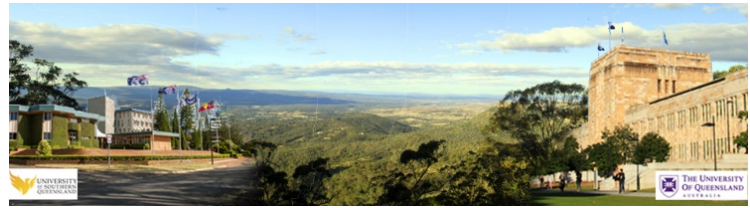


List of abstracts



List of abstracts.....	1
Bilger Lecture.....	3
Hydrogen and Ammonia Combustion – Japan’s Challenge and Technical Progress	3
Keynote 1.....	4
New opportunities and challenges from a growing role for hydrogen in future low-carbon industrial processes	4
Session 1 Hydrogen.....	5
Experiment and Simulation of Hydrogen Oxidation in the High-Pressure, Weak-Ignition Regime.....	5
Toluene addition to turbulent H ₂ /CH ₄ flames in bluff-body burners	5
Visible and thermal radiation from toluene-doped hydrogen flames	6
A comparative study of sound generation by turbulent hydrogen/methane premixed flames	6
Session 2 High-speed combustion	7
Hydrogen Boundary Layer Combustion with Multi-Porthole Injector Arrays.....	7
Scramjet Combustion Mode Establishment and Stability in a Reflected Shock Tunnel.....	7
Atomic Oxygen in Supersonic Combustion Experiment Inflows	8
Measurements of Density Fluctuations in a Scramjet Combustor	8
Keynote 2.....	9
Fundamental Aspects of Ammonia Oxidation	9
Keynote 3.....	10
A functional-group-based approach to modeling real-fuel combustion chemistry	10
Session 3 Turbulent flames	11
A priori analysis of flame wrinkling factor models in a turbulent premixed round jet flame	11
LES/PDF Modelling of Turbulent Premixed Flames Using an MMC – Shadow Position Mixing Model Incorporating Detailed Chemistry	11
A Method for Solving Two-Stream Mixing using the Generalised Binomial-Langevin Multiple Mapping Conditioning Model.....	12
An improved understanding of the stability of hydrocarbon flames with compositional inhomogeneity.....	12
Studying the Merging Fire Fronts in Field conditions	13
On the unsteady effects of flamelet models in a turbulent line fire.....	13
Session 4 Engines.....	14
Cycle to cycle variations of in-cylinder flow in a high-tumble spark ignition engine	14
Laboratory Simulation of Real-driving Emissions with a Heavy-Duty Diesel Engine	14
A transition flame speed approach for large-eddy simulation of a natural gas DISI engine	15
Preliminary experiments in a confined and pressurised	15
jet-in-hot-coflow combustor.....	15
Experimental investigation of iso-butanol-acetone (BA) and diesel blend as an alternative fuel for CI engines	16
Near-field autoignition study of a premixed jet in a cross-flow.....	16



Session 5 Special topics	17
A Multi-Density Incompressible Method for Industrial Scale Dispersion Calculations	17
Development length in smooth channels with wall reactions	17
On Relations of Combustion and Systems Modelling	17
Session 6 Flows with physical & chemical processes	18
Study of electric arc dynamics inside a plasma torch under the influence of external magnetic field using a non-equilibrium model	18
Thermal Plasma Destruction of Perfluoroalkyl Substances: Experimental investigation and modelling studies	18
Supercritical CO ₂ Turbulent Flow and Heat Transfer Behavior in a Concentric Rotating Annulus	19
Super-critical CO ₂ Behavior in a Concentric Annulus Based on Ideal Gas and Real Gas Properties	19
Keynote 4.....	20
Modelling Particle Synthesis in Turbulent Flames	20
Special Invited Talk.....	21
Indigenous Fire Practices	21
Session 7 Spray and Soot	22
Effect of Thermodynamic Pressure on Laminar Burning Velocity in Ammonia/Dimethyl-ether Premixed Flames.....	22
An Experimental Study of Ignition and Combustion Characteristics of Single Droplets of Vacuum Residues	22
Modelling a dilute spray flame using the eddy dissipation concept.....	23
Dilute spray flames of ethanol and n-heptane in the transition to mild combustion	23
Reactive π -diradicals found in soot forming flames.....	24
On the Combined Effects of Compositional Inhomogeneity and Ammonia Addition to Turbulent Flames of Ethylene	24
Session 8 Kinetics and Solid combustion.....	25
Decomposition of Carbonyl Sulfide.....	25
New Pathways for Formation of Toxic Species in Oxidation of 4-Chlorobiphenyl	25
Partial oxidation of spent tyre pyrolysis oil for the production of carbon black	26
Freeboard Effects on Instabilities in a Fixed Bed Biomass Combustor	26
Effects of Constant and Staged Torrefaction Temperatures on Biomass Combustion and Pyrolysis	26



Bilger Lecture

ACS21000K

Hydrogen and Ammonia Combustion – Japan’s Challenge and Technical Progress

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Abstract

There is a growing demand for fuel switching in the energy sector. In Japan, where a large amount of fossil fuel is imported, hydrogen and ammonia have been identified as the first feasibility choice as a fuel for decarbonized thermal power generation, and “Fuel Ammonia Industry” has been newly positioned as one of the government's “Green Growth Strategies”. The construction of a supply chain to import blue and green hydrogen and ammonia from overseas has been initiated as an international economic activity. In the field of decarbonized combustion science and technology, in addition to the development to improve the ammonia co-firing ratio in pulverized coal-fired power generation, research and development of liquid ammonia spray combustion, which can stably burn a large amount of ammonia in gas turbine power generation, is underway.

Keywords: Hydrogen, Ammonia, Thermal power generation, Carbon neutrality, Ammonia spray combustion.



Keynote 1

ACS21001K

New opportunities and challenges from a growing role for hydrogen in future low-carbon industrial processes

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Abstract

Net-zero hydrogen (H_2), that is H_2 produced with net-zero CO_2 emissions, is expected to play an important role in the decarbonizing of those high temperature processes used to produce basic materials such as iron/steel, alumina and cement/lime. Its use is expected to span being the dominant to a supplementary energy source, in combination with other energy types including electricity (e.g., via a thermal plasma or resistive heating), carbon-capture and storage/re-use and concentrated solar thermal energy, whose relative contributions will vary from process-to-process and region-to-region due by differences in commercial readiness, cost and technical challenges. The transformation to these new energy types is driven by the emergence of new markets for high-value low-carbon products, investor demand, new policies, carbon taxes and community expectation, together with the potential for lowering energy/heat costs in the emerging, low-carbon economy. Net-zero H_2 is expected to be the dominant pathway to green steel because this route is the closest to market of the various technology options, and because it will begin to be economic in its own right when the cost of net-zero H_2 reaches the target of US\$2/kg. This will bring a range of opportunities and challenges, which is driving new research needs and opportunities, both for the technologies themselves, for the supply chains needed to deliver H_2 with net-zero emissions and for improved predictive capability to de-risk the transition to utilize it in a highly bespoke industrial sector.

