Double Conditional Moment Closure simulation of n-heptane spray autoignition

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Autoignition of fuel sprays is a key feature of compression-ignition engine technology, and exhibits complex interactions between turbulence, chemistry, and multi-phase flow. A particular challenge for combustion modelling for diesel engine simulations is the need to account for three distinct modes of combustion: autoignition, flame propagation, and diffusion flames. This study focusses on Conditional Moment Closure methods for turbulent combustion modelling (Klimenko and Bilger, 1999), which provide a rigorous framework in which it is feasible to include detailed chemistry and potentially to account for a range of different combustion modes. First-order Single Conditional Moment Closure SCMC has been applied to Diesel engine combustion previously using mixture fraction as the conditioning variable (Bolla et al. 2013). In order to account for flame propagation and the development of a lifted diffusion flame after ignition, the conditional moments are allowed to vary in space, leading to CMC equations that can be four-dimensional partial differential equations (PDEs) (i.e. up to three spatial dimensions and one dimension for the conditioning variable), and incurring high computational costs. The objective of this study is to evaluate the performance of a new zero-dimensional first-order Double Conditional Moment Closure (DCMC) formulation that is able to describe autoignition, propagation and diffusion flames using two-dimensional PDEs (i.e. two-dimensions in conditioning variable space but with no spatial dimensions). The new DCMC formulation is presented and its performance compared directly with 2D axisymmetric SCMC results from Bolla et al. (2013) for the case of n-heptane spray autoignition in a combustion bomb (Picket 2011). The results indicate that the DCMC results are sensitive to the modelling of the conditional (cross-)dissipation rates of mixture fraction and progress variable but, with adequate models for the (cross-)dissipation rates, the zero-dimensional DCMC approach yields results in approximate agreement with the 2D axisymmetric SCMC results at a reduced computational cost. The computational advantages of the DCMC approach increases for practical combustion systems for which the SCMC would require three spatial dimensions.

Formulation

The double conditional moment closure equations are derived conditional on mixture fraction and progress variable \( c \), where the progress variable is normalised by a time-dependent function of mixture fraction,

\[
c(x, t) = \frac{\varphi(x, t) - \varphi_{\min}(\xi(x, t), t)}{\varphi_{\max}(\xi(x, t), t) - \varphi_{\min}(\xi(x, t), t)}.
\]

where \( \varphi = Y_{CO2} + Y_{CO} + Y_{H2O} + Y_{H2} \). The minimum value \( \varphi_{\min} = 0 \), and the maximum value is assumed equal to the value of \( \varphi \) conditioned on unity progress variable,

\[
\varphi_{\max}(\xi(x, t), t) = \langle \varphi | \xi = 0, \eta = \xi(x, t); t \rangle
\]

where \( \xi \) and \( \eta \) are the sample space variables for progress variable and mixture fraction respectively. Because the progress variable is time-dependent, the region of composition space described by the DCMC grows during autoignition, ensuring that the progress variable space remains well-resolved throughout the simulation.

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To enable a direct comparison with the results of Bolla et al. (2013), the DCMC equations are coupled with the same CFD code (Star-CD), keeping all of the RANS-based computational models unchanged, and employing the same fractional-step solution scheme. The doubly conditional dissipation rates of mixture fraction and progress variable are modelled in a manner that is equivalent to the modelling used by Nguyen et al. (2010) in the context of flamelet modelling, and following Nguyen et al. (2010) three alternative models for the cross-scalar dissipation rate of mixture fraction and progress variable are compared: first that the cross dissipation is zero; second, that the mixture fraction and progress variable gradients are perfectly aligned; and third, that the mixture fraction and progress variable gradients are always perfectly opposed. Using these models, the conditional (cross-)dissipation rates are computed in each CFD cell and then a global set of conditionally-averaged (cross-)dissipation rates is obtained through a pdf-weighted averaging procedure. The mixture fraction and progress variable distributions are assumed to be independent and they are each modelled by beta function marginal probability density functions.

Results
The 0D DCMC approach yields similar ignition delay times to the 3D SCMC and to the experimental measurements, in contrast to the 0D SCMC which always predicts an attached flame as shown in Fig. 1. However the lifted flame shape and lift-off length predicted by the DCMC are sensitive to the model used for the conditional cross dissipation rate of mixture fraction and progress variable. Simple modelling for the cross dissipation rate based on a transport for the mixture fraction-progress variable covariance equation is examined.

Figure 1. Temperature contour plots at 1.5ms after the start of injection for 3D SCMC, 0D DCMC, and 0D SCMC models. The 0D-DCMC conditional cross-dissipation rate is set to zero.

References
Bolla, M., Gundmundsson, T., Wright, Y., and Boulouchos, K., (2013) SAE Int. J. Engines 6(2) 1249-1261.
Autoignition of blends butanol-ethanol with diesel and biodiesel fuels in a constant-volume combustion chamber

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Extended Abstract

Diesel fuels can be blended with bioalcohols as a means to introduce a renewable fraction and to provide certain oxygen content. This renewable fraction could be additional to that already included in many diesel fuels with some biodiesel content, as it is usual in many countries. Some previous studies have reported reductions in the emissions of particulate matter and carbon monoxide when diesel engines operate with ethanol and butanol blends, although not unanimous trends have been reported in unburned hydrocarbons. The hydroxyl group of the alcohol molecule contributes to reduce soot formation and consequently particulate emissions, even more than other functional groups with similar oxygen content [1,2,3]. Among the alcohols to be used in diesel blends, ethanol and butanol have proved to have a significant potential to reduce life-cycle greenhouse gas emissions, as far as they can be produced by biological processes. Specifically, butanol can be produced from various methods, among which acetobutyllicum fermentation has superior interest, as far as the bio-acetone obtained as co-product is valued as such [4]. A previous work was published about blending stability, lubricity, viscosity and cold filter plugging point as the key properties of ethanol and butanol blends (among others) with diesel fuel [5]. Additionally, among the properties affecting the combustion process, cetane number is a limiting one. Alcohols exhibit low cetane numbers [6], and therefore, only minor concentrations of these alcohols in the blends are recommended to be used in unmodified diesel engines. The higher cetane number of butanol with respect to ethanol, together with its better miscibility, higher heating value and lower hydrophilic character, suggest that n-butanol is a better renewable component than ethanol in diesel blends [6,7], and consequently, its maximum concentration in diesel blends could be increased with respect to that recommended for ethanol.

