and instead the modules developed at Daresbury Laboratory have been reserved as stand-alone plugins for AMR based codes. These issues have been raised with the line manager of the relevant CoSeC staff member and the developers of HAMISH are meeting regularly with the relevant Daresbury staff members to ensure necessary progress with HAMISH.

Membership (Management team members are indicated by the underlines. There are 4 applications for new membership which are not included in this list. The applicants are invited to present in the next virtual annual meeting in 2021 before the final decision is taken regarding this membership. However, we expect that all these 4 applicants to be inducted as members)

Newcastle University: Prof. N. Chakraborty (Consortium chair and PI), A. Aspden, U. Ahmed; University of Brighton: Dr. K. Vogiatzaki; University of Brunel: Dr. J. Xia; University of Cambridge: Profs. R.S. Cant, E. Mastorakos, M. Kraft, and N. Swaminathan, and Dr. C. Armitage; University of Central Lancashire: Prof. G.M. Makhviladze, Drs. W. Liu, and J. Mai; Cranfield University: Dr. K.W. Jenkins; Daresbury Laboratory: Prof. D. Emerson, Drs. C. Moulinec and X. Gu; University of Edinburgh: Profs.

G. Jomaas, J. Torero, Dr. S. Welch, and D. Hyuk Shin; Imperial College, London: Profs. P. Aleiferis, W.P. Jones, R.P. Lindstedt, Drs. A. Guisti, F. Marquis, A. Morgans, S. Navarro-Martinez, G. Papadakis, S. Rigopoulos, and G. Rein; Liverpool John Moore University: Dr. S. P. Malkeson; Loughborough University: Profs. W. Malalasekara, J. McGuirk, Drs. A Garmory, I. Langella; Northumbria University: M. Jiangi; Queen Mary London: Prof. X. Jiang; University College London: Prof. K.H. Luo; University of Durham: Prof. P. Gaskell; University of Leeds: Prof. D. Bradley and Dr. G. Sharpe; University of Manchester: Dr. R. Prosser; University of Southampton: Drs. E.S. Richardson, K.K.J. Ranga Dinesh; University of Ulster: Profs. M. Delichatsios and V.B. Novozhilov, Dr. J. Zhang; Warwick University: Prof. J.X. Wen

World class and world leading scientific output: *ARCHER should enable high quality and world-leading science to be delivered. This should generate high impact outputs and outcomes that increase the UK's position in world science.*

- If all the publications relating to the work of the Consortium for this reporting period have been added to ResearchFish / will be added to ResearchFish by the end of the ResearchFish reporting exercise, please indicate this below.
- If submission of a full list of publications to the Consortium record/s in ResearchFish has **not** been possible for this reporting period please provide a list of publications that have resulted from work performed on ARCHER by the Consortium during this reporting period (this can be included as a separate attachment).
- For the reporting period please provide a bullet pointed list of key / important research findings that has resulted from work performed on ARCHER by the Consortium. Please reference any related publications.
- For the reporting period please include a bullet pointed list of any relevant press announcements and other communications of significance to an international community.

➢ **Key research outcomes and linked journal publications and book chapters**

Fundamental understanding and modelling of multi-phase combustion using high-fidelity simulations

S.P. Malkeson, U. Ahmed, C. Turquand d'Auzay, A.L. Pillai, N. Chakraborty, R. Kurose, "Displacement speed statistics in an open turbulent jet spray flame", Fuel, 286,1, https://doi.org/10.1016/j.fuel.2020.119242, 2020.

S.P. Malkeson, U. Ahmed, A.L. Pillai, N. Chakraborty, R. Kurose, "Evolution of Surface Density Function in an open turbulent jet spray flame", Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00186-2, 2020.

S.P. Malkeson, D.H. Wacks, N. Chakraborty, "Statistical behaviour and modelling of fuel mass fraction dissipation rate transport in turbulent flame-droplet interaction: A Direct Numerical Simulation study", Flow Turb. Combust., 105, 37–266, 2020.

A.A.S. Mukundan et al., "DNS and LES of primary atomization of turbulent liquid jet injection into a gaseous crossflow environment", Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.08.004.

G. Ozel-Erol, J. Hasslberger, M. Klein, N. Chakraborty, "A Direct Numerical Simulation analysis of turbulent V-shaped flames propagating into droplet-laden mixtures", Int. J. Multiphase Flow, 133, 103455, 2020.

G. Ozel-Erol, N. Chakraborty, "Inertial effects on globally stoichiometric spherically expanding flames propagating in droplet-laden mixtures", Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.218, 2020.

G. Ozel-Erol, U. Ahmed, N. Chakraborty, "Flame self-interactions in globally stoichiometric spherically expanding flames propagating into fuel droplet-mists.", Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.05.025, 2020.

G. Ozel-Erol, J. Hasslberger, N. Chakraborty, "Statistics of two-phase coupling in turbulent spherically expanding flames in mono-sized fuel-droplet mists.", Combust. Sci. Technol., https://doi.org/10.1080/00102202.2020.1769086, 2020.

G. Ozel-Erol, J. Hasslberger, N. Chakraborty, "Surface density function evolution in spherically expanding flames in globally stoichiometric droplet-laden mixtures", Combust. Sci. Technol. https://doi.org/10.1080/00102202.2019.1678373 , 2020.

V. Papapostolou, G. Ozel-Erol, C. Turquand d' Auzay, N. Chakraborty, "A numerical investigation of the minimum ignition energy requirement for forced ignition of turbulent droplet-laden mixtures", Combust. Sci. Technol., https://doi.org/10.1080/00102202.2020.1786376 , 2020.

H. Y. Tang, S. Rigopoulos, G. Papadakis, "A methodology for coupling DNS and discretised population balance for modelling turbulent precipitation", Int. J. Heat Fluid Flow, 86, 108689, 2020.

Fundamental physical understanding and modelling of conventional turbulent premixed, non-premixed and stratified mixture combustion

U. Ahmed, A. Herbert, N. Chakraborty, M. Klein, "On the validity of Damköhler's second hypothesis in statistically planar turbulent premixed flames in the thin reaction zones regime", Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.07.128, 2020.

P. Brearley, U. Ahmed, N. Chakraborty, M. Klein, "Scaling of second-order structure functions in turbulent premixed flames in the flamelet combustion regime", Fluids, 5(2), 89; https://doi.org/10.3390/fluids5020089 , 2020.