Keywords: industrial process heat; hydrogen production; hydrogen combustion; hybrids; decarbonisation.



Session 1 Hydrogen

ACS21021

Experiment and Simulation of Hydrogen Oxidation in the High-Pressure, Weak-Ignition Regime

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Abstract

This work investigates the oxidation of hydrogen in a turbulent flow reactor at pressure of 10 to 48 bar and temperature of 950 K with an equivalence ratio of 0.03. Pressure weakly promotes hydrogen oxidation at these conditions. Such impact is not only different from the inhibiting effect observed at 1-10 bar but also atypical of the usual promoting effect of pressure on reaction kinetics. Simulation of the measured species time history is conducted using existing chemical kinetic models, where significant differences are observed between model and experiment. Modification to the kinetic model proposed by Zhang et al. (Combust. Flame, 2017, p. 122) improves the prediction for a wide range of experimental data including those in this work and from the literature.

Keywords: Hydrogen oxidation, high pressure, turbulent flow reactor

ACS21012

Toluene addition to turbulent H₂/CH₄ flames in bluff-body burners

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Abstract

In the transition to renewable sources of energy, industries have begun to look at the integration of hydrogen for some high temperature applications. A key challenge which must first be addressed is the reduced thermal radiation of hydrogen flames compared with its sootier hydrocarbon counterparts. A novel solution to this may be to dope hydrogen flames with bio-oils to increase soot production and resulting enhanced thermal radiation. This study investigates the efficacy of toluene as a prevapourised dopant in pure and blended turbulent hydrogen/natural gas flames stabilised on bluff-body burners. Two bluff-body diameters (dBB) of 50 mm and 64 mm are used to emulate the recirculation component of industrial systems. The results showed a positive non-linear relationship between toluene addition and heat flux for all gas blends and bluff-body diameter. The blended cases required less than 1 mol% toluene to meet equivalent natural gas heat flux and the pure hydrogen cases required approximately 4 mol%. Increasing the bluff-body diameter had a negative effect on the overall heat flux. Hydrogen with an addition of 10 vol% compared to 20 vol% in natural gas had opposite effects for each bluff-body diameter, where a dilution effect was seen in the larger 64 mm diameter, but a chemical promoting effect was seen in the smaller 50 mm diameter.

Keywords: Hydrogen, Toluene, Radiation, Bluff-body



ACS21013

Visible and thermal radiation from toluene-doped hydrogen flames

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Abstract

Hydrogen is a promising alternative fuel for the displacement of carbon emissions from hydrocarbons in a range of applications. Hydrogen flames differ from those of “conventional” fuels in several ways, particularly in their radiative properties, both in the visible and infra-red regions of the spectrum. This leads to the lack of a clearly visible flame in the case of hydrogen, which has significant implications from a safety perspective in domestic settings. Reduced radiative heat transfer from hydrogen flames can also affect efficiency in both domestic and industrial applications. In this paper, the effect of the addition to hydrogen of a small quantity (1% by mole) of a highly sooting fuel—namely toluene—is explored. The addition of toluene was found to have a profound impact on the flame visibility and radiative heat transfer properties. In addition to characterising the effect of toluene, the visibility of pure hydrogen flames is also investigated, with particular focus on the impact of sodium impurities which gives rise to the previously encountered orange colour of “pure” hydrogen flames.

Keywords: Hydrogen flame, dual-fuelling, thermal radiation, soot formation

ACS21022

A comparative study of sound generation by turbulent hydrogen/methane premixed flames

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Abstract

This study presents a Direct Numerical Simulation (DNS) study of sound generation by turbulent, premixed hydrogen/methane flames. Two cases with 50% and 80% by volume of hydrogen in the mixture at the same Reynolds number of 10,300 were simulated. The average flame length is similar between the two, and the 50% case features a higher level of flame-turbulence interaction due higher velocity fluctuations relative to the laminar flame speed. The Overall Acoustic Sound Pressure Level (OASPL) of the 80% flame was consistently higher by about 3-5 dB than the 50% flame. This difference is found to be primarily related to the high frequency range of the sound spectrum. A theoretical framework to examine the impact of the flame dynamics on sound generation is used. It is found that a higher laminar flame speed in the 80% case is the main reason that this case is louder. Also, increases in the contribution of annihilation events are the key mechanism by which hydrogen addition impacts sound generation.

Keywords: Hydrogen, methane, turbulent premixed flames, sound.



Session 2 High-speed combustion

ACS21006

Hydrogen Boundary Layer Combustion with Multi-Porthole Injector Arrays

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Abstract

Multi-porthole injector arrays (MPIA) are a proposed method to promote boundary layer combustion with the goal to reduce skin friction and heat transfer within a scramjet. It is not known how resilient this method is to other flow disturbances, such as mainstream fuel injection through a porthole. Experimental studies were conducted to investigate the effectiveness of an MPIA to promote boundary layer combustion, while also investigating the effects of a porthole injector. Hydrogen was injected through each injector via two separate fuel systems. Skin friction measurements taken downstream of the MPIA showed reductions of skin friction up to 64%. Heat transfer data also showed reductions. The introduction of the porthole injector diminished the reductions achieved by the MPIA, however the skin friction remained below the unfuelled value for a portion of the flow path. The introduction of the porthole injector also increased the heat transfer to above unfuelled values. Schlieren imaging of the flow revealed the porthole injector allowed deeper penetration from the MPIA, spreading the layer of fuel away from the wall and diminishing its effectiveness to promote boundary layer combustion.

Keywords: Hypersonic, Hydrogen, Multi-porthole Injector Array, Skin Friction, Boundary Layer Combustion

ACS21007

Scramjet Combustion Mode Establishment and Stability in a Reflected Shock Tunnel

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Abstract

This paper examines the transient behaviour of the varying combustion modes of a Mach 8, scramjet combustor within a reflected shock tunnel. Flight-equivalent flows were delivered to the axisymmetric, cavity combustor via the T4 reflected shock tunnel. The combustor was fuelled with ethylene. Combustion modes were examined via static pressure sensors, with the full time-history of each sensor visualised. It was noted that, despite some sensors seeing measurement uncertainties during the test time, the progression to stable and steady combustion at supersonic, jet-wake anchored, and dual-mode conditions was achieved during the test time provided.

Keywords: Supersonic combustion, scramjet, shock tunnel, dual-mode combustion.