Blends of alcohols with diesel or biodiesel blends are not expected to provide autoignition times proportional to their composition. Instead, the most reactive components (those with shorter autoignition times) contribute to shorten the autoignition time more that the least reactive ones to enlarge it. Therefore, experimental autoignition studies with these blends are necessary to evaluate their autoignition behavior.

The impact of ethanol and butanol concentrations on diesel and biodiesel blends are analysed in this study at a constant initial temperature and pressure. Tests were carried out in a constant-volume combustion chamber, following the experimental procedure proposed in reference [8] and pressure signals were recorded and analysed with a diagnostic model described in [9]. Tests were made for blends of ethanol and diesel fuel as far as their miscibility permitted, butanol and diesel and butanol and biodiesel. In all cases, the combustion process occurred in two stages, and therefore, two different ignition delays were defined: the first was denoted as $\text{ID}_{\text{CF}}$ because it was associated to the cool flame stage, and the second, $\text{ID}_{\text{M}}$, is associated with the main combustion.

As expected, increasing the alcohol content always led to a significant increase in both $\text{ID}_{\text{CF}}$ and $\text{ID}_{\text{M}}$. Since their trends are very similar, only $\text{ID}_{\text{M}}$ is shown in Figure 1. Such an increase was sharper at high alcohol contents, which is in agreement with other studies [1]. In the case of ethanol-diesel blends, no experimental results were obtained from 15% ethanol to 65% content, due to the weak miscibility of blends within this range. No tests could be done for ethanol blends when delay times were higher than 120 ms, because the acquisition window was exceeded. For the same alcohol content, the increase in ignition delay was always larger for
ethanol than for butanol blends. For butanol blends, the increase in delay time was very similar when diesel or biodiesel were blended.

The pressure peaks in the combustion chamber were observed to decrease as the alcohol content increased, especially in the case of ethanol, as a consequence of their reduced heating value. However, for low ethanol and butanol contents, some increases in the pressure peaks were observed (up to 15% butanol content and up to 5% ethanol content). These increases can be explained by a combination of effects: increase in the amount of premixed gaseous fuel-air mixture before combustion and increase of the flame speed derived from the presence of alcohols in the blends. Further alcohol concentrations led to progressive reductions of the pressure peaks, not only as a consequence of their lower heating values, but also of the over-diluted gaseous mixtures, which also contribute to slower flame velocities.

References

Structures of Lean Premixed Turbulent H\textsubscript{2}/Air Flames at High Karlovitz Numbers

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Keywords: DNS, premixed turbulent flames, flame regimes, Karlovitz number

Abstract

Premixed turbulent flames are widely used in industrial combustion devices, where the turbulent Reynolds numbers and Karlovitz numbers tend to be very high [1]. These non-dimensional numbers are defined as

\[ Ka = \left( \frac{u'}{S_L} \right)^{3/2} \left( \frac{\delta_L}{l} \right)^{1/2} \]
\[ Re_T = \frac{u'}{S_L \delta_L} \]

where \( u' \) is rms turbulent fluctuation velocity, \( l \) is integral length scale of turbulence, \( \delta_L \) and \( S_L \) are laminar flame thickness and speed respectively. At high Karlovitz numbers, the smallest turbulent length scale can be smaller than the typical chemical time scale, which can lead to the distributed or broken flame regime and significantly change the chemical pathways [2]. It is hard to measure or simulate such a reaction zone due to the high spatial and temporal resolution required. However, with the availability of increasingly powerful supercomputers, direct numerical simulation (DNS) of turbulent reacting flow at high turbulent Reynolds numbers and high Karlovitz numbers has become a reality, although actual DNS simulations are still far and few in between, especially when detailed chemical mechanisms are employed. The goal of this work is to study the detailed structure of lean premixed turbulent H\textsubscript{2}/air flames at high Krlovitz numbers using DNS with detailed chemical mechanisms.

In the present DNS of turbulent hydrogen/air flames, the three-dimensional, time-dependent, compressible Navier-Stokes equations and chemical species transport equations are solved with six-order compact finite difference schemes for spatial discretization and the low-storage third-order Runge-Kutta time advancing scheme using the Pencil code [3]. Turbulence was generated in a periodic box, which was then fed into the inlet plane of the main simulation. A one-dimensional laminar flame was generated using detailed chemistry to initialize the three-dimensional turbulent flame simulation. The size of the computational domain is 0.628 cm in x-direction, 0.314 cm in y-direction and 0.314 cm in z-direction. The Navier-Stokes Characteristics Boundary Conditions (NSCBS) are applied at the inlet / outlet and periodic boundary conditions are imposed in the spanwise and lateral directions.

The key parameters for the DNS cases conducted are summarized in Table 1. All the three cases are in the distributed/broken reaction zone with high Ka and Re values, and the turbulence intensity in case C is much higher than in previously published results [4, 5, 6]. Analysis of the DNS results shows that in all cases, turbulent small eddies from the unburned mixture side penetrate deep into the flame zone. The thickness of the broken reaction zone is
much larger than that in the thin reaction zone regime. The formation of distributed flame zones has significant influence on the transport processes and consequently the local and global reaction rate. The global reaction rate, however, shows a nonlinear relation with the $Ka$ and $Re$ numbers. Detailed results and analysis for all the cases will be presented at the conference.