P. Brearley, U. Ahmed, N. Chakraborty, “The relation between flame surface area and turbulent burning velocity in statistically planar turbulent stratified flames”, Phys. Fluids, 32, 125111, 2020.
N. Chakraborty, M. Klein, H. G. Im, “A comparison of entrainment velocity and displacement speed statistics in different regimes of turbulent premixed combustion”, Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.241, 2020 .
Z.X. Chen, I. Langella, R. Barlow, N. Swaminathan, “Prediction of local extinctions in piloted jet flames with inhomogeneous inlets using unstrained flamelets.”, Combust. Flame, 212. 415-432, 2020.
Z. X. Chen, N. Swaminathan, “Influence of fuel plenum on thermoacoustic oscillations inside a swirl combustor.”, Fuel, 275, doi: 10.1016/j.fuel.2020.117868, 2020.
Z.X. Chen et al., “Application of machine learning for filtered density function closure in MILD combustion.”, Combust. Flame, 225. 160-179, 2020.
F. Farazi, M. Salamanca, S. Mosbach, J. Akroyd, A. Eibeck, L.K. Aditya, A. Chadzynski, K. Pan, X. Zhou, S. Zhang, M.Q. Lim, and M. Kraft, “Knowledge Graph Approach to Combustion Chemistry and Interoperability”, ACS Omega 5(29), 18342-18348, 2020.
D. Frederich, W.P. Jones, A. Marquis, “Thermo-acoustic Instabilities in the PRECCINSTA combustor investigated using a compressible LES-pdf Approach”, Flow, Turb. Combust., http://dx.doi.org/10.1007/s10494-020-00177-3, 2020.
X. HAN, D. Laera, D. Yang, C. Zhang, J. Wang, X. Hui, Y. Lin, AS Morgans, C-J. Sung, “Flame interactions in a stratified swirl burner: Flame stabilization, combustion instabilities and beating oscillations”, Combust. Flame, 212, 500-509, 2020.
A. Herbert, U. Ahmed, N. Chakraborty, M. Klein, “Applicability of extrapolation relations for curvature and stretch rate dependences of displacement speed for statistically planar turbulent premixed flames”, Combust. Theor. Modell., 24, 1021-1038, 2020.
E. Inanc, N. Chakraborty, A. M. Kempf, “Analysis of mixture stratification effects on unstrained laminar flames”, Combust. Flame, 219,339-348, 2020.
C. Kasten, F.B. Keil, N. Chakraborty, M. Klein, “Statistical Behaviours of turbulent scalar fluxes in high pressure turbulent premixed combustion in the context of Large Eddy Simulations”, Combust. Sci. Technol., 192, 192, 2050-2069, 2020.
F.B. Keil, N. Chakraborty, M. Klein, “Flame Surface Density transport statistics for high pressure turbulent premixed Bunsen Flames in the context of Large Eddy Simulation”, Combust. Sci. Technol., 192:11, 2070-2092, 2020.
F.B. Keil, N. Chakraborty, M. Klein, “Analysis of the closures of sub-grid scale variance of reaction progress variable for turbulent Bunsen burner flames at different pressure levels”, Flow Turb. Combust., 105,869–888, 2020.
F.B. Keil, M. Klein, N. Chakraborty, “Sub-grid reaction progress variable variance closure in turbulent premixed flames”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00121-5 , 2020.
J. C. Massey, Z.X. Chen, N. Swaminathan, “Modelling Heat Loss Effects in the Large Eddy Simulation of a Lean Swirl-Stabilised Flame”, Flow, Turb. Combust. doi: 10.1007/s10494-020-00192-4, 2020.
G. Ozel-Erol, M. Klein, N. Chakraborty, “Lewis Number effects on flame speed statistics in spherical turbulent premixed flames”, Flow, Turb. Combust. , https://doi.org/10.1007/s10494-020-00173-7 , 2020 .
V. Papapostolou, C. Turquand d’Auzay, N. Chakraborty, “A numerical investigation of the effects of fuel composition on the minimum ignition energy for homogeneous biogas-air mixtures”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00229-8, 2020.
V.S. Papapostolou, C. Turquand d’Auzay, N. Chakraborty, “Numerical investigation of the effects of spatial distribution of CO2 dilution on localised forced ignition of stoichiometric biogas-air mixtures”, Joint meeting of the French and the British sections of the Combustion Institute, Lille, France, 5th -6th November, 2020.
R. Rasool, N. Chakraborty, M. Klein, “Algebraic Flame Surface Density modelling of high pressure turbulent premixed Bunsen flames”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00128-y, 2020.
M.P. Sitte, C. Turquand d’Auzay, A. Giusti, E. Mastorakos, N. Chakraborty, “A-priori validation of scalar dissipation rate models for turbulent non-premixed flames”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00218-x , 2020.
G. Tan, U. Ahmed, L. Wang, N. Chakraborty, “Quantification of the flame structure at multi-scale levels”, Phys. Fluids, 32, 125110, 2020.
S. Trivedi, H. Kolla, J. H. Chen, R.S. Cant, “Analysis of flame-flame interactions in premixed hydrocarbon and hydrogen flames”, Phys. Rev. F, 5, 113201, 2020.
C. Turquand d’Auzay, V.S. Papapostolou, N. Chakraborty, “Ignition and kernel to flame transition in a non-premixed CH4/CO2/air planar turbulent jet”, Joint meeting of the French and the British sections of the Combustion Institute, Lille, France, 5th -6th November, 2020.
C. Turquand d’Auzay, V.S. Papapostolou, N. Chakraborty, “Effects of biogas composition on the edge flame propagation in igniting turbulent mixing layers”, Flow Turb. Combust. , https://doi.org/10.1007/s10494-020-00210-5 , 2020.
R. Yu, T. Nillson, G. Brethouwer, N. Chakraborty, A. Lipatnikov, “Assessment of an evolution equation for the displacement speed of a constant-density reactive scalar field”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00120-6, 2020.

Fundamental physical understanding and modelling of novel combustion analysis (e.g. flame-wall interaction, soot, interaction of electric field with combustion and MILD combustion)

U. Ahmed, N. Chakraborty, M. Klein, “Scalar gradient and strain rate statistics in oblique premixed flame-wall interaction within turbulent channel flows”, Flow, Turb. Combust., https://doi.org/10.1007/s10494-020-00169-3, 2020.

U. Ahmed, A. L. Pillai, N. Chakraborty, R. Kurose, “Surface density function evolution and the influence of strain rates during turbulent boundary layer flashback of hydrogen-rich premixed combustion”, Phys. Fluids, 32, 055112, 2020.

J.R. Bailey, E.S. Richardson, “DNS analysis of boundary layer flashback in turbulent flow with wall-normal pressure gradient”, Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.004, 2020.

N.A. K. Doan et al., “Identification of combustion mode under MILD conditions using Chemical Explosive Mode Analysis.”, Proc. Combust. Inst. 38, 10.1016/j.proci.2020.06.293 , 2020.

S. Gkantonas, J. M. Foale, A. Giusti, E. Mastorakos. "Soot Emission Simulations of a Single Sector Model Combustor Using Incompletely Stirred Reactor Network Modelling.", J. Engg. Gas Turbines and Power 142 (10), 101007, 2020.