ACS21016

Atomic Oxygen in Supersonic Combustion Experiment Inflows

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Abstract

Supersonic combustion experiments at hypersonic flight-equivalent conditions are frequently conducted in reflected shock tunnels. A downside of these experiments is the amount of radicals within the test flow that are ingested by an experimental model. Combustion is particularly sensitive to the atomic oxygen radical, O, which can cause dramatic reductions in ignition length at very low levels. Test flow compositions are typically simulated using a 5-species chemical reaction scheme that includes N₂, O₂, N, O and NO, resulting in significant mass fractions of O. However, studies have not observed these levels of O, indicating that the effect of freestream radicals may not be as dramatic as previously thought. This paper presents the hypothesis that by neglecting species, such as NO₂, the chemical pathways to accurately remove O were being artificially limited. By considering a 6-species reaction scheme that includes NO₂, the authors show that the mass fraction of O becomes negligible at supersonic combustion test conditions.

Keywords: Supersonic combustion, Testing facilities, Chemical kinetics, Scramjets, Hypersonics.

ACS21024

Measurements of Density Fluctuations in a Scramjet Combustor

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Abstract

In this study, a Focused Laser Differential Interferometer (FLDI) was used for the first time to measure the density differences, and, hence noise, generated due to supersonic turbulent combustion processes in a model 2-D axisymmetric scramjet engine. Measurements were taken at the front and back end of the combustor for unfuelled and reacting cases. The Power spectral density spectra plots show that the noise level generated inside the scramjet combustor for the unfuelled case is about two orders of magnitude more than that in the free stream. Further, at the rear end of the combustor, heat release due to supersonic combustion results in combustion-induced noise that is found to be higher than for the unfuelled case. Additionally, distinct tonal features were also observed for both cases.

Keywords: FLDI, Scramjet, Supersonic combustion noise.



Keynote 2

ACS21002K

Fundamental Aspects of Ammonia Oxidation

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Abstract

Ammonia has found use in combustion applications since the original patent by Lyon (US3900554A) relating to its use for nitric oxide reduction in flue gases through selective non-catalytic reduction (SNCR). It is also a well-established component in the production of fertilisers with correspondingly efficient manufacturing processes. The recent interest in the use of ammonia relates to its use as a hydrogen rich energy carrier. The current paper presents selected fundamental aspects of ammonia oxidation put in a chemistry related context. Implications for the translation of the resulting understanding to the study of turbulent combustion of ammonia blends in practical devices are outlined. It is argued that the comparatively low laminar burning velocities and flame extinction characteristics of ammonia are likely to result in more prevalent local extinction events leading to a greater prevalence of non-topological flame structures. Furthermore, the enhancement of the fuel reactivity through the blending with more reactive components, such as hydrogen and hydrocarbons, will impact the extent and effectiveness of the temperature window where SNCR reactions are active. It is further suggested that the direct interaction of ammonia fragments with aromatic species (c.f. aniline) and the condition dependent increase of nitric oxide may impact the propensity to form soot. It is shown that use of ammonia as part of fuel blends results in a fundamentally different flame structure for the formation of oxides of nitrogen. Finally, recommendations are made in relation to research directions that can deliver the understanding required for the optimal practical use of ammonia as an energy carrier.

Keywords: Ammonia, Oxidation, Chemistry, Turbulence, SNCR



Keynote 3

ACS21003K

A functional-group-based approach to modeling real-fuel combustion chemistry

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Abstract

Real fuels are complex mixtures of hundreds to thousands of molecules, and it is intractable to understand fully the combustion kinetics of each of these compounds. The combustion community has evolved various approaches for dealing with such complex mixtures, such as the use of multi-component surrogates mixtures, lumped fuel chemistry modeling, and short reaction mechanisms. Here we present recent efforts to develop a lumped fuel chemistry modeling approach based entirely on the functional group distribution in a real fuel mixture (denoted as FGMech). Our approach starts with a modeling framework like the recent HyChem approach by Wang et al. at Stanford University. This approach is generalized by establishing a workflow to establish model parameters without the need for any combustion experiments on the real fuel. Model parameters are developed following a data science approach coupled with simplified regression and group additivity models. This paper presents the effectiveness of the FGMech approach in modeling the combustion chemistry of various transportation fuels and heavy residual gasification.

Keywords: surrogates, functional groups, kinetics, heavy fuels, combustion



Session 3 Turbulent flames

ACS21011

A priori analysis of flame wrinkling factor models in a turbulent premixed round jet flame

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Abstract

A DNS dataset of a turbulent, premixed, methane-air, round jet flame in the Thin Reaction Zones (TRZ) regime is analysed to assess the performance of algebraic models for the flame wrinkling factor used in Large-Eddy Simulation (LES). The models proposed by Charlette et al. [1], Fureby [2], and Muppala et al. [3] are studied. The parameters such as the wrinkling factor, the flame surface density and their conditional averages with the filtered progress variable are examined using the DNS data. It is shown that the performance of the models deteriorates for high levels of subgrid turbulent velocity. Furthermore, the decreasing trend of the average wrinkling factor from the unburnt side to the burnt side of the flame observed in this round jet flame is not captured by the models. Despite these discrepancies, the Charlette and Fureby models reproduce the DNS profiles of the conditionally averaged flame surface density with reasonable accuracy. The Muppala model considerably overestimates both the average wrinkling factor and flame surface density with the default constants. Overall, the results suggest that the performance of the models needs significant improvement for places where large errors are observed such as for flame annihilation events.

Keywords: Combustion modelling, Premixed flame, Flame wrinkling factor, Large-Eddy Simulation. Preferred Colloquium: Turbulent Flames

ACS21020

LES/PDF Modelling of Turbulent Premixed Flames Using an MMC – Shadow Position Mixing Model Incorporating Detailed Chemistry

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Abstract

This paper presents the first application of a novel multiple mapping conditioning model with a shadow position reference in LES/PDF modelling of a piloted premixed methane-air jet flame using detailed chemistry. The stochastic equations governing the temporal evolution of shadow positions encompass a diffusion coefficient correlated to the model parameter λ that represents the ratio between a reference turbulent propagation speed and the laminar flame speed. Therefore, in this approach, adjusting the actual turbulent propagation speed does not require varying the mixing constant, which could affect the flame's inner structure and propagation speed at the same time. The obtained results show a significant difference between the predictions obtained for the inner structure of the flame using simple and detailed chemical mechanisms, which demonstrates the significance of incorporating detailed chemistry to obtain a more realistic prediction. Furthermore, the results demonstrate the sensitivity of the predicted flame length to the model parameter. In contrast, the predicted inner structure does not show considerable sensitivity to variations as expected.

Keywords: Premixed combustion, Multiple mapping conditioning, MMC-LES, Shadow position.