Table 1 Key parameters for DNS of premixed turbulent $H_2$/air flames

<table>
<thead>
<tr>
<th>Case</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalence ratio</td>
<td>0.35</td>
<td>0.35</td>
<td>0.35</td>
</tr>
<tr>
<td>Laminar flame speed $S_L$ (cm/s)</td>
<td>21.2</td>
<td>21.2</td>
<td>21.2</td>
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<tr>
<td>Laminar flame thickness $\delta_L$ (cm)</td>
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<td>0.0628</td>
<td>0.0628</td>
</tr>
<tr>
<td>rms velocity $u'$ (cm/s)</td>
<td>2066</td>
<td>3725</td>
<td>5747</td>
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<tr>
<td>Integral length scale $l$ (cm)</td>
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<td>0.0628</td>
<td>0.0628</td>
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<tr>
<td>Turbulent Reynolds number $Re$</td>
<td>97.5</td>
<td>175.7</td>
<td>271.1</td>
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<tr>
<td>Karlovitz number $Ka$</td>
<td>962</td>
<td>2329</td>
<td>4463</td>
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</tbody>
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Reference

Methane – air laminar jet flames in high-pressure combustion

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MOTIVATION

A combustion facility has been recently set up in our laboratory aiming to characterize the response of local burning velocity to flame stretch rates in high pressure environments (up to 30 bars). The theoretically predicted linear relation between flame speed and stretch rate [1], is confirmed experimentally on atmospheric flames [2]. Some measurements of the linear factor (the Markstein length) in high pressure flames have also been reported but are scarce [3], in spite of its relevance to practical issues. As a first step to fill this gap, the aim of this work is to characterize the flame speed dependence for a larger range of gas pressures.

EXPERIMENTAL RIG

The combustion chamber (Figure 1.a) is a steel cylinder (1 m height, 30 cm inner diameter) with four opposed optical ports fitted with fused silica windows (12 cm diameter, 2 cm thickness). The windows allow the optical access to the rim (Figure 1.b) consisting of a 1 cm Ø laminar jet burner surrounded by a 2.5 cm width annular air coflow for stabilizing purposes.

The burner was fed with methane-air mixtures at a given equivalence ratio and room temperature. After ignition under atmospheric conditions, jet flames were observed and optically characterized at different pressures by gradually increasing the chamber pressure with a downstream control valve.

Figure 1. a) Combustion chamber and optical diagnostic systems: PLIF system (Quantel) with an intensified high-speed CCD camera (dicam pro) and PIV system (New Wave 120XT Dual-Nd:YAG-Laser) with PIV CCD camera (pixelfly). b) Close view of the burner seen from a window. The burner rim and the coflow annulus can be identified on the centre of the image, with the spark igniter device disposed laterally and the chimney on the top to stabilize the upwards gas combustion flow.

RESULTS

Preliminary studies have been performed with a very rich methane-air mixture ($\phi = 1.5$) to assure the premixed flame anchoring by the accompanying diffusion flame. Planar flame burning velocity was determined in the range 1 to 9 bar by measuring the flame inclination angle in the lower conical part where stretch effects are negligible (Figure 2). The resulting values are plotted in Figure 3.
CONCLUSIONS
The high pressure combustion facility has shown an excellent performance to characterize laminar jet flames in the tested pressure range (1 to 9 bar). Measurements of the burning velocity of rich methane–air flames have revealed a net qualitative change of behaviour occurring at about 4 bar. For pressures below this value, the burning velocity follows a power-law pressure dependence with an exponent close to −0.655, which is in agreement with other authors. This behaviour corresponds to an overall reaction order $n \approx 0.7$, reminiscent of first-order kinetics. However, at pressures larger than 4 bar, the burning velocity remains almost constant, a typical signature of bimolecular kinetics. Analyses of flame radiation are now underway to relate the change in the prevailing kinetic path to a change in the radiative properties of the radical pool in the flame.

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REFERENCES
Influence of Flame Surface on the Bending Effect in Turbulent Premixed Flames

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1 Background

Turbulent burning velocity $s_T$ measures the mean burning rate of a turbulent pre-mixture. Since $s_T$ is a marker for healthy flame propagation, it serves as a critical parameter in combustion system design. Pre-mixture turbulence properties ($u', \ell_0$) have a significant effect on $s_T$ based on scaling relationships with properties of the flame

$$s_T = F(u'/s_L, \ell_0/\delta_L, L/\ell_0)$$

where $u'$ is the turbulent intensity and $\ell_0$ is the integral length scale and the flame properties are laminar flame speed $s_L$ and laminar flame thickness $\delta_L$. The “bending effect” [1] in turbulent premixed flames refers to the non-linear variation of $s_T(u')$ given all other properties constant. The present work investigates the principal mechanisms of bending using Direct Numerical Simulations (DNS) and the Flame Surface Density (FSD) approach.

![Figure 1:](image)

Figure 1: The present DNS cases plotted to show a) their placement in the regimé diagram, b) the exhibited nonlinear “bending” curve of $s_T(u')$, and c) the underlying flame surface quantities involved in bending: integrated strain ($\alpha_t$) and curvature ($s_d h_m$) terms.

2 Methodology

DNS of a statistically-planar methane-air stoichiometric premixed flame has been conducted using Senga2 – details of the solver and properties of the flame and unburned mixture have been provided
in previous articles [3]. The placement of each of the 5 simulations in the regime diagram is given in Fig. 1 a – turbulence intensity $u'$ is the sole parameter varied across the different simulations.

