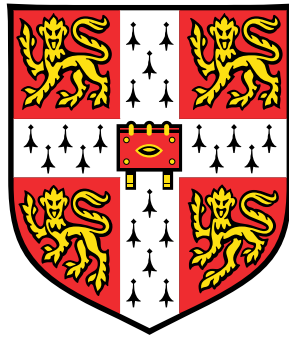


Simulating Extinction and Blow-off in Kerosene Swirl Spray Flames



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This dissertation is submitted for the degree of
Doctor of Philosophy

To my grandmother

Perhaps some day the precision of the data will be brought so far that the mathematician will be able to calculate at his desk the outcome of any chemical combination, in the same way, so to speak, as he calculates the motions of celestial bodies.

Antoine Lavoisier (1743–1794)

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification at this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation is estimated to contain approximately 60,000 words including appendices, figure captions, tables, and equations, and 65 figures.

Jenna Michelle Foale
31 October 2021

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Abstract

Alternative jet fuels are being developed for use with existing jet engines, however there are still knowledge gaps concerning how unusual compositions and properties of these fuels will affect combustion performance. Physical and chemical processes leading to problematic engine stability phenomena like flame extinction and lean blow-off (LBO) are still not well-understood for conventional spray flames, but alternative fuels provide additional challenges as they have been observed to have increased variability from expected behaviour at conditions close to LBO. Evaporation is known to be the limiting factor for combustion in spray flames, and experiments have shown both gaseous and spray flames exhibit increased amounts of local extinctions as the equivalence ratio is decreased. The flame structure and transient behaviour of spray flames behave very differently compared to gaseous flames at near-blow-off conditions and during the blow-off transient. Fuel starvation has been proposed in past experiments as a significant reason for why spray flames blow off more quickly and at richer equivalence ratio compared to gaseous flames, but has been explored very little in computational studies. The prediction of fuel starvation and LBO phenomena using numerical simulations with detailed chemistry are the primary focus in this work. Large Eddy Simulations (LES) with the Conditional Moment Closure (CMC) turbulence-combustion model are used, as this methodology has shown good results in simulating extinction and blow-off in both gaseous and spray flames in a lab-scale bluff body swirl spray flame configuration. The jet fuels simulated are the Dagaut Jet-A1 surrogate and the U.S. National Jet Fuels Combustion Program (NJFCP) fuels of interest: A2, C1, and C5. A2 is a conventional Jet-A used as a reference fuel, whereas C1 and C5 are synthetic kerosenes with unusual fuel chemistry or liquid property characteristics. These NFJCP fuels are represented using the Hybrid Chemistry “HyChem” lumped pyrolysis detailed kinetic mechanisms.

Simulations in non-premixed laminar counterflow flamelet configurations are conducted at pressures of 1 atm and 10 atm for stable scalar dissipation value flamelets up to extinction, and during the extinction transient. Species trends in the three HyChem fuels and the Dagaut Jet-A1 surrogate are compared in detail. In comparison with

experimental blow-off trends, only C5 deviates from expected behaviour and is the most robust fuel against extinction via high scalar dissipation rate. This highlights the interplay of both chemical and physical forces contributing to a real fuel’s tendency for LBO. Reignition of an extinguishing laminar flamelet using the HyChem A2 mechanism is also achieved through decrease of the scalar dissipation rate, although after a certain time the flamelet is not recoverable due to lack of chain-branching radical species.

A stable condition LES-CMC simulation using the HyChem A2 (Jet-A) chemical mechanism is used as a starting point and reference for lean blow-off simulations. The computational domain is based on the Cambridge bluff body swirl burner, with a structured LES mesh and a coarse structured CMC grid. The simulation is run using an Eulerian-Lagrangian framework for multiphase flow with the Abramzon and Sirignano evaporation model. Overall flame size and shape from the LES are fairly similar to experimental OH* and OH-PLIF with Mie scattering results, however there are significant differences in location of peak heat release rate and further work is required for validation of the simulations against experiments. CH is discussed as a promising experimental marker for local extinction and location of heat release.

Three fuel mass flow rates from the experimental blow-off curve for the Jet-A flame are simulated. The three simulations exhibited LBO at air flows between 5–20% greater than experimental bulk air blow-off velocities. Heat release rate decreased by at least 80% in the flame zone around the stoichiometric mixture fraction, however globally the combustor saw an increase in heat release rate due to the presence of unburnt droplets continuing to vaporise downstream. The asymmetric flame structure and duration of the blow-off transient in the simulations align very well with previous experiments with kerosene and other low-volatility fuels. The LBO transient lasted between 10–30 ms. Fuel starvation is suggested to be a driver of spray flame extinction, through decreased temperature and reduced evaporation caused by increased quantities of cold air in the system. Unburnt vaporised fuel remains in regions of temperature below 1200 K, where the fuel is no longer able to pyrolyse completely, resulting in non-flammable local mixtures. The quantity of local extinctions observed in both conditional and unconditional space is lower than expected compared to gaseous flames, and is linked to low values of the conditional scalar dissipation rate. Changing the model used to close the conditional scalar dissipation rate in the CMC equations is suggested as a potential way to improve the LBO results, as the Amplitude Mapping Closure model does not account for the very lean mixtures experienced at LBO conditions.