S. Gkantonas, M. Sirignano, A. Giusti, A. D'Anna, E. Mastorakos. "Comprehensive Soot Particle Size Distribution Modelling of a Model Rich-Quench-Lean Burner." Fuel, https://doi.org/10.1016/j.fuel.2020.117483, 2020.

S. Ivarone et al., “An a priori assessment of the Partially Stirred Reactor (PaSR) model for MILD combustion”, Proc. Combust. Inst., 38, doi:10.1016/j.proci.2020.06.234, 2020.

Z. Li et al., “Study of MILD combustion using LES and advanced analysis tools”, Proc. Combust. Inst., 38, doi: 10.1016/j.proci.2020.06.298, 2020.

X. Z. Jiang and K. H. Luo, “Reactive and electron force field molecular dynamics simulations of electric field assisted ethanol oxidation reactions,” Proc. Combust. Inst. 38 https://doi.org/10.1016/j.proci.2020.06.318, 2020.

I. Konstantinou, U. Ahmed, N. Chakraborty, “Effects of fuel Lewis number on the near-wall dynamics for statistically planar turbulent premixed flames impinging on inert cold walls”, Combust. Sci. Technol., https://doi.org/10.1080/00102202.2020.1799201, 2020.

A. Menon, J.W. Martin, G. Leon, D. Hou, L. Pascazio, X. You, and M. Kraft, “Reactive localized π-radicals on rim-based pentagonal rings: properties and concentration in flames”, Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.07.042 , 2020.

S. Mosbach, A. Menon, F. Farazi, N. Krdzavac, X. Zhou, J. Akroyd, and M. Kraft, “Multi-scale cross-domain thermochemical knowledge-graph”, J. Chemical Info. Modeling, https://doi.org/10.1021/acs.jcim.0c01145,2020.

L. Pascazio, J.W. Martin, K.L. Bowal, J. Akroyd, and M. Kraft, “Exploring the internal structure of soot particles using nanoindentation: A reactive molecular dynamics study”, Combust. Flame 219, 45-56, 2020.

L. Pascazio, J.W. Martin, A. Menon, D. Hou, X. You, and M. Kraft, “Aromatic penta-linked hydrocarbons in soot nanoparticle formation”, Proc. Combut. Inst, https://doi.org/10.1016/j.proci.2020.09.029, 2020.

P. Zhao, L. Wang, N. Chakraborty, “Effects of the cold wall boundary on the flame structure and flame speed in premixed turbulent combustion”, Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.214, 2020.

Simulation and modelling of fire, deflagration to detonation transition

M. Bambauer, J. Hasslberger, N. Chakraborty, M. Klein, “Vortex dynamics and fractal structures in reactive Richtmyer-Meshkov instability”, 13th International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, Braunschweig, Germany, 27th -31st July, 2020.

➢ Relevant grants and awards

- EPSRC research grant EP/S025154/1: Numerical exploration and modelling of novel environmentally friendly combustion technique: droplet-laden MILD combustion (£342,000, PI)
- EPSRC network grant EP/S032134/1: A network for hydrogen-fuelled transportation (Network-H2) (CI)
- EPSRC research grant EP/V003534/1: A combined experimental and numerical investigation of premixed flame-wall interaction in turbulent boundary layers (£776,896, PI)

Greater scientific productivity: *As well as speed increases, the optimisation of codes for the ARCHER machine will enable problems to be solved in less time using fewer compute resources.*

- For the reporting period please provide a brief update on the progress of software development activities associated with the Consortium and the impact this has had on Consortium members and the broader research community.

Generic porting and optimisation of major UKCTRF codes have already taken place for ARCHER. Other general porting of codes will be requested through the ARCHER helpdesk. During the reporting period, the main workhorse of Work Package 1 of

UKCTRF, SENGA2 (already ported on ARCHER) was updated, incorporating new functionality for droplets, coal/biomass particles and highly-detailed chemistry, as well as improvements made to time stepping and boundary conditions. The development of a fully compressible version of one of the major LES codes of this consortium, BOFFIN is now completed, and it has been demonstrated to reproduce the observed frequency and amplitude of self excited thermo-acoustic oscillation in gas turbine combustors.

The proposal on behalf of UKCTRF entitled Adaptive software for high-fidelity simulations of multi-phase turbulent reacting flows, submitted to EPSRC in response to their call on flagship software development in 2016 has come to an end. Prof. N. Chakraborty (Newcastle University) was the PI and Profs. R.S. Cant (Cambridge), D. Emerson (Daresbury Laboratory) and Dr. C. Moulinec (Daresbury Laboratory) were the Co-Is of this project.

This project focussed on the development, validation and documentation of a next-generation fully parallelised computational fluid dynamics (CFD) code called HAMISH, based on adaptive mesh refinement (AMR) which enables high-fidelity Direct Numerical Simulations (DNS) of advanced turbulent reacting flows such as flame-wall interaction, localised ignition, and droplet combustion including atomisation processes.

Such simulations cannot be achieved at present without limiting simplifications due to their prohibitive computational cost. AMR for large-scale highly-parallel simulations of compressible turbulent reacting flows is a significant new functionality, which offers major benefits in terms of computational economy for problems involving thin fluid-mechanical structures, e.g. resolution of both the flame and the boundary layer in flame-wall interaction, droplet surfaces in atomisation in spray combustion, shock waves in localised forced ignition, etc. Such structures have either been ignored or simplified severely in previous work due to the prohibitive computational cost of fixed global meshes, thus limiting the usefulness of the simulations. Hence AMR offers a step-change in capability for the computational analysis of turbulent reacting flows and provides data with the degree of detailed physical information which is not currently available from simulations using existing CFD codes. The software is validated with respect to the results obtained from the well-proven uniform-mesh DNS code SENGA2, which has already been ported to ARCHER and is currently widely used by members of the UK Consortium on Turbulent Reacting Flows. The newly developed code, HAMISH, is not only ported to ARCHER, but also is prepared for architectures supporting accelerators, thanks to OpenMP 4.5, which will support OpenACC, targeting a POWER8 cluster. The information on HAMISH and all the relevant documentation can be obtained from the following URL: http://www.ukctrf.com/index.php/flagship-software/ .

HAMISH was initially developed at Cambridge University as the next generation CFD solver based on adaptive mesh refinement (AMR) using Morton code and Octree algorithms. This technique is very efficient in capturing fine small-scale motions in reactive flows (such as droplets, flame/wall interaction), as it requires much less computing resources than classical methods because it is using dynamic mesh refinement. This code allows for new simulations in areas previously inaccessible due to high computational cost. The specific areas include flame-wall interaction, two-phase flow and droplet combustion, but the development of this code also benefits the wider Combustion community with respect to DNS/LES-based research. During 2019-2020, HAMISH was improved in the following respects:

(a) Simulation of 1-D planar laminar premixed flames to demonstrate the capability of AMR in capturing the sharp gradients within the flame.