3 Results and Discussion

In Fig. 1 b, the $s_T(u')$ curve has been shown as calculated by the parametric DNS study – the bending effect has been reproduced. While attempts have been made previously [2] to model the bending effect as observed experimentally, the present work is the first to highlight it in a DNS framework. Moreover, the source-terms of the FSD equation [4] have been analysed namely 1) $a_t$ is the turbulent surface strain and 2) $s_d h_m$ is the flame surface curvature term. In Fig. 1c, the integrated source-terms (normalized appropriately) have been used to illustrate the gradual change in sign of the flame surface density source with turbulent intensity. While at low $u'$, turbulent surface strain dominates and contributes positively to flame surface density, at high $u'$ flame surface curvature dominates and contributes increasingly negatively to flame surface density. Throughout the bending curve, however, flame surface area determines the turbulent burning velocity, i.e. $s_T/s_L \sim A_T/A_L$. Fig. 2 a and b show the local (non-integrated) surface strain and surface curvature terms across the turbulent flame brush with increasing $u'$.

![Figure 2: Local turbulent surface strain (a) and flame surface curvature (b) variations across the turbulent flame brush.](image)

These results highlight the importance of flame surface properties in determining the turbulent burning velocity and its variation with increasing turbulence intensity. It appears that $s_T$ is determined by flame surface area $A_T$ which is a function of turbulent straining $a_t$ and flame propagation $s_d h_m$.

References


Analysis of the co-variance of fuel mass fraction and mixture fraction in turbulent flame-droplet interaction: A Direct Numerical Simulation study

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Introduction

The closure of the mean reaction rate in the context of Reynolds Averaged Navier Stokes (RANS) simulations in turbulent inhomogeneous mixture combustion often requires the knowledge of the co-variance of the fuel mass fraction $Y_f$ and mixture fraction $\xi$, which is given by: $\overline{Y_f\xi''} = \overline{\rho Y_f' \xi''} / \overline{\rho}$ where $\rho$ is the density, and $\bar{q}, \bar{q} = \bar{pq}/\bar{p}$ and $q' = q - \bar{q}$ are the Reynolds average, Favre mean and Favre fluctuation of a general quantity $q$. Algebraic and transport equation based closures for $\overline{Y_f\xi''}$ have previously been proposed for purely gaseous phase combustion of inhomogeneous mixtures [1]. By contrast, the analysis of the statistical behaviour of $\overline{Y_f\xi''}$ and its transport for the combustion of droplet-laden mixtures has received limited attention. Furthermore, the validity of existing closures of $\overline{Y_f\xi''}$ and the unclosed terms of its transport equation, which were originally proposed for purely gaseous phase combustion, is yet to be assessed for turbulent spray flames. This gap in the existing literature is addressed here by analyzing the statistical behaviour of $\overline{Y_f\xi''}$ and the terms of its transport equation using a 3-D compressible Direct Numerical Simulations (DNS) database [2] of statistically planar turbulent flames propagating into droplet-laden mixtures where fuel is supplied in the form of mono-disperse droplets ahead of the flame for different initial values of droplet diameter $a_d$ and droplet equivalence ratio $\Phi_d$. The objectives of this study are to: (a) analyse the statistical behaviour of $\overline{Y_f\xi''}$ and the unclosed terms of its transport equation and (b) assess the validity of the existing models for the unclosed terms of the co-variance $\overline{Y_f\xi''}$ transport equation for turbulent spray flames in the context of RANS.

Mathematical Background & Numerical Implementation

A modified single-step irreversible chemical mechanism [3] was used to perform the present analysis. The activation energy and heat of combustion are taken to be functions of the gaseous equivalence ratio, $\Phi_g$, so that a realistic $\Phi_g$-dependence of the unstrained laminar burning velocity is obtained [3]. All species are taken to have unity Lewis number and are assumed to be perfect gases. Standard values have been taken for the ratio of specific heats ($\gamma=1.4$) and Prandtl number ($Pr =0.7$). The individual droplets are tracked in Lagrangian sense and the quantities transported for each droplet are the position, $\bar{x}_d$, velocity, $\bar{u}_d$, diameter, $a_d$ and temperature, $T_d$. The droplet and gaseous phases are coupled in the gaseous transport equations. Droplet evaporation leads to mixture inhomogeneities, which are characterized by the mixture fraction $\xi = (Y_F - Y_D/\gamma)/s/(Y_F + Y_D/\gamma)/s)$, where $Y_F = 1.0$ ($Y_D = 0.233$) is the fuel (oxygen) mass fraction in the pure fuel (air) stream. The fuel used here is n-heptane, $C_7H_{16}$, for which $s=3.52$ is the ratio of oxygen to fuel by mass and the stoichiometric fuel mass/mixture fraction is: $Y_{FSt} = \xi_{St} = 0.0621$.