Publications

The work from this thesis has been published in the following:

Conference papers

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Nomenclature

Roman letters

a	Thermal diffusivity, $\equiv \lambda/(\rho C_p)$ [m^2/s]
d_d	Droplet diameter
e	Subgrid scale conditional flux, [s^{-1}]
$\mathbf{f}$	Body force vector [N/m^3]
h, h_s	Enthalpy, sensible enthalpy [J/kg]
k	Turbulent kinetic energy [m^2/s^2]
m_d	Droplet mass
p	Pressure
r	Radial coordinate, radius
t	Time
$\mathbf{u}$	Velocity vector, $= (u_x, u_y, u_z)$
u'	Turbulent velocity fluctuation
$\mathbf{x}$	Cartesian coordinate vector, $= (x, y, z)$
x	Cross-stream coordinate
y	Axial coordinate
C_p	Isobaric specific heat capacity [$\text{J}/\text{kg}/\text{K}$]
D	Mass diffusivity [m^2/s]
Da	Damköhler number, $\equiv \tau_p/\tau_c$
E_a	Activation energy [J/mol]
$\mathbf{F}$	Force vector [N]
G	Error function distribution
$\mathbf{I}$	Identity matrix
Le	Lewis number, $\equiv a/D$
Ka	Karlovitz number, $\equiv \tau_c/\tau_K$
LHV	Heat of evaporation [J/kg]
N	Scalar dissipation rate [s^{-1}]

Nomenclature

Nu	Nusselt number
Pr	Prandtl number, $\equiv \nu/a$
$\tilde{P}$	Probability density function or filtered density function (in LES)
Q_α, Q_h, Q_T	Conditional means of mass fraction Y_α , enthalpy and temperature
Re	Reynolds number
R_u	Universal gas constant, ≈ 8.314 J/mol/K
S	Strain rate tensor (LES-resolved)
Sc	Schmidt number, $\equiv \nu/D$
Sh	Sherwood number
T	Temperature
T_a	Activation temperature
U_b	Bulk velocity
$\mathbf{U}_d, \mathbf{U}_p$	Droplet (d) or particle (p) velocity vector
V	Volume
Y	Mass fraction
X	Mole fraction
W	Molar mass

Greek letters

δ	Delta function, or time step
η	Sample space variable of ξ
λ	Thermal conductivity [W/m/K]
μ	Dynamic viscosity [Pa · s]
ν	Kinematic viscosity, $= \mu/\rho$ [m ² /s]
ξ	Mixture fraction [-]
ξ_{st}	Stoichiometric mixture fraction
ρ	Density, [kg/m ³]
τ	Reynolds stress, [m ² /s ²]
ϕ	Equivalence ratio
ϕ_{ov}	Overall equivalence ratio (total amount of liquid and gaseous fuel)
$\dot{\omega}_\alpha, \dot{\omega}_T$	Reaction rate for species α and temperature, [s ⁻¹]
Γ	Gamma function
Δ	LES-filter width
Π	Volumetric evaporation rate per unit volume [s ⁻¹]

Subscript indices

b	bulk, as in bulk air velocity
cmc	concerning the resolution of the CMC
d	droplet
exp	experimental measurement
F	fuel
G	gaseous
L	liquid or laminar
les	concerning the resolution of LES
NS	Navier-Stokes
res	resolved (by LES)
sat	saturation
sgs	sub-grid scale (unresolved by LES)
T	turbulent
V	vapour from the fuel

α	chemical species
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Superscript indices and overbar symbols

'	Fluctuations around the conventional mean, $Y' = Y - \bar{Y}$
"	Fluctuations around density-weighted mean, $Y'' = Y - \tilde{Y}$, or fluctuations around the conditional mean, $Y'' = Y - Q$
-	Average
$\sim$	Density-weighted Favre average for LES-filtered quantities

Acronyms

AMC	Amplitude Mapping Closure, model for $N \eta$
ATF	Artificially Thickened Flame
AJF	Alternative jet fuel
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy (number), $\equiv u \delta t / \delta x$
CMC	Conditional Moment Closure
DCMC	Doubly Conditional Moment Closure
DCN	Derived cetane number (inversely $\propto$ autoignition delay time)
DNS	Direct Numerical Simulation

Nomenclature

FDF	Filtered density function (= sub-grid PDF in LES)
FGM	Flamelet Generated Manifold
FPV	Flamelet Progress Variable
HRR	Heat release rate [W/m ³]
LES	Large-Eddy Simulation
PDF	Probability density function
NJFCP	National Jet Fuels Combustion Program (U.S.A.)
OH-PLIF	OH Planar Laser Induced Fluorescence
OS	Operator splitting
PDA	Phase Doppler Anemometry
PDF	Probability density function
PIV	Particle Image Velocimetry
RANS	Reynolds-Averaged Navier-Stokes
RMS	Root mean square
SAF	Sustainable aviation fuel
SDR	Scalar dissipation rate
SF	Stochastic Field
SGS	Sub-grid scale

Chapter 1

Introduction

1.1 Motivation

In 2020, aviation saw its largest curtailment in history. The pandemic caused massive revenue losses on the order of tens of billions of U.S. dollars per continent [Dichter et al., 2020; Mazareanu, 2021a] and a 90% reduction in European air passenger traffic (compared to a reduction by 61% globally) [Mazareanu, 2021a]. Based on analyses of responses to crisis events like 9/11 and the Great Recession, global air traffic is not expected to return to pre-pandemic levels until about 2024 [Bouwer et al., 2021]. Due to the significant decrease in air traffic, another result of the pandemic in Europe was the overall reduction of carbon dioxide emissions from flights by 57% in 2020 [Eurocontrol, 2021]. Of course, this reduction is only temporary—once passengers return to the skies, trends indicate that global passenger numbers will double every 15 to 20 years [Mazareanu, 2021b], particularly as the middle class in the Asia-Pacific region continues to grow.

This expected growth in air travel, and corresponding growth in emissions, means that it is more important than ever now to reduce emissions from aviation. Increased presence of pollutant compounds produced by current jet engines such as ozone (O_3), nitrogen oxides (NO_x), particulate matter ($PM_{2.5}$, which includes soot), and unburnt hydrocarbons [Yim et al., 2015] has direct human health consequences: lung cancer, as well as heart and respiratory diseases. In 2015 it was estimated that global aviation emissions cause roughly 16,000 premature deaths per year, with $PM_{2.5}$ exposure causing 87% of early deaths [Yim et al., 2015].