ACS21038

A Method for Solving Two-Stream Mixing using the Generalised Binomial-Langevin Multiple Mapping Conditioning Model

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Abstract

Newly-defined closures for the binomial-Langevin Multiple Mapping Conditioning (BLM-MMC) model are used to determine the proportion of stochastic particles that mix each time step. The parameter was previously treated as a constant. Two further developments were introduced to address the requirements associated with two-stream mixing configurations. First, the proportion of particles to mix is determined by requiring the MMC scalar variance to match the binomial-Langevin variance. To achieve this, particles are mixed using the Modified Curl's model and a uniform random mixing amount until the scalar variance is lower than the binomial-Langevin variance. To exactly match the variance, the amount of mixing for the final particle pair is calculated via deterministic sampling from the distribution so compliance is guaranteed. Second, a standard Gaussian variable is introduced and defined so that the mapping function of the binomial Langevin scalar corresponds to its conditional mean. This conventional conditioning variable is introduced because its distribution is always continuous, whereas during the initial mixing period for two streams the probability density function of the scalar must be discontinuous, leading to segregated mixing. These changes are shown to correctly model non-reacting homogenous mixing of two distinct streams.

Keywords: Multiple Mapping Conditioning, Two-Stream Mixing, binomial Langevin model, Curl's Mixing.

ACS21026

An improved understanding of the stability of hydrocarbon flames with compositional inhomogeneity

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Abstract

This paper presents experimental data that extends the current understanding of flame stability improvement due to compositional inhomogeneity utilising the well-documented Sydney inhomogeneous burner. The focus here is on three gaseous hydrocarbon fuels: Methane (CH₄), Ethylene (C₂H₄) and Propane (C₃H₈). The exploration of these light to heavier hydrocarbons (C₁ – C₃) enables a parametric study for a range of different air to fuel ratios (A/F) which correspond to different global jet equivalence ratios (ϕ). It was found that each fuel studied has a specific equivalence ratio where the improvement in flame stability due to inhomogeneity was the greatest. Between different fuels, the flame stability improvement was found to be well correlated with the air to fuel ratio.

Keywords: Inhomogeneous burner, Turbulent flames

ACS21027

Studying the Merging Fire Fronts in Field conditions

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Abstract

Merging fire fronts have been known for rapid fire spread and developing into extremely destructive wildfires, resulting in increased injuries, property losses, and deaths. To date, there has been few studies characterising merging fire behaviours outside of the laboratory. In our study, we conducted two experimental harvested crop burns in Victoria, Australia, in March and April 2021 to better understand merging fire fronts. A UAV with a thermal camera was used to capture high-resolution fire propagation of 109 merging fire fronts. During experiments 50 junction fire fronts (32 forward and 18 backward), 24 coalescence fire fronts and 35 inward parallel fire fronts were studied. The median rate of spread (ROS) of forward junction fires was highest (2.02 m/s), followed by linear and backward ROS, 0.57 m/s and 0.18 m/s, respectively. The ROS of forward junction fires in the first burn was twice as high as in the second burn, suggesting the influence of local drivers such as weather or fuel. However, the ROS of backward fire fronts was similar between the two burns. The forward junction fires were, on average, 3 times faster than the linear fire fronts, irrespective of the burn. In some cases, this difference could be as much as an 18-fold increase. A deceleration of forward junction fires toward the end of merging was observed, but this process was insignificant and almost unnoticeable (slopes=0.001-0.034) in contrast to other studies. We observed an increase in the current junction angle over time for all initial junction angles (slopes=0.26-0.47) except of 60°-90°. These slopes are considerably higher than in other studies but are consistent with our previous results. Although the current angles become twice as large at the end of merging, the ROS did not decrease significantly in contrast to other studies. The differences observed between the laboratory and field experiments demonstrate the necessity for additional experiments to better understand the relationship between fuel, weather and merging of fire fronts.

Keywords: Wildfires, Merging fire fronts, Junction fires, Spot fire coalescence

ACS21034

On the unsteady effects of flamelet models in a turbulent line fire

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Abstract

Advanced combustion models play a significant role in facilitating predictive numerical simulations in fires, which remain challenging due to the complex interaction of turbulence, chemical reactions and radiation. Among those, flamelet models are one of the most tractable categories to promote in fire applications with its affordable cost. To this end, large-eddy simulations (LES) / flamelet modelling is implemented with an OpenFOAM-based solver, to investigate a turbulent line fire, which is a target case in the Measurement and Computation of Fire Phenomena (MaCFP) workshop and is experimentally investigated at University of Maryland (UMD). The objective of the work is to reveal the role of unsteadiness in flamelet models, which can be either introduced by scalar dissipation (γ) or radiation. It is revealed that the unsteady radiative flamelets should be considered in the model to yield reasonable prediction in temperature, implying the importance of radiation-induced unsteadiness. Comparatively, the c-induced unsteady effect contributes less significantly to determining the temperature, while it strongly affects the prediction of radicals such as OH. A time scale analysis further reveals the comparable characteristic time-scale for radiation, mixing and flamelet residence, which justifies the significance of both unsteady effects in this flame.

Keywords: turbulent line fire, flamelet method, radiation, scalar dissipation, unsteadiness

Session 4 Engines

ACS21005

Cycle to cycle variations of in-cylinder flow in a high-tumble spark ignition engine

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Abstract

Latest generation spark ignition engines are designed to achieve a high tumble ratio for enhanced mixing and faster flame propagation. The result is increased engine efficiency and higher power output. However, higher tumble flow magnitude might lead to increased cyclic variations, which would deteriorate the engine operation stability. The present study performs endoscopic high-speed particle image velocimetry (eHS-PIV) in production engines with varied tumble ratios to analyse the cyclic variations of flow field and spatially averaged flow magnitude. The experimental results showed that the higher tumble engine induces more intense lateral flow vectors during the piston compression, which causes a more complex flow structure near top dead centre than the lower tumble engine. From the data obtained for 100 engine cycles, the cyclic variations in the flow magnitude were measured initially lower for the higher tumble engine due to a more clearly defined flow structure. However, as the flow structure became more complex during the flow breakdown occurring near top dead centre, higher cyclic variations were measured in the flow magnitude for the higher tumble engine. This leaves an important task of flow magnitude and cyclic variation optimisation for the engine development.

Keywords: SI engine, Tumble flow, Cyclic variation, eHS-PIV

ACS21010

Laboratory Simulation of Real-driving Emissions with a Heavy-Duty Diesel Engine

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Abstract

The current study investigated the influence of driving style and traffic conditions on real-world transient emissions and fuel consumption of a heavy-duty diesel engine. Six different transient engine cycles classified as timid, normal and aggressive at peak and off-peak hour were developed from the real-world measurements performed using Portable emissions measurement systems (PEMS) on an urban route. The on-road engine parameters were converted to laboratory engine parameters using the guidelines of the US Code of Federal Regulations, Title 40 Part 86. Gaseous and particle emissions and fuel consumption were measured and analysed for different driving styles and traffic conditions. The results have shown specific driving style has a significant impact on emissions than traffic conditions. Urban driving generates a lot of transient micro trips which significantly increase the turbocharger lag effects and overshoot emissions.

Keywords: Transient cycle, NOx, CO, PM, Turbocharger lag.