(b) 1-D head-on quenching of laminar premixed flames to demonstrate the capability of HAMISH in dealing with reacting flows in the presence of a wall.

(c) 2-D ignition problem, which demonstrates the capability of HAMISH to dynamically refine the mesh based on the position of the ignition front.

(d) Fully-developed laminar channel flow which shows that HAMISH is capable of refining the mesh in the boundary layer next to the wall.

(e) 3-D non-reacting Taylor-Green vortex which demonstrates HAMISH can deal with vortical motion typical of turbulent flows.

(f) 3-D premixed turbulent flame propagation under isotropic homogeneous decaying turbulence so that it can be shown that this code can be used for standard simulations for DNS of turbulent reacting flows in canonical configurations.

There are also plans in place for adding more functionality to the code to support the wider research interests of the community.

Recent research carried out by UKCTRF members has also had a major impact on industry and policy. The development of an improved CFD model by the research group at the University of Warwick has been adopted by the sponsor FM Global and used by their engineers in numerical simulations to reduce the number of large-scale fire tests, which typically cost $50K USD per test. The findings from a recently completed KTP project at Warwick have been adopted in the consulting practices at DNV GL, the world's leading classification society and a recognized advisor for the maritime industry. The outcome has resulted in a £400K increase in the annual sales turnover and is expected to lead to £2M increase in annual sales turnover in three years' time.

UKCTRF members based at Warwick have also started a new EU project (HySEA) with the support of international companies Air Products, Air Liquide, Shell, FIKE and FM Global to conduct research that will result in recommendation to update both the International and European Standards concerning protection of hydrogen energy applications through explosion venting.

Increasing the UK's CSE skills base (including graduate and post doctorate training and support): *This builds on the skills sets of trained people in HPC, both in terms of capacity and raising the overall skill level available to the sector.*

- For the reporting period please provide information on the number of PhDs and Post-Docs that have been trained in the use of ARCHER as a result of work relating to the Consortium.
- For the reporting period please provide a bullet pointed list of training activities undertaken by the Consortium, providing information on the target audience and level of attendance.

Most users of the consortium are Early Career Researchers ((ECRs) i.e. PhD students, Postdoctoral Research Associates). In the 1st Annual Progress Review meeting of the new incarnation of UKCTRF (http://www.ukctrf.com/index.php/upcoming-events-2019/), ECRs gave 11 oral presentations out of 18 oral presentations and about 40 ECRs attended the meeting. In the virtual student users meeting in 2020 (https://www.ukctrf.com/index.php/past-events-2020/), **12** PhD student users delivered 10 minute long presentations over Zoom. This substantiates the high level of involvement of ECRs in the consortium activities. UKCTRF members and their respective institutions have expertise and training facilities of parallel computation (i.e. MPI, OpenMP) and access to the training facilities organised by institutional and Tier-2 facilities. For this reason, no special training on parallel computation is organised by the consortium. However, the training sessions, webinars organised by EPCC for ARCHER users, eCSE calls and the specialised training courses organised by Daresbury Laboratory are publicised to consortium members by the UKCTRF administration. The training options and other facilities (e.g. effective file management and efficient usage of RDF) have been publicised to the consortium users in the Annual Progress Review meeting. The EPCC's consortium contact for ARCHER is also invited to join the Impact Advisory Panel (IAP) and is in close contact with the management team to explore the possibility of having training sessions which might be beneficial for the consortium users. We also used the fund for workshop organisation to award first and second prizes for the best oral presentation and best image/videos to the ECRs based on the feedback of the attendees and Impact Advisory Panel (IAP) members (http://www.ukctrf.com/index.php/upcoming-events-2019/).

The previous incarnations of UKCTRF (i.e. Consortium On Computational Combustion For Engineering Applications (COCCFEA)) had the option for summer schools on computational combustion. Under new regulations of EPSRC, it was not possible to include the summer school in the proposal for UKCTRF. However, both academic experts and industrial members of IAP commented in the kick-off meeting that there is a need for such training activities at regular intervals. It was decided by the management team that the demand for this training will be catered through the EPSRC funded Centre of Doctoral Training Centres (DTCs) based at the University of Leeds and Imperial College, London. Furthermore, the International Combustion Institute arranges training workshops for ECRs every year which also covers the cost of travel and accommodation of PhD students. It has been decided by the UKCTRF Management team that the availability of such facilities will be disseminated more extensively among the consortium members in the future and they will be encouraged to make use of all available opportunities. Most UKCTRF members are also the members of the British Section of the Combustion Institute (BSCI) and BSCI organised a weeklong course on combustion theory and modelling in 2019. Most ECRs associated with UKCTRF members benefit from this course.

The consortium has a strong link to the UK Fluids Network through its Combustion Science and Technology and Droplets and Sprays Special Interests Group, where the PI of the UKCTRF is involved as the co-leader and this link is utilised to broaden the UKCTRF user base, interaction and exchange of ideas with experimentalists, training activities of ECRs and also for the outreach purpose.

Increased impact and collaboration with industry: *ARCHER does not operate in isolation and the 'impact' of ARCHER's science is converted to economic growth through the interfaces with business and industry. In order to capture the impacts, which may be economic, social, environmental, scientific or political, various metrics may be utilised.*

- For the reporting period please provide where possible information on Consortium projects that have been performed in collaboration with industry, this should include:
  - Details of the companies involved.
  - Information on the part ARCHER and the Consortium played.
  - A statement on the impact that the work has / is making.
  - If relevant, details of any in kind or cash contributions that have been associated with this work.
- For the reporting period include a list of Consortium publications that have industrial co-authorship.

- For the reporting period please provide details of the any other activities involving industrial participation e.g. activities involving any Industrial Advisory panels, attendance / participation in workshops and Consortium based activities.

➢ Collaboration with industry as outlined in the original Pathways to Impact for the consortium

The consortium recognises the importance of maximising the impact and dissemination of their work and thus established an IAP to ensure a strong knowledge-exchange activity with industrial partners (Rolls Royce Plc., Siemens Plc., Shell Plc., and Renuda Ltd.), and international academic experts (Dr. W. Meier from Institute of Combustion Technology, DLR, Germany, Prof. D. Roekaerts, Technical University, Delft, Netherlands, and Prof. L. Vervisch, CORIA, Rouen, France). The IAP is currently chaired by Dr. M. Zedda from Rolls Royce Plc., who is actively involved in RANS and LES simulations of turbulent reacting flows in complex engineering configurations for the purpose of designing new generation energy-efficient and environment-friendly industrial combustion devices for automotive and gas turbine applications.