The present study utilises a widely-used three-dimensional compressible DNS code SENGA [2]. High-order finite-difference and explicit Runge-Kutta schemes are used for spatial differentiation and time advancement, respectively. A rectangular domain of size $63.35D_0/S_b(\Phi_g=1) \times 42.17D_0/S_b(\Phi_g=1) \times 42.17D_0/S_b(\Phi_g=1)$ has been considered, where $D_0$ and $S_b(\Phi_g=1)$ are the unburned gas diffusivity and the unstrained laminar burning velocity of the stoichiometric mixture. The simulation domain is discretised using a Cartesian grid of size $384 \times 256 \times 256$, ensuring that both the thermal flame thickness of the stoichiometric mixture, $\delta_{th}$ (which is equal to $1.6D_0/S_b(\Phi_g=1)$ for the present thermochemistry), and the Kolmogorov length-scale, $\eta$, are resolved. The boundaries in the mean direction of flame propagation (i.e.
x-direction) are considered to be partially non-reflecting. The droplets are distributed uniformly in space throughout the y- and z-directions and in the region \(0 \leq x S_b(\phi_g=1)/D_0 \leq 16.53\) ahead of the flame. The reacting flow field is initialised based on the steady laminar solution for desired values of \(a_d\) and \(\phi_d\) for \(\tau = (T_{ad}(\phi_g=1) - T_0)/T_0\), where \(T_0\) and \(T_{ad}(\phi_g=1)\) are the unburned gas temperature and adiabatic flame temperatures of the stoichiometric mixture, respectively. Initial turbulent velocity fluctuations, generated using a standard pseudo-spectral method, have been superimposed on top of the steady laminar spray flame solution. The cases considered here have initial values of normalised root-mean-square (rms) turbulent velocities of \(u'/S_b(\phi_g=1) = 7.5\) and non-dimensional longitudinal integral length scale \(L_{x_1}/\delta_{th} = 2.5\). The ratio of droplet diameter to the Kolmogorov scale is \(a_d/\eta = 0.3, 0.4, 0.5\) for \(a_d/\delta_{th} = 0.06, 0.08, 0.1\), respectively.

Results & Discussion

Figures 1a-c present the instantaneous distributions of normalised fuel mass fraction \(Y_F/Y_{Fst}\), mixture fraction \(\xi\) and non-dimensional temperature \(T = (\bar{T} - T_0)/(T_{ad}(\phi_g=1) - T_0)\) (where \(\bar{T}\) is the instantaneous dimensional temperature) fields in the central \(x - z\) plane for \(a_d/\delta_{th} = 0.08\) and \(\phi_d = 1.0\) at a time \(t = 4D_0/S_b(\phi_g=1)^2\). The black dots indicate the droplets which reside immediately adjacent to the plane. The droplets shrink due to evaporation as they approach the flame, but may not completely evaporate until they have passed through the flame. In many cases, the evaporation of droplets is not complete on their arrival at the flame front and the reaction takes place predominantly under fuel-lean (i.e. \(\xi < \xi_{ad}\)) conditions. Therefore, the heat release and the resultant burned gas temperature are lower than the adiabatic flame temperature of the stoichiometric mixture [3]. This observed behaviour affects the statistical variation of the unclosed terms of the co-variance \(\nabla_T Y_F\nabla_T \tilde{\xi}\) transport equation which must be accounted for in the modelling of these terms. This paper assesses and identifies model expressions for the unclosed terms of the co-variance \(\nabla_T Y_F\nabla_T \tilde{\xi}\) transport equation for turbulent droplet-laden flames in the context of RANS.

![Figure 1](image_url) Instantaneous fields of (a) normalized fuel mass fraction, \(Y_F/Y_{Fst}\), (b) normalised temperature \(T\) with reaction progress variable c isolines (left to right \(c = 0.1, 0.3, 0.5, 0.7\) and \(0.9\)) in white and (c) mixture fraction \(\xi\) fields at the central \(x - z\) plane for the case with \(a_d/\delta_{th} = 0.08\) and \(\phi_d = 1.0\) at time \(t = 4D_0/S_b(\phi_g=1)^2\). Droplets are shown as black dots (not to the scale).

References

Abstract:

In the conversion of existing pulverized fuel plant from coal to biomass, it is necessary to ensure that the combustion behavior of the solid biomass fuels is engineered to match, as far as practical, that of the original plant design. While biomass feedstock characteristics vary considerably, one controllable variable for pulverized fuel is the size of the particles. Modelling for adaptation and design of boiler plant can be improved with detailed knowledge of the combustion behavior of individual particles of varying fuels. In this study, a laboratory-scale experiment has been used to examine the relationship between particle size and burn-out. The experimental method also allowed measurement of particle surface temperature and the rate of gas-phase potassium release from the combustion of individual particles.

Typical power plant biomass fuels including pine, eucalyptus, wheat straw and willow with particle sizes ranging from 0.5mm up to 3mm and with differing moisture content, aspect ratios and pretreatments were selected for study. Single particles were supported in a water-cooled cover and then exposed above a flame, simulating biomass combustion. Measurements of ignition delay, volatile burning time and char burn-out time were undertaken using high speed image capture. From the analysis of the large data sets obtained from these measurements, empirical relationships between particles mass have been obtained (e.g. figure 1). The data also enabled examination of the effects of particle size and shape on the duration of combustion.

Figure 1 – relationship between particle mass and burn-out for samples of willow
Thermo-gravimetric measurements on separate samples complement the single particle measurements as a means of validating the demarcation between the different stages of combustion and providing kinetic data.

Particle surface temperature was measured using an infra-red thermographic camera. The temporal profiles of particle surface temperatures were obtained from this and have been used to inform and verify modelling of the single particle combustion experiment.

A photo-detection device was also developed as a means of simple flame-emission spectroscopic measurement of gas-phase potassium release. The temporal profiles of gas-phase potassium release from the combusting particle for various biomass materials were observed (e.g. figure 2). This simple technique has provided interesting and useful insights into potassium release mechanisms, differences between various biomass materials and a means for estimating the proportion of potassium retained in char and ash particles at varying stages of burn-out.