It has always been in the aviation sector’s interest to reduce emissions like soot and to increase engine efficiency, the evidence being that fuel-burn per passenger-kilometre has decreased by 50% since 1990 [Dichter et al., 2020]. However, with the goal set by

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the Intergovernmental Panel on Climate Change (IPCC) to reach net-zero emissions by 2050, aviation will need to redouble efforts to explore various ways of reducing its greenhouse gas emissions. Interest has spiked in “zero-emission” alternative propulsion for aircraft using electricity or hydrogen to replace conventional kerosene-powered planes with smaller aircraft [Dichter et al., 2020]. Nonetheless, these new technologies face many hurdles in implementation. Batteries for electric aircraft are lower in energy density than jet fuel, such that using today’s technology an aircraft would require 50 kg of battery weight to equal the energy of 1 kg of kerosene. For a hydrogen combustion-powered aircraft, to get the same energy density, liquefied hydrogen would necessitate four times the volume of jet fuel, meaning that either the number of passengers or quantity of cargo would need to be reduced [Dichter et al., 2020].

In the near-term, it is critical to kick start funding into researching these radically different technologies in order to meet goals on climate change, despite the current debt of the industry [Bouwer et al., 2021]. However, major companies such as Airbus report that none of these concepts will exist beyond that of a limited number of prototypes by 2035 [Hepher & Frost, 2021], and even then only for shorter range aircraft carrying fewer than one hundred passengers. Hydrogen may only become widely used in aircraft around the year 2050 [Hepher & Frost, 2021]. In order to continue to reduce emissions while still servicing the growing interconnectivity of the globe, improved gas turbine and combustion technology in addition to the use of sustainable aviation fuels (SAFs) must be undertaken in parallel to the development of “zero-carbon” technologies.

SAFs, also known as “drop-in” fuels or alternative jet fuels (AJFs), are seen as the most practical way forward, working with existing technology to decrease emissions. These alternative fuels do not require changing the entire fuel system or energy exchange mode of an aircraft. SAFs also have the potential to significantly reduce carbon emissions both during flight and during life-cycle emissions. This could be through carbon sequestration via growth of biofuel feedstock or conversion of a waste material to fuel, and could range in CO₂ reductions from anywhere between 30-100% [Blakey et al., 2011; Dichter et al., 2020; Rye et al., 2010].

It is important to get a deep understanding of the chemical and physical behaviour of potential alternative jet fuels as soon as possible, as projections indicate that in order to meet the carbon dioxide reductions set forth by the IPCC, a vast number of biofuel refinery facilities will need to be built every year to keep up with consumption and deployment of increasing amounts of SAFs [Bullerdiek et al., 2021; Staples et al., 2018].

Alternative fuels for use in aviation are already being developed and standardized to mitigate emissions as well as improve fuel stability limits, although currently they account for less than 1% of total consumed jet fuel [Dichter et al., 2020]. These are fuels that are characteristically similar to commercially used Jet-A/A-1 kerosenes (composed primarily of paraffins) and meet existing jet fuel specifications [Rye et al., 2010]. However, different fuel feedstocks (such as Jatropha, algae, rapeseed) combined with processes like Fischer-Tropsch or hydroprocessing produce alternative jet fuels with dramatically different and unique compositions. Properties of interest (ignition characteristics, flame structure, extinction limits, and combustion speciation) are very sensitive to fuel composition and play active roles in engine performance and stability, affecting flame blow-off, high altitude relight, combustor efficiency and emissions [Zhang et al., 2016]. Fundamental studies are thus needed to better understand the combustion characteristics of alternative jet fuels to ensure their behaviour will not go out of bounds from experience with existing jet fuels. Better fundamental understanding will also streamline fuel testing programs, allowing for manufacturers to identify unusable alternative fuels before expensive component and engine tests are carried out [Zhang et al., 2016].

In combustion terms, the *stability* of an engine can refer to the range of fuel-air ratios over which stable combustion is possible, or to the maximum air velocity at which a flame can still survive, which is at the fuel-lean end of flame-sustaining fuel-air ratios [Lefebvre & Ballal, 2010]. In general, engine-makers want to continually widen flame stability limits in order to enable engines to operate in unfavourable conditions, such as at high altitude where external temperatures and pressures are low. A major operational stability concern in existing gas turbine engines is the issue of flame blow-out or blow-off. A visual example of an unusual large scale external flame blow-off event from an SR-71 afterburner is shown in Fig. 1.1. Flame blow-off occurs when the flame is pushed over the edge of its stability limits and is typically caused by air velocity exceeding the maximum value the system can withstand before flame extinction [Lefebvre & Ballal, 2010]. This maximum air velocity limit of a system is known as the blow-off velocity U_{BO} . This phenomenon can cause the flame in a jet engine combustor to extinguish unexpectedly— a potentially dangerous situation for a pilot and passengers if an engine were to fail during take-off or landing.

Lean blow-off (LBO), which is also known as *global extinction* or *weak extinction*, is a concern in industry due to current emphasis on lean-combustion engine designs to reduce emissions, where lean-combustion refers to burning fuel with an excess of air. As air is increased in the fuel/air mixture, the combustion process is weakened and



Fig. 1.1 Photograph of a flame detachment event exiting the afterburner of an SR-71 after a high gravity manoeuvre. Photograph is reproduced with permission from Campbell & Chambers [1994].

more vulnerable to small perturbations in the flow [Muruganandam et al., 2004]. One component of the flame blow-off phenomenon are *local extinctions*, which are small holes in the flame where no combustion occurs. Local extinctions have been experimentally observed to increase in frequency and duration for premixed gaseous flames as the flame is operated closer to U_{BO} [Muruganandam & Seitzman, 2005; Nair & Lieuwen, 2007], as well as in Jet-A non-premixed spray flames [Muruganandam et al., 2004]. Flame lift-off is another precursor of blow-off in premixed flames [Shanbhogue et al., 2009] and turbulent jet non-premixed gaseous flames [Peters & Williams, 1983], where the flame is “lifted” by the high air velocity away from the site of fuel/air injection. Once air velocity is increased beyond U_{BO} , then the blow-off transient followed by global extinction of the flame occurs.