ACS21017

A transition flame speed approach for large-eddy simulation of a natural gas DISI engine

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Abstract

A transition flame speed approach is used for Large-Eddy Simulation (LES) of a Compressed Natural Gas Direct Injection Spark Ignition (CNG DISI) engine. The G-equation combustion model is utilised in conjunction with the Reyes laminar and Damköhler turbulent flame speed models. In this transition approach, the flame propagates with a laminar flame speed until it reaches a specified cut-off radius, and then evolves with a turbulent flame speed. Three distinct cut-off radii of 2, 3, and 5 mm are used and the LES results are compared with the experimental and GT-POWER results. Changing the cut-off radius significantly impacts both the pressure trace and the Mass Fraction Burned (MFB) profile, highlighting the significance of correctly capturing the early stage of flame development. Consistent with the literature, a cut-off radius of 3 mm results in the best agreement with the experimental results.

Keywords: CNG, Large-Eddy Simulation (LES), G-equation modelling, Direct Injection (DI), Flame Development.

ACS21014

Preliminary experiments in a confined and pressurised jet-in-hot-coflow combustor

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Abstract

Combustion in hot, low oxygen environments, such as mild combustion is not well understood at pressure. To meet this gap in understanding, a confined-and-pressurised jet-in-hot-coflow (CP-JHC) burner has been developed to facilitate optical diagnostics of turbulent flames in hot and vitiated coflows for the studies of flame stabilisation, structure and soot formation at elevated pressures. The CP-JHC burner has been designed for steady operation at 10 bar(a) with internal temperatures of up to 1975 K with a water-cooled, 4.6-mm central jet issuing into a hot oxidant stream produced by a non-premixed natural gas/H₂ burner. This work describes the key features and operational capabilities of the CP-JHC burner and presents a selection of results from initial experiments. Temperature measurements of the hot coflow with heat inputs of 8.7-17 kW are used to estimate the enthalpy deficit of the stream, with thermal efficiency increasing with increasing heat input, and decreasing with increasing pressure. Preliminary mean and instantaneous images of turbulent natural gas/H₂ and C₂H₄ flames, with and without chemiluminescence filters, are discussed in context of ignition pathways and soot formation at elevated pressures to highlight the need for future studies in this newly developed burner.

Keywords: Elevated-pressure combustion, Mild combustion, Turbulent flames, Chemiluminescence imaging



ACS21039

Experimental investigation of iso-butanol-acetone (BA) and diesel blend as an alternative fuel for CI engines

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Abstract

Bio-butanol is a potential fuel for compression ignition engines (CI) because of its beneficial physicochemical properties and its ability to be produced from agricultural waste through fermentation. The feasibility of using bio-butanol from biomass is not yet clear due to the high production cost caused by low yields and expensive processes for separating it from butanol-acetone (BA) fermentation. Instead using the intermediate fermentation products of butanol (that is BA) as a fuel has already been found to produce clean combustion. Butanol-acetone is, therefore, proposed as a fuel for CI engines which could lead to extra reductions in BA production cost, and could improve combustion by reducing temperature. Butanol produces in four isomers: n-butanol, iso-butanol, sec-butanol, and tert-butanol. The effects of iso-BA-diesel blends on combustion, performance and emission characteristics were investigated at three engine speeds and full load. The results were compared with neat diesel and 10% and 20% iso-BA-90% diesel blends. Brake power (BP) was slightly reduced while Brake specific fuel consumption (BSFC) increased for iso-butanol-diesel blends due to the low heating value. Exhaust gas temperature (EGT) and Nitrogen of oxide (NOx) emissions were reduced with the inclusion of iso-butanol in the test blends, relieving combustion and reaction temperature which resulted in NOx emissions reduction. Carbon monoxide (CO) emissions were reduced due to the high oxygen content. However, unburnt hydrocarbon (UHC) emissions rose due to iso-BA-diesel blend showing higher UHC because iso-butanol has the most terminal C single bond H bonds, so the reaction rate of iso-butanol in butanol-acetone is lower, resulting in insufficient time to complete the reaction, causing an increase in UHC emissions. Thus, iso-butanol-acetone could be a good alternative fuel for CI engines because of its production manner and reduced emissions.

Keywords: iso-butanol, diesel engine, emissions.

ACS21040

Near-field autoignition study of a premixed jet in a cross-flow

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Abstract

In this work, we conduct an analysis of the ignition characteristics in the near field of a premixed jet flame in a vitiated cross flow, a configuration that closely represents the second stage of an axially staged gas-turbine combustion system. This concept has gained significant attention among gas-turbine manufacturers due to its greater fuel flexibility and lower NOx emissions. A premixed methane-air jet with an equivalence ratio of 0.7 is injected into a vitiated cross flow comprising combustion products from a methane-air mixture at an equivalence ratio of 0.5 and atmospheric pressure. The simulation is performed using a compressible high-order accurate numerical solver (S3D). The simulation results show that the flame is lifted from the jet inlet with an anchoring point on the leeward side of the jet. Significant radical concentrations are found upstream of the anchoring point. Very close to the jet inlet, intermediate radicals are produced due to OH consumption. Whereas adjacent to the anchoring point, intermediates are due to autoignition reactions. Further, it is identified that coherent structures in the near field have an important role in the spatial location of autoignition.

Keywords: axially staged combustion, direct numerical simulation, premixed jet in a cross-flow.



Session 5 Special topics

ACS21035

A Multi-Density Incompressible Method for Industrial Scale Dispersion Calculations

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Abstract

Dispersion calculations using computational fluid dynamics for problems on an industrial scale are very time consuming and carry irreducible uncertainty. Generally, for industry-based problems, it is necessary to examine the effect of a release whether it be toxic or flammable over a large area which makes detailed calculations prohibitively time consuming and expensive. With a view to speed up the process, a method for modelling the dispersion of species using a multi-density incompressible Navier-Stokes solver is introduced. The method is set up within exploCFD: a hybrid analytical-numerical toolchain that relies on the open source CFD solver SU2, which does not have a facility for multispecies calculations. The analytical method uses what is termed a false temperature to calculate the density of the released material. The approach is approximate but is far more accurate than many methods in use in industry which rely solely on conservation of mass. The proposed approach is also much faster than using a Lagrangian approach for tracing the species. The method is used to model some of the BA Hamburg tests as part of the validation of the methodology. The results show very good agreement with the experiment falling mostly within a fraction of a percent of the measured value. The predicted results from this method overwhelmingly sit within the band 50%-200% of the measured values which is the most commonly used Model Evaluation Protocol metric for dispersion models.

Keywords: Toxic Dispersion, Flammable Dispersion, Fast Dispersion modelling

ACS21030

Development length in smooth channels with wall reactions

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Abstract

In micro/nanoscale flows the assumption of a no-slip condition at solid boundaries becomes invalid and slip conditions must be considered. The presence of this wall slip increases the development region in micro/nanoscale channels. This work derives analytical expressions for the velocity profiles and an approximation to the slip length in a channel in the slip flow regime for a channel with slip governed by wall reactions, such as adsorption, in the limiting case of very small slip coefficient.