The role of the IAP is to: (i) offer advice on the research activities in the consortium; (ii) support research activities by disseminating information and sharing experimental and computational data from their research group (as appropriate); and (iii) indicate any avenues of research which need immediate attention from the point of view of fundamental understanding and industrial requirements. The IAP provides an impartial assessment of the activities of the consortium. Consortium members and colleagues from relevant industrial sectors (MMI Engineering Ltd., Renuda, Rolls Royce, Shell, Siemens etc.) are invited to present their research findings and exchange ideas with the consortium and advisory panel members in these annual progress review meetings.

The representatives of Renuda Ltd., Rolls Royce Plc Shell Plc., and Siemens Plc. (i.e. Prof. R. Cracknell, Drs. M. Zedda, N. Tonello and S. Sadasivuni) attended the 1st Annual Progress meeting of the consortium and offered their valuable inputs. The industrial colleagues of IAP identified that focused research is needed on explosions modelling, spray and soot modelling, bio-fuel combustion and thermo-acoustic interaction. This industrial view is consistent with the priority areas identified by the consortium. It was felt by industrial colleagues and UKCTRF members alike that it will be useful if the models developed using fundamental insights obtained from DNS data can be implemented in an open-source code such as OpenFOAM or Code Saturne to demonstrate its validity. This will help the assimilation of research outcomes of UKCTRF members into the industrial sector relatively quickly and contribute towards the development of the next generation energy-efficient and environment friendly combustion devices. It is recognised that this exercise will require interactions between various research groups and their concerted efforts and will be a desired outcome at the end of this consortium. This exercise will also help identify those methodologies which will be useful for pre-processing and post-processing of industrial simulations.

➢ Projects that have been performed in collaboration with industry

- Lithium-ion battery safety in transport, storage and utilization, Innovate UK Faraday Challenge, is led by Jaguar Land Rover (JLR), July 2019 ~ February 2021 (£397,398.21 of £5M). The consortium includes 8 other industrial organisations.
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021) – there are 3 industrial partners in the consortium as well as an industrial advisory board.
- Rolls-Royce via the EU (DREAMCODE 970,848€) (ruud.eggels@Rolls-Royce.com): LES study of spray droplet breakup and combustion
- Siemens Industrial Gas Turbines, £190,000 (ghenadie.bulat@siemens.com): This involved an LES study of thermo-acoustic instabilities in Industrial Gas Turbines
- Alstom Switzerland (now GE), £155,000: The development of an advanced computational method for simulating the properties of liquid fuelled spray and non-premixed, partially and perfectly premixed turbulent flames in the context of Large Eddy Simulation. Alstom have also used the method and computer code in a study of the dynamic response of their EV combustor (khawar.syed@ge.com).
- 'Mixing and Crystallisation' Workshop, Imperial College, 2019, organised by consortium members G. Papadakis and S. Rigopoulos. This consortium had significant participation from industry.
- 2 industrial CASE awards at Newcastle University: One with Ricardo, and the other with Reaction Engines. Each company contributing £6.5k/yr.
- Rolls-Royce provided funding for the PhD position at Cambridge University Engineering Department to perform detailed kerosene spray flame simulations for gas turbine and aircraft engine applications
- Rolls-Royce provided funding for the PhD position at Cambridge University Engineering Department to work on the prediction of soot emissions using Conditional Moment Closure methods.

➢ Publications that have industrial co-authorship

- S.P. Malkeson, U. Ahmed, C.T d'Auzay, A.L. Pillai, N. Chakraborty, R. Kurose, Displacement speed statistics in an open turbulent jet spray flame, Fuel 286, 119242, https://doi.org/10.1016/j.fuel.2020.119242, 2020.
- S.P. Malkeson, U. Ahmed, C. Turquand d'Auzay, A.L. Pillai, N. Chakraborty, R. Kurose, "Displacement speed statistics in an open turbulent jet spray flame", Fuel, 286,1, https://doi.org/10.1016/j.fuel.2020.119242, 2020.

- V. Papapostolou, C. Turquand d'Auzay, N. Chakraborty, "A numerical investigation of the effects of fuel composition on the minimum ignition energy for homogeneous biogas-air mixtures", Flow Turb. Combust. https://doi.org/10.1007/s10494-020-00229-8, 2020.
- V.S. Papapostolou, C. Turquand d'Auzay, N. Chakraborty, "Numerical investigation of the effects of spatial distribution of CO2 dilution on localised forced ignition of stoichiometric biogas-air mixtures", Joint meeting of the French and the British sections of the Combustion Institute, Lille, France, 5th -6th November, 2020.
- V. Papapostolou, G. Ozel-Erol, C. Turquand d' Auzay, N. Chakraborty, "A numerical investigation of the minimum ignition energy requirement for forced ignition of turbulent droplet-laden mixtures", Combust. Sci. Technol., https://doi.org/10.1080/00102202.2020.1786376, 2020.
- M.P. Sitte, C. Turquand d'Auzay, A. Giusti, E. Mastorakos, N. Chakraborty, "A-priori validation of scalar dissipation rate models for turbulent non-premixed flames", Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00218-x , 2020
- C. Turquand d'Auzay, V.S. Papapostolou, N. Chakraborty, "Effects of biogas composition on the edge flame propagation in igniting turbulent mixing layers", Flow Turb. Combust. , https://doi.org/10.1007/s10494-020-00210-5 , 2020.
- C. Turquand d'Auzay, N. Chakraborty, "The localised forced ignition and early stages of flame development in a turbulent planar jet", Proc. Combust. Inst. , 38, https://doi.org/10.1016/j.proci.2020.07.148, 2020.
- C. Turquand d'Auzay, V.S. Papapostolou, N. Chakraborty, "Ignition and kernel to flame transition in a non-premixed CH4/CO2/air planar turbulent jet", Joint meeting of the French and the British sections of the Combustion Institute, Lille, France, 5th -6th November, 2020.

Strengthening of UK's international position: *The impacts of ARCHER's science extend beyond national borders and most science is delivered through partnerships on a national or international level.*

- For the reporting period please provide a bullet pointed list of projects that have involved international collaboration. For each example please provide a brief summary of the part that ARCHER and the Consortium have played.
- For the reporting period please provide a list of consortium publications with international co-authorship.
- For the reporting period please detail any other international activities that the Consortium might be involved in (workshops, EU projects etc.).

Projects involved international collaboration

- The EPSRC research grant CHAMBER (2017-20) involves collaboration with NTNU in Norway
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021)
- The EPSRC research grant EP/S025154/1 (2019-2022) involves collaboration with the University of Naples and University of Ghent
- The EPSRC research grant EP/V003534/1 involves collaboration with Kyoto University and University of Darmstadt.