However, studies on the structures of non-premixed flames and spray flames during the blow-off transient show that spray flames behave distinctly differently from non-premixed flames during LBO [Cavaliere et al., 2013; Yuan et al., 2018]. These studies suggest that not only local extinctions, but also *fuel starvation* phenomena may contribute to the blow-off of spray flames. The notion of fuel starvation, which is caused by reduced fuel vaporisation and pyrolysis, is an important distinction in the blow-off process for spray flames compared to gaseous flames, and warrants deep exploration in experimental and numerical studies as a potential driving cause for spray flame blow-off. The underlying physics of the LBO phenomenon are still not fully understood and are difficult to predict accurately with current computational models [Esclapez et al., 2017], especially for spray flames relevant for gas turbine applications.

LBO is a very important stability criterion for selecting a fuel appropriate for aircraft engines [Colket et al., 2017]. It has also been observed that fuel-chemistry has the largest effect at lean conditions, making LBO a critical factor when developing new aviation fuels [Colket et al., 2017]. Improving understanding of the physics of LBO will aid engine designers and computational modellers to create more stable engines for future fleets of jet aircraft, saving money on expensive trial-and-error experimental testing.

The National Jet Fuels Combustion Program (NJFCP) was founded in the U.S. to conceive a coordinated international industrial and academic collaboration to address the issue of fundamental characterization of jet fuel composition and chemistry in the context of gas-turbine combustion [Colket et al., 2017]. The aims of the program are to use reference fuels (petroleum-derived) and computational modelling to characterize fuel behaviour. There are still improvements to be made in simulating transient physics and finite-rate kinetic phenomena in conventional heavy hydrocarbon fuels, which warrants deeper exploration and study in order to create standards for comparison. Alternative fuels can then be characterized experimentally and computationally using fundamental fuel kinetics and combustion data and compared against referee fuels for effects on LBO, relight and cold start [Colket et al., 2017].

The research group where this doctoral work was performed fits into this program with the task of researching LBO of kerosene spray flames in a well-studied bluff-body swirl burner [Cavaliere et al., 2013; Giusti & Mastorakos, 2017; Tyliczszak et al., 2014; Yuan et al., 2015; Zhang et al., 2015], both experimentally and numerically. Prior to the start of this work, experimental data using this burner was collected on conventional and synthetic jet fuels under study in the NJFCP to explore LBO behavior of alternative fuels with unusual fuel chemistry or liquid properties [Allison et al., 2018; Sidey et al., 2017]. This will be discussed in the subsequent literature review. The fundamental studies in the current work are part of the NJFCP effort to update and validate chemical kinetic models (fuel chemistry), Large Eddy Simulation (LES) turbulence-combustion models, as well as spray and evaporation models. Success in these realms will allow for future jet engine designers to have the necessary tools on hand to design new gas turbine combustors which will increase flame stability and operability limits while decreasing emissions. This will be achieved through replicating experimental findings using advanced combustion models to capture LBO phenomena of kerosene spray flames in the Cambridge bluff-body swirl burner.

This thesis endeavours to contribute a stronger understanding of the chemical and physical processes involved at the lean limit of operability for jet fuels.

Key contributions of this work include:

- emphasizing the role of fuel starvation as a driving cause of LBO in spray flames.
- evidence of fuel starvation phenomena in simulations, such as asymmetric flame shapes, presence of unburnt droplets, and shrinking flame isosurfaces.
- an attempt to simulate the blow-off curve of a practical aviation fuel.
- detailed analysis of intermediate species, including soot precursors and markers of extinction and heat release, and their response to varying amounts of scalar dissipation rate, pressure, and air velocity.

1.2 Strategy

Kerosene is a complex liquid fuel composed of many heavy hydrocarbon species. To capture the differences in chemical composition and physical properties of various jet fuels in reacting simulations requires detailed chemical mechanisms capable of modelling the fuel pyrolysis and the oxidation of the pyrolysis products. In addition, each fuel’s physical properties must be implemented correctly for accurate spray characteristics. A comprehensive turbulence-combustion model which accounts for species variation in time and space coupled with a transient computational fluid dynamics solver should be used along with detailed chemistry to capture key transient phenomena like LBO, extinction, and the formation of pollutant precursors. Additionally, experiments must be undertaken to allow for the computational model to be assessed for validity through comparison with real results.

Experiments studying non-premixed LBO of the conventional and alternative kerosenes from the NJFCP were conducted in the Cambridge bluff body swirl spray burner [Allison et al., 2018; Sidey et al., 2017] to study chemistry effects on LBO, and to make a blow-off curve comparing the LBO of the fuels at different fuel flow rates. They looked at three NJFCP fuels of interest: A2, C1, and C5. A2 is a conventional Jet-A kerosene, which is used as a reference fuel, whereas C1 and C5 are synthetic kerosenes with unusual fuel chemistry or liquid property characteristics. C1 has an unusually low derived cetane number (DCN) which corresponds to a longer autoignition delay time, whereas C5 has unusual liquid viscosity and its distillation mixture of hydrocarbons all boil at approximately the same temperature. The work of Allison et al. [2018]; Sidey et al. [2017], which includes time-averaged and instantaneous OH* chemiluminescence and OH-Planar Laser Induced Fluorescence (PLIF) with Mie

scattering results, provides a useful comparison for numerical models to validate their approach. Studying the fuels in a simple lab-scale combustor geometry rather than a realistic gas turbine combustor [Esclapez et al., 2017] allows for clearer isolation of effects of fuel chemistry and spray characteristics on local extinctions and LBO.

Under the NJFCP, detailed chemical mechanisms such as the Hybrid Chemistry “HyChem” lumped pyrolysis approach [Wang, 2018; Wang et al., 2018a,b; Xu et al., 2018] have been developed for numerical simulations to have tailored chemical mechanisms to describe the behaviour of compositionally different kerosenes like A2, C1 and C5. To assess the HyChem approach against more established detailed mechanism approaches such as the surrogate model for jet fuel [Dagaut, 2002], comparisons need to be made between chemical mechanisms using flame simulations.