Figure 2 – temporal profiles of potassium release from single particles of wood combusting in a methane flame

Keywords: biomass combustion, particle size, burn-out, potassium release
Effects of stoichiometry on premixed flames propagating in planar microchannels

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Abstract

Recent studies have shown that for flames freely propagating in narrow channels differential diffusion-induced instabilities may result in non-symmetric solutions and/or oscillating and rotating propagation modes [1]. This has been shown in the context of lean mixtures for which a single species transport equation with a single Lewis number of the deficient reactant can be used to represent the propagation problem. Here the effect of varying the stoichiometry on the symmetry breaking is investigated, using a two-reactant model and within the framework of the diffusive-thermal (constant-density) approximation. The computations show that near-stoichiometric mixtures stabilize the flame to symmetric solutions and that both the fuel and oxidizer Lewis number ($Le_F$ and $Le_O$, respectively) are responsible for the break of symmetry.

We consider a premixed flame propagating to the left at velocity $U_f$ in a planar adiabatic channel of height $h$. The mixture is at initial temperature $T_u$ and immersed in a Poiseuille flow given by the velocity components $u(y) = 6U_0(y/h)(1 - y/h)$ and $v(y) = 0$, with $U_0$ the mean velocity. The chemical reaction is modeled through $\nu_F F + \nu_O O \rightarrow \text{Products} + Q$, where $F$ and $O$ denote the chemical symbols of the fuel and the oxidizer, $\nu_F$ and $\nu_O$ the corresponding molar stoichiometric coefficients, and $Q$ is the heat of combustion per mole products.

In what follows, we define the equivalence ratio of the mixture as usual $\phi = s Y_{F_2}/Y_{O_2}$, where $s = \nu_O W_O/(\nu_F W_F)$, and $Y_{F_2}$ and $Y_{O_2}$ correspond to the mass fraction of fuel and oxidizer in the fresh unburnt region at $x \to -\infty$. To avoid the discussion of lean and rich mixtures separately, a convenient parameter $\Phi = (\nu_1 W_1 Y_{2_1})/(\nu_2 W_2 Y_{2_a})$ is introduced [2]. The subscripts 1 and 2 stand for the deficient and abundant reactants, respectively, and replace the subscripts $F$ and $O$ as appropriate.

Introducing non-dimensional variables $Y_1 = Y'_1/Y_{1_a}$, $Y_2 = \Phi Y'_2/Y_{2_a}$ and $\theta = (T - T_u)/(T_a - T_u)$, with $Y'_1$ and $Y'_2$ the deficient and abundant reactant mass fraction, respectively, and $T_a$ the adiabatic temperature of the mixture, and using $h$ and $h^2/D_T$ as the reference units of length and time, respectively, the steady problem reduces to the integration of the following equations in a reference frame moving with the flame:

\begin{align}
\sqrt{d}\{u_f + 6my(1-y)\} \frac{\partial \theta}{\partial x} &= \Delta \theta + d \omega, \quad (1) \\
\sqrt{d}\{u_f + 6my(1-y)\} \frac{\partial Y_i}{\partial x} &= \frac{1}{Le_i} \Delta Y_i - d \omega \quad i = 1, 2, \quad (2)
\end{align}

where the reaction rate, with unity reaction order, is given by

$$\omega = \frac{\beta^2}{2L^2} Y_1 Y_2 \exp\left\{ \frac{\beta(\theta - 1)}{1 + \gamma(\theta - 1)} \right\}, \quad (3)$$

with $L = Le_1 Le_2 (1 + A)/\beta$ and $A = 1 + \beta(\Phi - 1)/Le_2$, and subject to the boundary conditions

\begin{align}
x \to -\infty : & \quad \theta = Y'_1 - 1 = Y'_2 - \Phi = 0, \\
x \to +\infty : & \quad \partial \theta/\partial x = \partial Y'_i/\partial x = 0, \quad i = 1, 2, \quad (4)
\end{align}
The following parameters appear in the formulation: the Zel’dovich number $\beta = \frac{E(T_a - T_u)}{RT_a^2}$, with $R$ the universal gas constant, the heat release parameter $\gamma = \frac{(T_a - T_u)}{T_a}$, the reduced mass flow rate $m = \frac{U_0}{S_L}$, with $S_L$ the burning velocity of the planar flame, the propagation velocity of the flame $u_f = \frac{U_f}{S_L}$, and the Damköhler number $d = \frac{(h/\delta_T)^2}$, with $\delta_T = \frac{D_T}{S_L}$ representing the thermal flame thickness.

In the computations shown in Fig. 1, we selected $Le_F = 0.3$, $Le_O = 1.4$, $\beta = 10$, and $\gamma = 0.8$ as representative of hydrogen-oxygen mixtures in nitrogen-diluted inert gas. Flame propagation in channels of the order of 1 mm, $d = 20$, was considered. For assisted flow, $m < 0$, the flame is symmetric. Increasing $m$ towards positive values we find a bifurcation point, marked with $\circ$ in Fig. 1 (left), where the symmetry of the flame is broken, and only non-symmetric solutions are found. Such flames are stable and propagate faster than their symmetric counterparts (dashed curve), hard to find experimentally because of their unstable nature. Near-stoichiometric mixtures (see $\phi = 1$ curve) possess, however, such a markedly stable character than only symmetric stable solutions was found for all values of $m$, as anticipated in a different context in [3]. For lean mixtures, the present problem reduces to that solved before in [1].

References


Dynamic gas interactions with polycyclic aromatic hydrocarbon clusters

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Abstract

The initial formation of soot particles is still poorly understood. A complete description of this process would have widespread implications, from reducing the amount of soot released into the environment to controlling the manufacturing process of industrial carbon particles. The best description to date of nascent soot particles are aggregates of small polycyclic aromatic hydrocarbons (PAH) containing 10-20 rings \cite{1, 2}. Gas interactions are of primary importance in these early stages of soot formation; pressure effects the aggregation of the particles, acetylene grows and oxidation shrinks the PAH. Understanding how accessible gas species are to these self assembled PAH clusters becomes of primary importance to describing these early soot precursors.