Consortium publications with international co-authors for the reporting period

- U. Ahmed, N. Chakraborty, M. Klein, Scalar Gradient and Strain Rate Statistics in Oblique Premixed Flame–Wall Interaction Within Turbulent Channel Flows, Flow, Turb. Combust., https://doi.org/10.1007/s10494-020-00169-3, 2020.
- U. Ahmed, A.L. Pillai, N. Chakraborty, R. Kurose, Surface density function evolution and the influence of strain rates during turbulent boundary layer flashback of hydrogen-rich premixed combustion, Phys. Fluids 32 (5), 055112, https://doi.org/10.1063/5.0004850, 2020.
- U. Ahmed, A. Herbert, N. Chakraborty, M. Klein, On the validity of Damköhler's second hypothesis in statistically planar turbulent premixed flames in the thin reaction zones regime, Proceedings of the Combustion Institute, https://doi.org/10.1016/j.proci.2020.07.128, 2020.
- M. Bambauer, J. Hasslberger, N. Chakraborty, M. Klein, "Vortex dynamics and fractal structures in reactive Richtmyer-Meshkov instability", 13th International Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, Braunschweig, Germany, 27th -31st July, 2020.
- K.L. Bowal, L. Pascazio, H. Wang, D. Chen, and M. Kraft, "Surface properties of heterogeneous polycyclic aromatic hydrocarbon clusters", Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.123, 2020.
- P. Brearley, U. Ahmed, N. Chakraborty, M. Klein, Scaling of Second-Order Structure Functions in Turbulent Premixed Flames in the Flamelet Combustion Regime, Fluids 5 (2), 89, https://doi.org/10.3390/fluids5020089, 2020.
- N. Chakraborty, M. Klein, H. G. Im, "A comparison of entrainment velocity and displacement speed statistics in different regimes of turbulent premixed combustion", Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.241, 2020 .

• F. Farazi, M. Salamanca, S. Mosbach, J. Akroyd, A. Eibeck, L.K. Aditya, A. Chadzynski, K. Pan, X. Zhou, S. Zhang, M.Q. Lim, and M. Kraft, “Knowledge Graph Approach to Combustion Chemistry and Interoperability”, ACS Omega 5(29), 18342-18348, 2020.
• A. Herbert, U. Ahmed, N. Chakraborty, M. Klein, Applicability of extrapolation relations for curvature and stretch rate dependences of displacement speed for statistically planar turbulent premixed flames, Combustion Theory and Modelling 24 (6), 1021–1038, https://doi.org/10.1080/13647830.2020.1802066, 2020.
• E. Inanc, N. Chakraborty, A. M. Kempf, “Analysis of mixture stratification effects on unstrained laminar flames”, Combust. Flame, 219,339-348, 2020.
• C. Kasten, F.B. Keil, N. Chakraborty, M. Klein, “Statistical Behaviours of turbulent scalar fluxes in high pressure turbulent premixed combustion in the context of Large Eddy Simulations”, Combust. Sci. Technol., 192, 192, 2050-2069, 2020.
• F.B. Keil, N. Chakraborty, M. Klein, “Analysis of the closures of sub-grid scale variance of reaction progress variable for turbulent Bunsen burner flames at different pressure levels”, Flow Turb. Combust., 105, 869–888, 2020.
• F.B. Keil, N. Chakraborty, M. Klein, “Flame Surface Density transport statistics for high pressure turbulent premixed Bunsen Flames in the context of Large Eddy Simulation”, Combust. Sci. Technol., 192:11, 2070-2092, 2020.
• F.B. Keil, M. Klein, N. Chakraborty, “Sub-grid reaction progress variable variance closure in turbulent premixed flames”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00121-5, 2020.
• S.P. Malkeson, U. Ahmed, C.T d'Auzay, A.L. Pillai, N. Chakraborty, R. Kurose, Displacement speed statistics in an open turbulent jet spray flame, Fuel 286, 119242https://doi.org/10.1016/j.fuel.2020.119242, 2020.
• S.P. Malkeson, U. Ahmed, A.L. Pillai, N. Chakraborty, R. Kurose, Evolution of Surface Density Function in an Open Turbulent Jet Spray Flame, Flow, Turbulence and Combustion, https://doi.org/10.1007/s10494-020-00186-2, 2020.
• A. Menon, J.W. Martin, G. Leon, D. Hou, L. Pascazio, X. You, and M. Kraft, “Reactive localized π-radicals on rim-based pentagonal rings: properties and concentration in flames”, Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.07.042 , 2020.
• S. Mosbach, A. Menon, F. Farazi, N. Krdzavac, X. Zhou, J. Akroyd, and M. Kraft, “Multi-scale cross-domain thermochemical knowledge-graph”, J. Chemical Info. Modeling, https://doi.org/10.1021/acs.jcim.0c01145,2020.
• G. Ozel-Erol, J. Hasslberger, M. Klein, N. Chakraborty, “A Direct Numerical Simulation analysis of turbulent V-shaped flames propagating into droplet-laden mixtures”, Int. J. Multiphase Flow, 133, 103455, 2020.
• G. Ozel-Erol, M. Klein, N. Chakraborty, “Lewis Number effects on flame speed statistics in spherical turbulent premixed flames”, Flow, Turb. Combust. , https://doi.org/10.1007/s10494-020-00173-7, 2020 .
• G. Ozel-Erol, J. Hasslberger, N. Chakraborty, “Statistics of two-phase coupling in turbulent spherically expanding flames in mono-sized fuel-droplet mists.”, Combust. Sci. Technol., https://doi.org/10.1080/00102202.2020.1769086, 2020.
• G. Ozel-Erol, J. Hasslberger, N. Chakraborty, “Surface density function evolution in spherically expanding flames in globally stoichiometric droplet-laden mixtures”, Combust. Sci. Technol. https://doi.org/10.1080/00102202.2019.1678373, 2020.
• L. Pascazio, J.W. Martin, A. Menon, D. Hou, X. You, and M. Kraft, “Aromatic penta-linked hydrocarbons in soot nanoparticle formation”, Proc. Combut. Inst, https://doi.org/10.1016/j.proci.2020.09.029, 2020.
• R. Rasool, N. Chakraborty, M. Klein, “Algebraic Flame Surface Density modelling of high pressure turbulent premixed Bunsen flames”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00128-y, 2020.
• M.P. Sitte, C. Turquand d’Auzay, A. Giusti, E. Mastorakos, N. Chakraborty, “A-priori validation of scalar dissipation rate models for turbulent non-premixed flames”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00218-x , 2020.
• G. Tan, U. Ahmed, L. Wang, N. Chakraborty, “Quantification of the flame structure at multi-scale levels”, Phys. Fluids, 32, 125110, 2020.
• S. Trivedi, H. Kolla, J. H. Chen and R. S. Cant: “Analysis of Flame-Flame Interactions in Premixed Hydrocarbon and Hydrogen Flames”, Phys. Rev. Fluids 5, 113201, 2020.
• R. Yu, T. Nillson, G. Brethouwer, N. Chakraborty, A. Lipatnikov, “Assessment of an evolution equation for the displacement speed of a constant-density reactive scalar field”, Flow Turb. Combust., https://doi.org/10.1007/s10494-020-00120-6, 2020.
• P. Zhao, L. Wang, N. Chakraborty, “Effects of the cold wall boundary on the flame structure and flame speed in premixed turbulent combustion”, Proc. Combust. Inst., 38, https://doi.org/10.1016/j.proci.2020.06.214 , 2020.