The Conditional Moment Closure (CMC) turbulence-combustion model has demonstrated success in predicting local extinction and LBO in both gaseous [Garmory & Mastorakos, 2011; Zhang & Mastorakos, 2016] and high-volatility spray flames [Giusti & Mastorakos, 2017; Tyliczszak et al., 2014] using LES. Conditional Moment Closure was originally developed by Bilger [1993] and Klimenko [1990] independently and jointly reviewed in Klimenko & Bilger [1999]. CMC is a statistical and deterministic coupled turbulence-combustion model which utilises non-premixed flamelets¹, mixture fraction², and scalar dissipation rate³ concepts. The main assumptions of CMC are that most fluctuations of quantities of interest, Q , can be associated with fluctuations of a single conditioning variable, typically the conserved scalar mixture fraction, and that the fluctuations around conditional averages are small [Klimenko & Bilger, 1999]. This allows for a simple first-order closure for the highly non-linear chemical reaction source term. As CMC is able to solve the temporal and spatial evolution of conditionally-averaged flame structures, it is capable of solving for finite-rate chemical phenomena, such as: local extinctions, blow-off, autoignition, and pollutant formation. Another benefit of the CMC approach is that it can use detailed chemical mechanisms in a computationally feasible manner by solving for CMC transport equations on a comparatively coarse mesh to those commonly seen in computational fluid dynamics (CFD).

LES is a CFD tool that directly solves Navier-Stokes equations for the large-scale eddies and vortices of turbulent flows, which contain most of the kinetic energy and

¹Laminar flame counterflow configurations used to approximate the structure of turbulent flames.

²Conserved scalar between zero for pure oxidizer and one for pure fuel. Relates the fractions of mass from the fuel and air to the transport and combustion of species mass fractions.

³Rate at which fluctuations in the mixture fraction are dissipated. High scalar dissipation rates are associated with local extinctions [Peters, 1983].

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depend more on combustor geometry, while the small scales of turbulence, which are more universal in nature, are instead filtered out and approximated with turbulence models. This considerably reduces computational cost compared to Direct Numerical Simulations (DNS), which require very fine meshes to discretise the Navier-Stokes equations in order to forgo any turbulence modelling. LES can perform transient simulations at a feasible computational cost and accuracy using turbulence submodels such as the constant Smagorinsky model [Smagorinsky, 1963] used in this work.

When used with LES, the CMC model has shown good predictive capability as the LES is able to resolve fluctuations in the scalar dissipation rate and mixture fraction that may not have been taken into account using the simple first-order closure and single-conditioning variable. CMC can be referred to as a “subgrid” turbulence-combustion model, as it resolves the turbulence and chemistry interactions which occur at the smallest scales, which are not spatially resolved by the LES. LES-CMC is capable of predicting various transient phenomena and has been modified to include spray evaporation source terms in the governing CMC equations [Mortensen & Bilger, 2009] as well as in the mixture fraction and mixture fraction variance equations solved by the LES [Jiménez et al., 2001; Pera et al., 2006; Réveillon & Vervisch, 2000].

Modelling of spray combustion is executed in this thesis using an Eulerian-Lagrangian framework, where Eulerian refers to the continuous gaseous “carrier” phase and Lagrangian refers to the point-based representation of parcels of droplets and their equations of motion. The multiphase flow is two-way coupled, such that the gaseous phase influences the disperse spray phase and vice versa. The droplets are injected as a polydisperse⁴ dilute spray in the same manner as in Sitte [2019] using the Abramzon & Sirignano [1989] single droplet evaporation model with Stefan flow correction. The dilute spray model is used without spray breakup, droplet collisions, film deposition or agglomeration in order to make the simulations feasible within the time constraints necessary for using detailed chemistry. The focus regarding spray in this work is the effect of fuel evaporation on local extinctions and LBO, alongside the chemical species behaviour during these events. Building on the findings of Cavaliere et al. [2013] and Yuan et al. [2018], this work emphasizes how fuel starvation through reduced evaporation and pyrolysis contributes to extinction in spray flames.

Two types of simulations using the CMC combustion model are executed in this work using the detailed kerosene mechanisms: 0D-CMC, and LES-CMC. 0D-CMC is a simplified version of LES-CMC into a zero-dimensional transient laminar flamelet model in which temperature and species are dependent only on time and the mixture

⁴Droplets vary in size. The Rosin-Rammler distribution is used in this thesis.

fraction. The 0D-CMC equation only includes an unsteady term, a diffusion term via a user-prescribed maximum scalar dissipation rate, and a chemical source term which is solved using the detailed chemical mechanisms. Turbulence and spray effects are not represented in this framework.

Simulations using 0D-CMC are run in a counterflow diffusion flame configuration at various scalar dissipation rates and two pressures to explore the different chemical and extinction behaviours of the conventional and alternative kerosenes in a simpler context without spray effects. Scalar dissipation rate is used analogously to air velocity in these simulations. In order to cause extinction of the flamelet, a critically high scalar dissipation rate was found for each of the fuels above which the flamelet could not be sustained and would extinguish to inert conditions. After the analysis of kerosene extinction in 0D-CMC, the results are used as an input for initialising the three-dimensional LES-CMC simulations as well as quantifying useful metrics for determining extinction in the turbulent flames.

The LES-CMC simulations in this work utilise the lab-scale Cambridge bluff body swirl burner analysed previously in experiments [Allison et al., 2018; Cavaliere et al., 2013; Sidey et al., 2017; Yuan et al., 2018] and in numerical studies [Giusti & Mastorakos, 2017; Tyliczszak et al., 2014; Zhang et al., 2015; Zhang & Mastorakos, 2016]. The version of LES-CMC used to model spray combustion in this thesis is very similar to versions used in Giusti & Mastorakos [2017]; Sitte [2019]; Sitte & Mastorakos [2019]. Spray terms are included in the mixture fraction and mixture fraction variance transport equations solved in the LES, as well as in the CMC transport equations for species, temperature and enthalpy. LES-CMC simulations are conducted only for the HyChem A2 chemical mechanism, as due to time constraints LES-CMC of C1 and C5 went beyond the scope of this doctoral thesis. The HyChem A2 kerosene is simulated at three different fuel mass flow rates, corresponding to the middle three conditions of the blow-off curve in Allison et al. [2018], and blow-off is induced in the simulations by increasing the bulk air flow rate beyond the experimental U_{BO} values.