Chen and coworkers found that there is a size dependent melting phenomenon in PAH clusters which significantly changes the surface topology of the clusters.\cite{3} At low temperatures they forms long turbostratic stacks of molecules held together by Van der Waals interactions. At high temperatures thermal motion breaks apart these structures opening the structure. Previously surface reactivity of these clusters were explored by applying a static probe to integrate the accessible surface area for potential chemical reactions using the concept of solvent excluded surface\cite{4}, however the dynamic interactions were not considered and it was not possible to determine whether penetration of the cluster was possible.

We present an investigation of the dynamic interactions between gas-phase molecules and coronene clusters. The study considers temperatures corresponding to both liquid and solid clusters. Nitrogen was used as a probe as it posses similar adsorption properties to reactive species present in soot gas phase re-
actions (i.e. O₂, NO, C₂H₂). We found two main scattering regimes: specular and diffuse. Specular scattering involved the direct reflection of the nitrogen by the cluster giving a short interaction time. Diffuse scattering led to a significant interaction time of the gas on the cluster surface. During diffuse scattering the nitrogen, attracted to the surface, hops between sites/wells of low potential energy. For solid clusters we found three main sites where the nitrogen spends extended time, hydrogen sites, pockets between stacks and pinned on the top carbon surface of the coronene. Increasing the temperature beyond the melting point of the clusters broke apart the stacks of coronene and allowed nitrogen to penetrate the cluster. We present a dynamic model for the interaction of gas-phase molecules with nascent soot particles. This can be used to improve the modelling of soot oxidation, growth and effect of pressure.

References


Combining low order network modelling with incompressible flame LES for thermoacoustic instability in an industrial gas turbine combustor

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Abstract

Ultra low NOx emissions from gas turbine combustors can be achieved using lean premixed combustion. However, this makes the combustor highly susceptible to thermoacoustic instability, which arises due to a two-way coupling between acoustic waves and unsteady heat release from the flame, and can cause fatigue failure of the combustor hardware. Predicting thermoacoustic instabilities is extremely challenging due to the range of length scales involved, from tiny chemical reaction scales to long acoustic wavelengths. It is for this reason that low order thermoacoustic network models are attractive, modelling the acoustic waves using linear theory. The combustor geometry is simplified into a network of connected simple modules, with the linear acoustic wave strengths tracked across module boundaries. The flame region is assumed to be ‘acoustically compact’, meaning that the flame can be represented as a thin sheet [1]. The unsteady heat release rate of the thin flame is assumed to respond weakly nonlinearly to upstream acoustic forcing. This means its response frequency matches the forcing frequency, but with a gain and phase change that depend on forcing amplitude as well as frequency. The resulting frequency response is known as a Flame Describing Function (FDF). In this work, the FDF is obtained via incompressible LES, which assumes that the flame responds primarily to hydrodynamic flow disturbances. The use of incompressible simulations allows much larger time steps, hence computational speed up, while the use of LES allows the large scale unsteady flow features to be captured accurately. Two incompressible LES codes, BOFFIN [2] and OpenFOAM [3], are tested, incorporating a complex (15-step [4]) and a simple (4-step [5]) chemical reaction mechanism for methane respectively. By combining the FDF with the low order network modelling tool, OSCILLOS [6], both the frequencies and growth rates of a combustor’s thermoacoustic modes can be predicted. The accuracy of above combined approach has been verified by measurements on a lab scale combustor [7]. In this work, this approach is extended to predict the thermoacoustic modes of a full-scale combustor [8] taken from a Siemens industrial gas turbine operated under 3 bar and 6 bar (see Fig. 1). Two low order network representations for the combustor geometry are built (see Fig. 2), and multiple acoustic forcing cases involving two forcing amplitudes (0.1 and 0.2) and seven forcing frequencies (200-1500 Hz) are applied at the combustor entrance. The responding flame heat release rates are numerically simulated and processed with fast Fourier transform to form a weakly non-linear FDF (see Fig. 3a). By incorporating the FDF into OSCILLOS, all the thermoacoustic modes under 3 bar pressure are predicted to have negative growth rates and be stable, in agreement with the experiments. The predicted modal frequencies are also in good agreement with the measurements (see Fig. 3b), giving confidence in this coupled approach for real industrial combustors.

Keywords: Thermoacoustic instability, incompressible LES, flame describing function (FDF), OSCILLOS, BOFFIN

References


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Figure 1: (Left) the original combustor from Siemens SGT-100 gas turbine; (right) the schematic of high pressure test facility built in German Aerospace Centre (DLR)

(a) Short model: without water spray section  
(b) Long model: with water spray section

Figure 2: Two low order network models of the DLR test facility (blue line: closed inlet; green line: open outlet; red line: compact flame sheet).

Figure 3: (a) FDF from BOFFIN LES, with polynomial fitting for forcing amplitude $A_U = 0.1$ (black) and 0.2 (red) at 3 bar pressure; (b) contour map of the complex s-plane with modal frequency $f$ versus growth rate $\sigma$. The predicted thermoacoustic modes of ‘Short model’ under forcing amplitude of 0.1 are marked by white stars at the minima, while frequencies of the corresponding measured modes are indicated by black dashed lines.

Modelling the Acoustic Response of Fuel Sprays in Gas Turbines

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ABSTRACT

This work forms part of the development of a methodology for the simulation and subsequent prediction of combustion instabilities within liquid fuelled gas turbines. Combustion instabilities predominantly occur when a small perturbation of heat release causes a sound wave to be generated, which then travels upstream to the fuel injector. This may then cause a change to the mass flow rate of air or fuel, or change the interaction between them, which can in turn then cause a periodic variation in heat release rate. If the characteristic time of this cyclic process is such that Rayleigh’s criterion is positive across the combustion chamber at any characteristic frequency then there will be amplification of this instability until the sound energy absorbed by the combustor components or leaving the chamber equals the amount of energy being generated through this mechanism.