Involvement in international activities

- Characterisation of pressurised liquid hydrogen (LH2) releases (P-LH2), EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 September 2019 – 30 August 2021).
- Predicting flame acceleration and Deflagration to Detonation Transition in industrial scale explosions incorporating the Turbulence effects (TurbDDT) EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 March 2019 – 30 February 2021).
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021)

- Consortium members are involved in the biennial International Sooting Flame Workshop where simulation results on sooting flames will be presented.
- Knowledge-graph and eco-system of autonomous software agents, integrating chemistry into multi-domain use-cases. ARCHER has been critical in conducting Density Functional Theory (DFT) calculations for species thermodynamic data.
- Investigating various potential mechanisms for soot inception. ARCHER was instrumental for carrying out the required first-principles quantum chemistry and molecular dynamics calculations to shed light on a number of properties of PAHs and their interactions.
- ARCHER and UKCTRF resources have been utilised to perform detailed kerosene spray flame simulations at stable and blowoff conditions and synthetic kerosene chemistries were explored in the same context of a lab-scale burner for jet engine applications, as a part of US-based National Jet Fuels Combustion Program.
- Prediction of soot emissions using advanced turbulent reacting flow modelling and soot models in collaboration with the University of Naples and the group of Prof. A. D'Anna. Part of the simulations on soot modelling was undertaken on Archer. Archer and UKCTRF have provided the hours and HPC equipment to perform investigations on various flames. The following publication was co-authored by international collaborators:
  S. Gkantonas, M. Sirignano, A. Giusti, A. D'Anna, E. Mastorakos. "Comprehensive Soot Particle Size Distribution Modelling of a Model Rich-Quench-Lean Burner." Fuel 270, 2020
- Advanced flame-wall interaction simulations are in the process of being conducted on SuperMuc in collaboration with Prof. M. Klein, University of Bundeswehr, Munich and FUGAKU supercomputer in collaboration with Prof. R. Kurose, Kyoto University.
- Advanced high-fidelity simulations on turbulent stratified mixture combustion are in the process of being conducted on SuperMuc in collaboration with Prof. A. M. Kempf, University of Duisburg.
- A number of consortium members are in collaboration with Dr Isaac Boxx, DLR Stuttgart in a study hydrogen enriched fuels for Industrial Gas Turbines. This is a combined experimental and LES study. The measurements are being conducted in DLR and are funded by the EU.

Invited lectures by consortium members

- Dr. A. Giusti - Lecture at the Summer School on Advanced Research in Turbomachinery (ART), Florence, Italy, 6-10 July 2020.
- Prof. W.P. Jones- Combustion LES and the stochastic fields method APS Division of Fluid Dynamics, November 23–26, 2019 Seattle, Washington
- Prof. W.P. Jones-Large Eddy Simulation: Inert Flows, AECC Research Institute, Zhuzhou, China, April 2013
- Prof. W.P. Jones-LES: Approaches to Combustion, AECC Research Institute, Zhuzhou, China, April 2013
- Prof. W.P. Jones-LES of Particle Laden Flows: Dispersion, Evaporation and Combustion, AECC Research Institute, Zhuzhou, China, April 2013
- Prof. W.P. Jones-Combustion LES, Combustion Institute Summer School, 7-12 July, 2019
- Prof. W.P. Jones-Large Eddy Simulation: Inert Flows. Beihang University, Beijing, November 2018
- Prof. W.P. Jones-LES: Approaches to Combustion. Beihang University, Beijing, November 2018
- Prof. W.P. Jones-LES of Particle Laden Flows: Dispersion, Evaporation and Combustion, Beihang University, Beijing, November 2018
- Prof. W.P. Jones-Probability and the Scalar pdf Evolution Equation, Beihang University, Beijing, November 2018

Scientific committee of international conferences

- Profs. N. Chakraborty and A. Morgans are steering group members of Computational Science Centre for Research Communities (CoSeC).
- Prof. N. Chakraborty is a steering committee member of ExCALIBUR programme.
- Prof. N. Chakraborty recently served as an editor of the Engineering and Material Science chapter for the science case for Exascale computing commissioned by EPSRC.

Editorships

- Prof. N. Chakraborty to co-edit a special issue on high pressure turbulent premixed combustion for the journal entitled Combustion Science and Technology
- Prof. N. Chakraborty co-edited a special issue on numerical modelling of reacting and non-reacting multi-phase flows for the journal Fluids.
- Prof. N. Chakraborty to co-edit a special issue of Energies on Turbulent premixed combustion
- Prof. E. Mastorakos - Associate editor of *Combustion and Flame*, Editorial Board member of *Combustion Theory and Modelling*, and *Flow, Turbulence and Combustion*)

- Prof E. Mastorakos - Guest Editor in Topical Issue "Advances in Turbulence, Heat and Mass Transfer" in *Flow, Turbulence and Combustion*, 2019.

Other Highlights for the Current Reporting Period: Please provide details of any other significant highlights from the reporting period that are not captured elsewhere in the report.

Relevant achievements and impacts

- In 2018-2019 academic year 100+ journal and 120+ conference papers arose from this consortium Altogether 500+ publications over last 5 years and 30% of these publications involve international collaboration.
- The UKCTRF contributed £500 per research group towards the cost of attending the international conferences for those who had accepted papers for oral presentation in 2019 (9 in total) (http://www.ukctrf.com/wp-content/uploads/2019/08/UKCTRF-Conference-Funding.pdf). In 2020, 8 awards have been made for oral presentation of the accepted paper in the 38th International Symposium of Combustion. The award amount varies from £500 to £1000 depending on whether it is a virtual or in-person presentation.
- Prof. W. P. Jones has been awarded the Alfred C. Egerton Gold Medal, which recognizes distinguished, continuing, and encouraging contributions to the field of combustion. It is one of the highest awards of the Combustion Institute, presented biennially during the International Symposium on Combustion.
- Profs. R. Stewart Cant, M. Delichatos and M. Kraft have been elected as Fellows of the Combustion Institute.
- Prof. E. Mastorakos is one of the recipients of the Sugden Award 2020, for best Combustion paper by a section member in 2020.
- Prof. N. Chakraborty was the editor of the Engineering and Materials chapter of Exascale Computing Science case commissioned by EPSRC. This science case will be presented to the HM Treasury. The combustion section of this science case was authored by Profs. N. Chakraborty and D. Emerson, which was commended by international experts who served as reviewers. One reviewer noted:
  1. Combustion simulations: Highest priority – internationally leading
  2. Materials chemistry: High priority – internationally competitive
  3. High powered lasers and quantum electrodynamics: High priority – internationally competitive
  4. Plasma accelerators and light sources: High priority – internationally competitive
  5. Magnetic confinement fusion: High priority – internationally competitive
  6. Mesoscopic simulations of multiphase flows: High priority – internationally competitive
  7. Computational aerodynamics: High priority – internationally competitive
  8. Quantum mechanics-based materials modelling: High priority – internationally competitive
  9. Simulations of turbulent flow: High priority – internationally competitive
  10. Atomic, molecular and optical R-matrix calculations: High priority – internationally competitive