Keywords: Reacting flows, Microfluidics, Nanofluidics, Wall reactions

ACS21019

On Relations of Combustion and Systems Modelling

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Abstract

Modelling turbulent reacting flows offers a spectrum of well-developed modelling methodologies of varying complexity and precision. We review major classes of combustion models and examine the possibilities of extending these models for modelling general complex systems.

Keywords: Turbulent combustion modelling, multiscale phenomena, chaotic order, complex systems.



Session 6 Flows with physical & chemical processes

ACS21029

Study of electric arc dynamics inside a plasma torch under the influence of external magnetic field using a non-equilibrium model

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Abstract

The magnetic induced arc rotation has a significant effect on the arc structure and the resultant flow field inside the plasma torch. A two-temperature and transient plasma fluid model is developed in OpenFOAM to study the electric arc dynamics under the influence of external magnetic field. The arc rotation is created by imposing a constant axial magnetic field inside the torch to mimic the magnetic field generated by a permanent magnet or solenoid. The arc rotation observed in the present study is consistent with previous experiments and modelling works. The operating arc current is varied between 25A and 100A. The non-equilibrium parameter, which measures the deviation of electron temperature over the heavy species, is observed to be higher around the arc column fringes where the incoming cold gas contacts with hot plasma. The difference between maximal temperatures of electron and heavy species increases as the arc current decreases. The results from the two-temperature models are also compared with the single-temperature model developed previously.

Keywords: plasma fluid, electron temperature, external magnetic field.

ACS21031

Thermal Plasma Destruction of Perfluoroalkyl Substances: Experimental investigation and modelling studies

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Abstract

The defluorination of PFAS is investigated via thermolysis in a thermal steam-plasma reactor under a variety of experimental conditions including pollutant concentration, dosing rate and torch power. Accompanying computational fluid dynamics (CFD) simulations were performed for PFBA destruction in order to assess the internal operation of the reactor and decomposition pathways. It was found that under most conditions, the thermal plasma torch was capable of achieving an excess of 99% defluorination, with the only trials failing to achieve this being those operating with a lower energy density. CFD simulations found that local thermodynamic equilibrium is achieved in the hotter regions of the reactor where the pollutant is completely destroyed, with trace quantities of unreacted PFBA persisting along the water-cooled reactor walls. These results indicate that as long as energy density and mixing are sufficient at the point of the pollutant injection, effective pollutant destruction can be achieved by the plasma reaction.

Keywords: Perfluoroalkyl Substances, Thermal Plasma Destruction, Steam Plasma

ACS21032

Supercritical CO₂ Turbulent Flow and Heat Transfer Behavior in a Concentric Rotating Annulus

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Abstract

Supercritical CO₂ is already adopted in the industrial and power generation sector as a heat transfer fluid and its application is increasing worldwide. The concentrating rotating annulus turbulent flow is often encountered in external combustion turbomachinery utilizing supercritical CO₂. In supercritical CO₂ turbomachinery, the rotational speeds are high and there is a sharp axial temperature gradient. Therefore, existing solutions cannot be readily adapted to this new problem. The present study reports on supercritical CO₂ turbulent flow through a concentric annulus with the inner heated cylinder rotating and outer cylinder stationary. The computational mesh generation and solution for the given geometry were conducted using CFD fluent. The k- ω SST turbulent model was employed to obtain the simulation results. The entrance length axial velocity profile, turbulent characteristics, heat transfer coefficient, and friction coefficient were investigated along with varying clearance ratio and mass flow rate. The result showed that the one-fold increase in the annulus clearance causes an around the twenty-fold decrease in the entrance length to become the profile is fully developed. The higher the mass flow rate greater the entrance length. The turbulent eddy frequency decreases with increasing clearance. The effect of clearance on the convection heat transfer coefficient and friction coefficient was found insignificant.

Keywords: Concentric rotating annulus, Supercritical CO₂ flow, Heat transfer coefficient, Friction coefficient.

ACS21033

Super-critical CO₂ Behavior in a Concentric Annulus Based on Ideal Gas and Real Gas Properties

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Abstract

Supercritical CO₂ turbine technology has already been introduced as the next-generation energy conversion technology utilizing supercritical CO₂ as the working fluid where the heat of external combustion is transferred through the heat exchanger. The component development and optimum design of such technologies are often encountered to understand the supercritical CO₂ flow behavior. The annulus flow is very common in supercritical CO₂ external combustion turbomachinery. This study investigated the flow behavior of supercritical CO₂ through the concentric horizontal annulus based on the ideal gas and real gas properties. The Ansys workbench was employed to generate the computational mesh and the steady-state k- ω SST turbulent model has been employed to obtain the solution in fluent. The model was validated using the experimental results. The axial pressure drop gradient and friction factor were investigated as a function of the Reynolds number and Taylor number. The stability of the Taylor-Couette flow was also investigated. The result showed that the fluid properties have a significant effect on the pressure drop gradient whereas the effect is insignificant on the friction factor. The friction factor computed by the fluent were compared with the friction factor read from the moody chart and found a close agreement. The critical rotational speed found is 500 rad/s ($Ta = 10^7$) at which the flow transition expected from Couette flow to Taylor vortex flow through the annulus.

Keywords: Concentric annulus, Supercritical CO₂ flow, Pressure gradient, Friction factor, Taylor vortex.



Keynote 4

ACS21004K

Modelling Particle Synthesis in Turbulent Flames

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Abstract

Modelling nanoparticle synthesis in turbulent flames faces enormous challenges due to the large range of scales that need to be covered and a certain lack of detailed measurements that allow for an unambiguous assessment and validation of sub-models that describe specific aspects of the synthesis process. For this reason, a new burner for spray flame particle synthesis has been developed and a coordinated research programme attempts to characterize the burner and the process dynamics with the aid of a variety of measurement techniques and simulation approaches. We present predictions using a multiple mapping conditioning approach as being representative for the quality of current modelling attempts but also show selected experimental results that highlight issues, uncertainties and challenges that can be associated with design, characterization and modelling spray flame nanoparticle synthesis processes.

Keywords: spray flame particle synthesis, multiple mapping conditioning



Special Invited Talk

Indigenous Fire Practices

Presenter: Uncle Wayne Fossey

Uncle Wayne Fossey is the Elder in Residence for the University of Southern Queensland and a Director of the Bunya People's Aboriginal Corporation (BPAC). BPAC is an innovative Aboriginal organisation that works with all people to care for country across the broader Bunya Mountains landscape, north of Toowoomba on the Great Dividing Range. BPAC were established in 2012, continuing the legacy of the Bunya Mountains Elders Council, who came together to revive Aboriginal leadership and decision-making for the management of the Bunya Mountains. Uncle Wayne will present some of the work of BPAC in the Booburrgan Ngmmunge region (the traditional name for the Bunya Mountains used by many Aboriginal people).