The primary focus of the LES-CMC simulations in this work are to examine: the local extinction and fuel starvation behaviour, the evolution of key pyrolysis and intermediate species, and the flame structure during the blow-off transient. This is done using existing tools such as LES-CMC for sprays and the HyChem A2 mechanism for Jet-A, run with only small modifications, in order to gain more physical insight into the causes of flame extinction in non-premixed spray flames using a practical low-volatility fuel.

1.3 Objectives

Numerous questions persist around understanding LBO of spray flames. Is spray flame LBO driven primarily by increased amounts of local extinctions as in gaseous non-premixed flames? Or does the notion of fuel starvation play a more prominent role? Is it possible to replicate asymmetric flame structures observed in experiments of LBO using current turbulence-combustion methods? How does the different chemistry of conventional and synthetic jet fuels respond to increased scalar dissipation rate and how does this contribute to blow-off tendencies of different jet fuels?

This work uses detailed mechanisms of conventional and synthetic aviation fuels in transient numerical simulations of combustion to:

- predict local extinction and lean blow-off behaviour of heavy hydrocarbon spray flames.
- understand the role of heavy hydrocarbon chemistry and formation of intermediate species in flame stability, with emphasis on local extinction and fuel starvation phenomena as drivers of LBO in spray flames.
- evaluate the CMC combustion model and detailed kerosene chemical mechanisms on their capabilities in replicating blow-off trends and asymmetric flame structure behaviour observed in experiments.
- provide a stronger understanding of the physics and chemistry of kerosene spray flames at the lean condition limits of engine operability.

1.4 Outline

The structure of the thesis is as follows: Chapter 2 contains the literature review, which first briefly reviews conventional and alternative kerosene fuels and the U.S. National Jet Fuels Combustion Program. Then the review discusses studies of local extinction and LBO phenomena primarily as they relate to non-premixed flames. The review includes configurations relating to laminar flamelets, premixed and non-premixed gaseous flames, and lastly spray flames.

In Chapter 3 background information on the modelling of turbulent non-premixed flames is provided, including the mixture fraction concept, micro-mixing via scalar dissipation rate, and the transient flamelet concept. The CFD technique Large Eddy

Simulation is presented, as well as Lagrangian-Eulerian spray modelling. The Conditional Moment Closure subgrid turbulence-combustion model and its implementation in an LES spray context is described. The two types of detailed kerosene chemical mechanisms used in this work are discussed. The experimental and computational set-ups are documented and the solutions strategies are reported. Discussion of difficulties encountered and subsequent reduction in scope of work are also included.

In Chapter 4, the results from laminar counterflow simulations of the three NJFCP kerosenes and the Dagaut kerosene surrogate are presented at various conditions: atmospheric and high pressures, and varying scalar dissipation rates. Their extinction scalar dissipation rate values are compared against expected trends with experiments with mixed success. The extinction transient of the A2 fuel is analysed using relevant intermediate species and heat release rate markers. The ability for a flamelet to reignite is also assessed.

Chapter 5 shows results from the stable base case LES-CMC simulation results for the Jet-A spray flame. Experimental results are presented for comparison, with the LES-CMC capturing reasonably similar behaviour, although seeming to exhibit some behaviour characteristic of conditions closer to LBO. Time-averages and instantaneous results are discussed with emphasis on the occurrence of local extinctions and the behaviour of small intermediate and pyrolysis species. The flame structure, heat release rate and evaporation are analysed.

In Chapter 6, the LBO curve of the simulated Jet-A spray flame is presented and compared with experimental blow-off bulk velocities. The LES-CMC results compare with relatively good agreement with the experiments. The blow-off for three different fuel mass flow rate cases are simulated and discussed. Metrics for determining blow-off are detailed, particularly using reduction in heat release rate in the region of stoichiometric mixture fraction. Blow-off times are presented, with very good agreement with experimental blow-off times of other low-volatility fuels. Average species mass fractions and local extinctions are quantified along the mixture fraction stoichiometric isosurface over time. Local extinctions in mixture fraction space are also observed, however the quantity of local extinctions is notably lower than those observed in gaseous non-premixed flames. This points to reductions in the evaporation rate, the major limiting factor in spray flame stability, which results in fuel starvation and lower temperatures, as a major contributor to the blow-off of spray flames.

Chapter 7 contains the summary and conclusions of this thesis. Recommendations for future work are made.

Chapter 2

Literature review

The literature review is divided into two sections. Section 2.1 is a brief and general overview of kerosene fuels used for aviation and the U.S. National Jet Fuels Combustion Program, which provides context for the kerosene fuels studied numerically in this doctoral work.

Section 2.2 of the literature review covers the development of understanding of flame phenomena relating to local extinctions and lean blow-off. Counterflow laminar flamelet extinction studies as well as turbulent non-premixed gaseous and spray flames in both experiments and simulations are reviewed. Seminal works studying extinction and blow-off in premixed flames are also discussed. The literature covered in the review generally pertain to non-premixed bluff body swirl-stabilised flames with recirculation zones using hydrocarbon fuels, which feature local extinctions or lean blow-off. Due to the transient nature of local extinctions and blow-off, steady-state approaches (e.g., RANS or steady flamelets) are largely excluded from this review.

2.1 Conventional and alternative jet fuels

2.1.1 Description of aviation fuels

Kerosene is a complicated mixture of thousands of heavy hydrocarbon chemical compounds, which is why it is sometimes referred to as a “multi-component” fuel. As such there is no single definitive chemical compound or species to describe aviation kerosene [Maurice et al., 2001]. Even at industrial scale, kerosene blends can vary significantly from shipment to shipment [Edwards & Maurice, 2001].