A key factor in determining the stability or otherwise of a combustion system is how the fuel and air delivery to the reaction zone responds to an acoustic pressure wave. It has been identified that one of the weaknesses in the existing methodology is how to include the response of the spray, for example, alteration of fuel droplet size, velocity and number density post atomisation caused by the periodic changes of mass flow rate through the fuel injector. Therefore, this project seeks to model the acoustic response of gas turbine fuel injectors with two aims: firstly to develop a method of accurately including spray response into CFD calculations and secondly to use these calculations to further understand thermo-acoustic instabilities and how these can be managed.

Work at Loughborough University has recently shown that compressible URANS simulations coupled with characteristic boundary conditions implemented in an unstructured pressure based solver as part of OpenFOAM can be used to obtain the acoustic impedance of orifices of various length-to-diameter ratios [1]. This approach was subsequently applied to single phase simulations for predicting the acoustic impedance of generic fuel injector passages [2] and very good agreement with the experimental measurements was achieved. Experimental studies have been carried out to identify the phase averaged variation of fuel droplet properties through the use of PDA (Phase Doppler Anemometry). Based on the acoustically excited unsteady flow field calculated, we also conducted preliminary numerical studies on the transportation of fuel drops using the Lagrangian method. In these simulations the fuel drops are treated as solid particles and their influence on the continuum phase is ignored (i.e. one-way coupling). The simulation results obtained showed good qualitative agreement with the PDA data in terms of droplet momentum but the variation in droplet size and its distribution cannot be captured by this simplified simulation because the effect of the acoustic waves on atomisation is neglected,
methods of including this effect in the calculations forms a key part of our ongoing research. Future work will focus on using PDA derived phase averaged spray statistics to include the effect of the periodic change in mass flow rate through the injector on the droplet size, velocity, distribution and number density in LES and URANS computations with the ultimate goal being the accurate prediction of the flame transfer function in reacting flow simulations.

More recent work has focussed on the implementation of characteristic boundary conditions within the compressible version of PRECISE-UNS, an unstructured second order in space and time finite volume solver developed by Rolls-Royce plc, which will allow the testing of industry standard methods for the resolution of fully reacting flow. This implementation has been tested for its ability to convect pressure waves of a known frequency and amplitude through a duct with different outlet conditions such as those simulating a pressure node (figure 1a.) or velocity node with measurements made as to the dependence of these results on mesh sizing and time step. the ability of PRECISE-UNS to accurately resolve the mean flow field of a real lean-burn injector geometry has also been tested using URANS and RANS methods assuming both incompressible and compressible flow (figure 1b). This work so far has allowed a comparison of the acoustic impedance of a Rolls-Royce designed representative lean-burn fuel injector calculated using OpenFOAM, PRECISE-UNS and experiments utilising the multi-microphone technique.

![Figure 1](image-url)

**Figure 1**: a) An instantaneous contour plot of the fluctuating component of pressure (Pa) for the case where the upstream boundary condition is set to act as a pressure node and the downstream to inject a pressure wave at 53Hz. b) The unforced mean velocity magnitude (m/s) behind the representative lean-burn fuel injector geometry as simulated using a compressible URANS methodology in PRECISE-UNS.

REFERENCES


Dispersion of entropy waves advecting through combustion chambers

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Unsteady combustion in modern gas turbines generates large entropy waves, also known as hot spots. When these are accelerated through the stator vanes, they generate acoustic waves via a mechanism known as indirect combustion noise [1]. The upstream-propagating acoustic waves interact with the flame and can contribute to the thermoacoustic feedback loop [2], while the downstream-propagating waves contribute to the global noise [3]. The strength of each acoustic wave is directly proportional to the amplitude of the entropy wave reaching the inlet of the first stator blade.

Low-order models can be used to predict the noise generated by an entropy wave with reasonable accuracy, and at a fraction of the cost of numerical methods [4, 5]. These analytical models neglect the advection of the entropy wave through the turbulent combustion chamber, assuming the entropy wave arrives at the turbine inlet in the same form as that in which it was generated by the flame. The first computational analysis of the advection of entropy waves through a turbulent flow was performed by Morgans et al. [6]. For a fully resolved turbulent channel flow, they found that the entropy wave was strongly deformed by the shear dispersion of the flow, but all of the entropy was eventually convected downstream of the flow without loss in time-integrated amplitude.

The aim of this work is to extend the study of entropy wave advection to the case of a real gas turbine combustor geometry, whose flow includes far more complex features, such as recirculation zones and swirl. The particular combustor considered is the SGT-100 combustor [8, 9] shown in Fig. 1. Simulations are performed using the ReactingFOAM solver of OpenFOAM [7]. For entropy wave advection, a similar approach to that in [6] is used; the entropy wave is assumed to originate in the areas where mean heat release occurs. It is then advected as a passive scalar with the flow, using either the mean flow velocity or the instantaneous velocity at each point.

Example results, showing the effect of advection by the mean flow, are shown in figure 2. The outlet entropy wave strength indicates that a large amount of entropy is still able to reach the outlet. The flow features typical of industrial combustion chambers do have a significant effect on the entropy waves; in particular the recirculation zone results in an effective loss of entropy wave amplitude. This study will prove useful in deriving entropy wave advection models that pertain to real combustor flows.
Figure 1: The SGT-100 combustor simulated for the study [8, 9].

Figure 2: Source term of entropy (black) and entropy at the outlet of the combustor chamber (red).

References