Session 7 Spray and Soot

ACS21037

Effect of Thermodynamic Pressure on Laminar Burning Velocity in Ammonia/Dimethyl-ether Premixed Flames

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Abstract

Ammonia (NH₃)-based economy has been of great interest to replace conventional fossil fuels and thus mitigate carbon dioxide emissions. The present work considers blending ammonia with dimethyl ether (DME) to promote the flame speed of NH₃ flames under elevated inlet pressures using the 1D freely propagating flame model in Chemkin-Pro 2019. For this, the reaction mechanism is first validated by comparing numerical results with the experimental data available in the literature. Operating NH₃ in the presence of DME is found to enable the laminar burning velocity (SL) of NH₃ flames to be enhanced significantly. Reaction pathway and sensitivity analyses reveal that this change is due to the enhanced reaction rate arising from the variation in the major reaction steps and the sensitivities. Furthermore, the inlet pressure is shown to play a critical role in the SL of binary mixtures, but minimally impact NH₃/air. This difference is mainly because the relative importance of termination versus branching reactions for NH₃/DME flames under high pressure conditions is more remarkable. In general, the present work offers a guideline on the selection of fuel flexibility, and sheds light on the pressure dependence and fundamental enhancement mechanism of NH₃/DME-fueled flames.

Keywords: Ammonia, Dimethyl ether, Laminar burning velocity, Pressure dependence.

ACS21004

An Experimental Study of Ignition and Combustion Characteristics of Single Droplets of Vacuum Residues

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Abstract

The ignition and combustion characteristics of suspended single droplets of vacuum residues (VRs) were studied experimentally with a focus on the effect of asphaltene. Four VRs with different asphaltene content were tested and the droplet size, ignition delay time and flame duration were determined. Five stages of ignition and combustion of VRs were observed including (1) ignition of more volatile components evaporated from the droplet surface; (2) steady combustion of more volatile components evaporated from droplet surface; (3) splashing combustion of fuel vapours evaporated from droplet interior; (4) disruptive combustion due to the thermal decomposition of low volatile component (asphaltene) and (5) ignition and combustion of coke. The four VRs showed similar ignition delay time, suggesting that the ignition process of VRs was controlled by the vaporisation of more volatile components.

Keywords: Asphaltene; Combustion; Droplets; Vacuum Residues

ACS21023

Modelling a dilute spray flame using the eddy dissipation concept

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Abstract

A steady state model of a piloted dilute spray burner was developed and validated against experimental data. A realisable k-epsilon turbulence model was implemented in a steady state simulation. The eddy dissipation concept for resolving turbulence-chemistry interactions was used, with a Lagrangian-Euler description for the droplet and continuous phase interactions. Velocity and temperature radial profiles were compared between computations and experimental data. The velocity profiles showed reasonable agreement closer to the jet exit, with over-predicted evaporation causing discrepancies away from the jet centreline. Temperature was better represented further downstream, with strong qualitative agreement, but over-prediction of temperature away from the centreline. This is likely also due to the enhanced evaporation observed making more reactants available. Adequate quantitative agreement for velocity and temperature is noted at all axial locations, with strong qualitative agreement, indicating that this model is appropriate to capture the main features of a reacting spray flame. OH radial profiles were compared against temperature profiles at different axial locations, noting a constant jet spreading rate, and peak temperatures occurring at the peak OH concentration. Future work will investigate the application of this model in a cross-flow, as well as addressing the over-prediction of droplet evaporation.

Keywords: sprays, combustion, droplets, modelling

ACS21008

Dilute spray flames of ethanol and n-heptane in the transition to mild combustion

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Abstract

The structure and stabilisation mechanisms of ethanol and n-heptane spray flames are investigated in this study. The burner configuration involves a dilute spray of dispersed droplets which is produced and transported via a carrier gas stream of air to the reaction zone, where the flames are stabilised by a hot coflow of combustion products. A range of coflow conditions were implemented for the different flame cases, allowing the effects of the coflow oxygen (O₂) concentration and temperature to be examined independently. The resulting flames were analysed using three simultaneous laser diagnostic techniques, enabling the combined planar imaging of the hydroxyl (OH) and formaldehyde (CH₂O) radicals, along with the location of droplets. For both fuel types, a noticeable shift in stabilisation behaviour was observed with a variation in the coflow O₂ concentration from 11% to 3%, while the coflow temperature was not seen to have a significant impact. These flames also show an interesting departure from the typical behaviour observed for gaseous and prevaporised flames under similar conditions, particularly regarding the transition to the mild regime and the lift-off behaviour.

Keywords: Spray combustion, Mild combustion, Laser diagnostics, Flame stabilisation



ACS21003

Reactive π -diradicals found in soot forming flames

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Abstract

The formation of carbonaceous nanoparticles that grow into soot presents an ongoing challenge to the combustion community. In particular, what is the mechanism by which the gas phase aromatic soot precursors cluster to form nanoparticles? This transition is critical to understand to inhibit the formation of these toxic combustion products, but also to synthesis new carbon nanodots, fullerenes or graphene in flames and plasma gas environments. In this paper, evidence for new localised π -radicals is shown using high resolution atomic force microscopy and electronic structure theory that form thermally stable bonds in flames. Evidence is also shown for a π -diradical enabled by these localised π -radicals. These reactions occur in a barrierless chain reactions that are thermally stable. Finally, using ab initio molecular dynamics the reaction mechanism between colliding diradicals is revealed with a significant enhancement due to internal rotors. These species provide promising candidates for the clustering species involved in soot formation and provide some new strategies to reduce soot emissions.

Keywords: Soot, Inception, Nanoparticle, diradical

ACS21036

On the Combined Effects of Compositional Inhomogeneity and Ammonia Addition to Turbulent Flames of Ethylene

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Abstract

The paper is part of a broader program aimed at investigating the effects of co-firing clean fuels such as ammonia or hydrogen with hydrocarbons. The focus is on flame structure and stability as well as soot formation in turbulent mixed-mode combustion, which is highly relevant in practical combustors. While it is known that the addition of ammonia suppresses soot, visual inspection of compositionally inhomogeneous flames of ethylene-ammonia indicates a subdued level of soot suppression. Measurements of soot volume fraction, f_v and laser-induced fluorescence in selected UV and visible bands are made in selected flames to test this hypothesis. The paper reports measured profiles of f_v and LIF with a brief discussion of the results. It is found that, with the addition of ammonia, the peak soot volume fraction for inhomogeneous conditions is higher than that at the homogeneous limit.