Kerosene is a distillation of crude oil composed primarily of clean-burning heavy paraffins. Kerosene is less volatile than gasoline, making it a safer, cleaner and more

energy dense fuel choice [Maurice et al., 2001]. Kerosene was first used for aviation by Sir Frank Whittle in his turbojet engine in 1941. Aviation fuel development and kerosene blends went through numerous trial-and-error iterations under U.S. military programs for decades, starting with JP-1 (jet propellant #1)—the “ideal jet fuel” and first fuel specified for aviation gas turbines, which was limited only to military use due to its prohibitively low freezing point [Maurice et al., 2001]. In the 1960s commercial jet aviation began to take off, and the first commercial aviation kerosene was developed based on the JP-1 blend but with property adjustments made to ease mass refinery production, known as Jet-A in the U.S. and Jet A-1 internationally [Maurice et al., 2001]. Jet-A/A-1 has since been used worldwide for commercial jets.

Jet-A kerosene is made up of several classes of hydrocarbons, and although an infinite variety of mixtures could potentially be used operationally, blends must consist primarily of n-paraffins/isoparaffins (approx. 60%), cycloparaffins (approx. 20%), and aromatics (approx. 20%) [Maurice et al., 2001]. Paraffins (a.k.a. alkanes) are made of singly-bonded carbon chains in which each carbon atom is fully saturated with hydrogen, forming straight-chain or branch-chain molecules [Bonifazi et al., 1983]. This molecular structure is very stable and less likely to react with other materials, and a high hydrogen-to-carbon ratio results in a higher heat release by weight, making paraffins cleaner burning than other heavy hydrocarbons [Bonifazi et al., 1983]. Cycloparaffins (or naphthenes) form ring structures which decreases the H to C ratio, but they are still stable and clean, with the advantage to paraffins that their freezing points are lower [Bonifazi et al., 1983]. Aromatics on the other hand are fully-unsaturated six-carbon ring compounds with a lower heat content by weight; they contribute to combustor coking, smoke generation and high-luminosity flames [Bonifazi et al., 1983]. Despite these negative attributes, aromatics are commonly included in kerosene blends in order to enhance O-ring seal swelling to reduce fuel leaks.

To meet specifications for aviation, kerosene is formulated with the specific fuel system, operational requirements and refinery capabilities in mind as an afterthought to the design of the aircraft and engines [Maurice et al., 2001]. The physical property specifications that need to be met (and which are the constraining factors in the proportions of hydrocarbon classes) are those like boiling range, volatility, heat of combustion, freezing point, thermal stability, etc. [Edwards & Maurice, 2001; Rye et al., 2010].

However, as concerns over energy security and emissions grow, interest has developed concerning fuels derived from alternative sources to crude oil [Rye et al., 2010]. To save costs by avoiding redeveloping the entire fuel system or aircraft structure for

2.1 Conventional and alternative jet fuels

a drastically different type of fuel, “drop-in” alternative fuels are being considered—defined as a fuel that is characteristically very similar to Jet-A/A-1 and meets existing jet fuel specifications [Rye et al., 2010]. Some examples of operationally proven drop-in fuels are synthetic kerosenes derived from either fossil sources (e.g., coal, natural gas and oil sands) or biomass sources (e.g., *Jatropha*, algae, rapeseed), and have been tested as blends with Jet-A1 on numerous commercial airlines and engines [Blakey et al., 2011; Rye et al., 2010]. Using fossil-derived synthetic kerosene improves energy security by diversifying aviation fuel supply, but unsurprisingly results in a similar emission profile as that of petroleum-derived kerosene [Rye et al., 2010]. Using biomass-derived kerosene blends can improve environmental impact significantly with regard to soot, particulate matter (PM) and unburned hydrocarbons (uHCs), as well as reduce CO₂ emissions; however great care must be taken with biomass feedstock choice and cultivation, as the clearing of land and cultivation of feedstock could add substantially more CO₂ to the atmosphere when compared to the original growth in the region [Blakey et al., 2011]. Nonetheless, the desire to use alternative jet fuels has grown strong in efforts to mitigate climate change.

A major organisation involved in carrying out this mission is the National Jet Fuels Combustion Program (NJFCP), a U.S. based program with military and federal backing created in order to address the development of alternative jet fuels through international industrial and academic collaboration.

2.1.2 The US National Jet Fuels Combustion Program

The overarching strategy of the NJFCP is to “apply previously developed scientific knowledge and advanced diagnostic procedures to characterise the impact of fuel composition and chemistry on gas-turbine combustion” [Colket et al., 2017]. As there is a lack of knowledge regarding the physical and chemical properties of alternative jet fuels or SAFs, extensive testing and research utilising university labs, combustor rigs and engine testing facilities are necessary to evaluate the impact of using SAFs particularly with respect to aero-engine operation extremes like lean blowout, high-altitude relight, and cold start [Colket et al., 2017].

The aims of the program are to use reference fuels (petroleum-derived) and computational modelling to characterise fuel behaviour in referee combustor rigs in coordination with industry. Using the knowledge gained from studying conventional jet fuel behaviour at extreme operating conditions, alternative fuels can be characterised experimentally and computationally using fundamental fuel kinetics and combustion data and com-

pared against the reference fuels for effects on LBO, relight and cold start [Colket et al., 2017].

The fuels under inspection fall into two categories: A and C. Category A indicates the fuel is a conventional petroleum kerosene, and is used as a reference fuel. Category C indicates that it is an alternative test fuel designed to explore kerosene blends with unusual properties. The three fuels of particular interest for study in the NJFCP and in this report are: 1) Jet-A/A-1 (also referred to as A2), a conventional petroleum-derived jet fuel, 2) C1, an alternative fuel comprised primarily of paraffins (and very few aromatics) and which has a very low derived cetane number, and 3) C5, a synthetic fuel designed with evaporation characteristics to cause boiling at a single temperature. More details on these fuels can be read in the Methodology chapter.