Relevant grants and awards

- S. Gkantonas, A. Giusti and E. Mastorakos were awarded the British Flame best poster award at biennial IOP Early Career Researchers in Combustion for their work on Incompletely Stirred Reactor Network Modelling for Aero-Engine combustors.
- S. Gkantonas earned a visiting research scholar grant at Michigan State University (USA) to work on topology tracking techniques and fuel effects on the flame structure of premixed jet flames.
- S. Gkantonas was awarded a Tizard New Opportunities Fund award by Churchill College for investigating soot emissions from marine engines at the Cambridge Centre for Advanced Research and Education in Singapore. One of our papers that followed up and heavily relied on one of the papers in this report won the Gaydon Prize by the British Section of the Combustion Institute (CI(BS)), for "the most significant UK contribution to the International Symposium on Combustion".
- S. Gkantonas (University of Cambridge) was awarded the British Flame and IOP Combustion Physics Group poster award at the IOP Early Career Researchers Meeting in University of Sheffield (19th Sep): Incompletely Stirred Reactor Network Modelling for Soot Emissions Prediction in Aero-Engine Combustors
- ERC Consolidator Grant AFIRMATIVE (Acoustic-Flow Interaction Models for Advancing Thermoacoustic Instability prediction in Very low Emission combustors), 2018-23, €1.98M
- Lithium-ion battery safety in transport, storage and utilization, Innovate UK Faraday Challenge, led by Jaguar Land Rover (JLR), July 2019 ~ February 2021 (£397,398.21 of £5M).
- Characterisation of pressurised liquid hydrogen (LH2) releases (P-LH2), EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 September 2019 – 30 August 2021).

- Predicting flame acceleration and Deflagration to Detonation Transition in industrial scale explosions incorporating the Turbulence effects (TurbDDT) EU Horizon 2020 Marie Curie Fellow (€195.5K, 01 March 2019 – 30 February 2021).
- Pre-normative research for safe use of liquid hydrogen (PRESLHY), Horizon 2020 (€104.5K within a €1.9M consortium, 1 April 2018 – 31 March 2021).
- EPSRC network grant EP/S032134/1 (1st October 2019-30th September 2023): A network for hydrogen-fuelled transportation (Network-H2) (£96,6316, Prof. N. Chakraborty, Co-I).
- EPSRC research grant EP/S025154/1 (12th August 2019-11th August 2022): Numerical exploration and modelling of novel environmentally friendly combustion technique: droplet-laden MILD combustion (£791,000, PIs: Prof. Nilanjan Chakraborty, Newcastle University; Prof. N. Swaminathan, Cambridge University).
- EPSRC research grant EP/V003534/1 (3rd May 2021-2nd May 2025): A combined experimental and numerical investigation of premixed flame-wall interaction in turbulent boundary layers (£776,896, PI: Prof. Nilanjan Chakraborty, Newcastle University; Co-Iis: Drs. Umair Ahmed, Andrew Aspden, Newcastle University).

HEC Consortia Model: Over the coming months EPSRC will be looking at the future of the HEC Consortia model and potential future funding. We would like to use this opportunity to ask the Consortia Chairs for input:

- What are the key benefits that your community have experienced through the existence of the HEC Consortia?
- What elements of the financial support provided by the HEC Consortium's grant have worked well and what could be improved in the future?

Key benefits for the community due to the existence of the UKCTRF

The existence of this consortium enabled the community to achieve the following:

- Exploit HPC resources to perform leading-edge reacting flow simulations involving Reynolds Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS);
- Obtain fundamental physical information and develop high-fidelity modelling methodologies for analysing turbulent reacting flows with relevance to energy, gas turbine, automotive and fire safety engineering;
- Develop a forward-looking software development strategy to efficiently exploit today's and future HPC hardware;
- A platform to collaborate and share expertise within the community to avoid duplication of research and remain internationally competitive;
- Supporting both externally funded (e.g. EU and industrial) and internal (e.g. university funded) projects, which do not have dedicated HPC support of their own;
- Development of highly skilled manpower in the form of early career researchers who have received an extensive training on the reacting flow physics and modelling, mathematical analysis, high-performance computing and software development.

Elements of the financial support provided by the HEC Consortium's grant have worked well and what could be improved in the future

The funding for travel and subsistence, workshop/meeting arrangement and website development has worked well so far. The financial support could be improved by considering the provision for funding of the following aspects:

(i) The previous incarnations of UKCTRF (i.e. Consortium on Computational Combustion for Engineering Applications (COCCFEA)) had the option for summer schools on computational combustion. Under the new regulation of EPSRC, it was not possible to include the summer school in the proposal for UKCTRF. However, both academic experts and industrial members of IAP commented in the annual progress review meeting that there is a need for such training activities at regular intervals. It is recognised that EPSRC funded CDTs can offer some of these training activities but does not meet all the requirements. Especially, some funding for courses on advanced parallelisation techniques in collaboration with EPCC will be particularly helpful.

(ii) The job of annual reporting and handling other activities related to administrative duties of the consortium is becoming increasingly time consuming for a single academic as the consortium chair, even with a small percentage (~15%) of secretarial support, so provision for part of a Research Associate's (RA's) time for the help in the aforementioned administrative activities will be useful for the next incarnation of the HEC consortia.

Web-Content Approval:

Please indicate which sections of the annual report could be used to produce content for the Consortia pages on the ARCHER website: https://www.archer.ac.uk/community/consortia/

Section Heading	Yes / No / Maybe	Comments
Membership	Yes	Happy to disseminate on the website
World class and world leading scientific output	Yes	Happy to disseminate on the website
Greater scientific productivity:	Yes	Happy to disseminate on the website
Increasing the UK's CSE skills base	Yes	Happy to disseminate on the website
Increased impact and collaboration with industry	Yes	Happy to disseminate on the website
Strengthening of UK's international position:	Yes	Happy to disseminate on the website
Other Highlights for the Current Reporting Period	Yes	Happy to disseminate on the website

To Note: New web-content generated from the annual reports will not be published without the approval of the relevant Consortium Chair.