Keywords: mixed-mode combustion, turbulent flames, compositional inhomogeneity, ammonia

Session 8 Kinetics and Solid combustion

ACS21025

Decomposition of Carbonyl Sulfide

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Abstract

Reduced sulfur species (H₂S, CS₂ and COS) arise as important by-products in numerous industrial processes, such as recovery of sulfur from sour gases, gasification of coal and conversion of biomass. This contribution investigates the pyrolysis process of COS by combining jet-stirred reactor (JSR) experiments with the ab-initio calculations and kinetic modelling, to probe the unusual behaviour of carbonyl sulfide (COS) during its thermal conversion process. The experiments identified the pyrolysis of COS commencing at 1100 K in the process accompanied by the formation of CO and the disappearance of COS. However, the literature mechanism tends to underestimate the onset of pyrolysis of COS by 80 K. By conducting sensitivity analysis, we pinpoint the reaction $\text{COS} + \text{S} \rightarrow \text{CO} + \text{S}_2$ as the controlling step. This step displays different kinetics depending on the temperature range, due to intersystem crossing (ISC) process. The quantum chemistry calculations for $\text{COS} + \text{S} \rightarrow \text{CO} + \text{S}_2$ performed with CBS-QB3 method capture the intersection seam between the singlet and triplet reaction surfaces. For low temperature range (< 800 K), the reaction shifts from triplet reactants into the singlet pathway through the crossing-over point that exhibits a lower activation energy ($E_a \approx 9.8$ kJ/mol). Under higher temperature (>1000 K), triplet pathway appears dynamically preferable due to its elevated exothermicity (i.e., more stable product species), although with higher activation barrier ($E_a = 31.5$ kJ/mol). The reaction mechanism based on this compartment leads to excellent agreement between the kinetic model and the experimentally-measured quantities, such as the onset temperature and the conversion profiles of detected species.

Keywords: Carbonyl sulfide, pyrolysis, inter-system crossing (ISC), jet-stirred reactor (JSR), sulfur chemistry

ACS21028

New Pathways for Formation of Toxic Species in Oxidation of 4-Chlorobiphenyl

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Abstract

We investigate the oxidation of 4-chlorobiphenyl (4-CB) in three laminar flow reactors: an alumina reactor exhibiting significant catalytic effects including promotion of O₂ (1Δg) and chlorination-dechlorination reactions at temperatures as low as 350°C; a high purity quartz reactor which produced significantly lower O₂ (1Δ) and negligible chlorination-dechlorination; and, a high purity quartz reactor with surfaces passivated by a boron oxide coating, in which typical gas-phase oxidation behaviour was observed at elevated temperatures. The laboratory-scale apparatus consisted of a 4-chlorobiphenyl vaporiser and a laminar flow reactor equipped with a sampling system for intercepting the volatile organic compounds (VOCs) and condensable products, such as polychlorinated dibenzo-p-dioxins and dibenzofuran (PCDD/Fs). 3-Monochlorodibenzofuran (3-MCDF) and some important VOCs species were formed at low temperature by the effect of surface generated singlet oxygen (1Δg) in the alumina reactor and (to a lesser extent) in the high purity unpassivated quartz reactor. The low and high temperature reaction mechanisms have been studied by quantum chemical techniques to explain formation of the product species.

Keywords: VOC, PCDD/F, pollutant formation in fires, surface effects in flow reactors

ACS21015

Partial oxidation of spent tyre pyrolysis oil for the production of carbon black

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Abstract

Carbon black (CB) was prepared by partial oxidation of spent tyre pyrolysis oil (STPO) using a drop tube furnace. The effect of process variables, including the reaction temperature (T_{reaction}: 1100 to 1400°C), residence time (R_{time}: 5 to 60s) and feedstock to oxygen ratio (F/O: 0.002 to 0.009 v/v) on the yield and elemental carbon content of CB were examined and optimised using the response surface methodology (RSM). T_{reaction} and F/O were shown to significantly influence both the yield and elemental C content of CB. The CB yield was strongly influenced by T_{reaction} and R_{time}, while CB properties were critically determined by T_{reaction} and F/O. The optimal T_{reaction}, R_{time} and F/O were 1330.8°C, 60s and 0.009. The corresponding CB yield and elemental carbon content under the optimum conditions were 53.5% and 95.7%, respectively. Furthermore, the CB showed reasonably low ash (<0.03%), volatile (~0.5%), sulphur (<0.7%) and high C (≥ 95%) contents. The BET surface area and indicative average particle size were ~ 14 m²g⁻¹ and <150 nm, consistent with group 8 rubber-grade CB from fossil fuel feedstocks.

Keywords: Carbon black, Partial oxidation, Response surface methodology, Spent pyrolysis tyre oil

ACS21009

Freeboard Effects on Instabilities in a Fixed Bed Biomass Combustor

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Abstract

Biomass combustion at the lab scale is mostly performed using fixed bed configurations. In the counter current configuration, combustion air is staged and supplied both from beneath the packed fuel bed (primary air, Q_p) and above the fuel bed (secondary air, Q_s). The location and amount of secondary air significantly influences combustion efficiency through combustion of post-bed volatiles in the freeboard. However, secondary air can also lead to instabilities which affect freeboard temperatures and may lead to incomplete combustion and noise-pressure coupling, both of which should be avoided. This paper into combustion instabilities examines the role of primary and secondary freeboard height along with secondary air staging ratios Q_s/(Q_s+Q_p)=0.25, 0.50, and 0.75, spanning globally fuel rich (Q_s+Q_p=300 L/min) or stoichiometric combustion (Q_s+Q_p=560 L/min). Results show that introducing secondary air at the later stage of 550mm downstream of the packed bed and Q_s/(Q_s+Q_p)=0.75 and 0.50 causes instabilities at both rich (300 L/min) and stoichiometric (560 L/min) conditions. Instabilities were also observed at rich conditions (300 L/min) if the secondary air is located closer to the packed bed (300 mm). The variation in post-secondary air freeboard height (secondary freeboard) did not generate any instabilities. Once initiated, the occurrence of these combustion instabilities was irregular (erratic) not periodic.

Keywords: Fixed bed combustion, Biomass, Wood Pellets, Freeboard Height, Instabilities-

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Effects of Constant and Staged Torrefaction Temperatures on Biomass Combustion and Pyrolysis

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Abstract

Torrefaction is a thermal pre-treatment method used to enhance the thermochemical, hydrophobic, and grindability properties of raw biomass. It is typically undertaken in an inert or oxygen deficient environment. In this study, the sensitivity of woody biomass fuels to two types of heating commonly reported in torrefaction research were investigated. Biomass fuel, in the form of 6.5 mm pellets torrefied at 300 °C was subjected for 30 minutes in a tube furnace to either a (i) (sudden) "constant heating" or a (ii) "staged heating" involving a gradual ramp-up. This paper analyses torrefied fuel properties through TGA (and indicator of thermochemical properties) and an immersion testing method (to assess hydrophobicity). Thermogravimetric profiles highlighted the elimination of hemicellulose and the decrease in the cellulose fraction in both torrefied samples from (i) and (ii). However, the extent of degradation in holocellulose fraction of biomass was much higher in samples torrefied using (ii) staged heating compared to (i) constant heating. Furthermore, staged heating also showed better hydrophobicity than the latter. The overall results highlight the need for research (into torrefied biomass) to also report the temporal evolution of heating when studying torrefaction due to its apparent effect on the overall properties of biomass.