In this thesis, these fuels are studied in a computational context to understand the physical mechanisms causing their LBO and local extinction behaviour and to evaluate current modelling tools in their ability to capture such behaviour with practical fuels. Detailed chemical mechanisms using the Hybrid Chemistry “HyChem” lumped pyrolysis approach, based on the idea that fuel cracking occurs very quickly, have been developed recently to represent the three NJFCP kerosene fuels for computational studies [Wang et al., 2018a,b; Xu et al., 2018].

These fuels have been studied with regard to LBO in experiments [Allison et al., 2018; Bell et al., 2018; Colket et al., 2017; Heyne et al., 2017; Khandelwal et al., 2021; Pathania et al., 2020, 2021; Rock et al., 2020; Sidey et al., 2017; Won et al., 2019] and simulations [Esclapez et al., 2017; Foale et al., 2019, 2021; Hasti et al., 2018; Piehl et al., 2018]. The most important findings of these works will be discussed in more detail toward the end of the next section, along with other relevant literature discussing local extinction and lean blow-off in spray flames.

2.2 Local extinction and lean blow-off

2.2.1 Extinction in laminar non-premixed flamelets

As combustion theory developed, transient phenomena such as extinction were studied in laminar flame contexts to aid understanding of extinction in turbulent flames. Building on the work of Fendell [1965], Liñán [1974] produced a seminal work where asymptotic expansion methods were applied to analyse the laminar mixing zone with one-step irreversible chemistry and large activation energy; it demonstrated that extinction was predicted to occur when the strain rate of the flame exceeded a certain

value. Liñán [1974] attributed a too-short chemical reaction time scale as the cause of full extinction of the flame. Peters [1983] used the laminar counterflow results from Liñán [1974] to derive a quenching condition in the context of laminar flamelets using an instantaneous scalar dissipation rate. An ensemble of laminar flamelets in this work was successfully used to predict local quenching in a lifted non-premixed turbulent jet flame. Peters [1983] also proposed for the scalar dissipation rate rather than flame velocity to act as the parameter describing non-premixed flamelet extinction. The technique of using ensembles of non-premixed laminar flames to model turbulent flames was developed further in Peters [1984, 1986] and applied to turbulent flame modelling with detailed chemistry in Rogg et al. [1986], resulting in excellent agreement with experiments.

Sets of global reaction schemes for methane-air and propane-air non-premixed counterflow flames in Jones & Lindstedt [1988] were used to show the approach to extinction with increasing strain rate causes a drop in the peak temperature of the flame which steepens as the extinction strain rate is approached. Heat release rate was also noted to increase considerably with increasing strain up to extinction, in agreement with the experimental findings in Tsuji [1982].

Simulations of laminar counterflow non-premixed methane-air experiments in Cheliah et al. [1991] showed that for undiluted methane flames, increasing pressure caused increased strain rates at extinction. However this positive-increasing relationship was less strong at particularly high pressures. The maximum scalar dissipation rate experienced in the burner configuration was noted to exceed the stoichiometric extinction scalar dissipation rate by more than an order of magnitude.

Unsteady laminar counterflow flames of non-premixed hydrogen and air were simulated in Darabiha [1992] with complex chemistry and variable strain rates. They showed that close to extinction, the heat release rate behaved nonlinearly and the flame was very sensitive to low frequency perturbations. Sufficiently long duration perturbations pushing the strain rate beyond the critical extinction value caused the flame to completely extinguish. For shorter durations the flame could recover from the strain perturbations. Impulse-applied and sinusoidal varying strain rates in laminar counterflow non-premixed flames were also investigated by Im et al. [1995] which replicated the findings of Darabiha [1992] that the flame was more easily extinguished when characteristic times were sufficiently long. The findings suggested that the laminar flamelet regime could be applied to higher Reynolds number contexts in turbulent flames, for despite the existence of eddies with sufficiently higher strain rates than

the extinction rate, most of these high strain eddies do not have sufficiently long characteristic times to cause extinction.

Cuenot et al. [2000] applied these ideas from the unsteady strain rate simulations to make an unsteady laminar flamelet model based on steady strained flamelet libraries. The model used an “equivalent” strain rate calculated from the strain rate history, with good agreement between the new model and the original numerical simulation.

More recently, Foale et al. [2019] simulated unsteady laminar flamelets up to extinction scalar dissipation rates using the laminar flamelet version of the Conditional Moment Closure equations (0D-CMC) and detailed chemical mechanisms of conventional and synthetic jet fuels from the NJFCP to determine if the relative extinction behaviour exhibited by the jet fuels in turbulent experiments could be predicted in a laminar flame context, with mostly good agreement. The C1 fuel extinction was predicted to occur at lower scalar scalar dissipation rate than the other fuels, which was in line with experimental trends. However the C5 fuel was more robust to extinction than the Jet-A fuel, contrary to experimental findings, which suggested that it was physical liquid property attributes not captured in laminar flamelet simulations that caused the C5 flame to blow-off at higher equivalence ratio than Jet-A.

Laminar counterflow non-premixed methane and n-dodecane ($n\text{-C}_{12}\text{H}_{26}$) simulations were conducted using 0D-CMC and detailed chemistry at various pressures in Paxton et al. [2019] to assess formaldehyde (CH_2O) and chemiluminescence species (CH^* , OH^*) as experimental observables in extinction transients. CH_2O mass fraction was shown to persist after the extinction transient, as there was no longer OH present to consume the CH_2O . The well known experimental relation $\text{OH} \times \text{CH}_2\text{O}$ was deemed to have a good correlation with heat release rate for premixed flamelets, whereas OH^* was well-correlated with heat release rate in the non-premixed flamelets. CH^* was affirmed to be a useful indicator of imminent extinction.

2.2.2 LBO and local extinction in turbulent premixed flames

Present understanding of flame stabilisation and blow-off is derived from gaseous premixed flame bluff body stabilisation experiments by Longwell et al. [1953] and Zukoski & Marble [1956]. These studies approached the understanding of the physics of flame stabilisation through relative chemical and mixing time scales, following in the same vein as Damköhler [1940]. Longwell et al. [1953] suggested that the wake of a bluff body behaves as a homogeneous chemical reactor, and that flame extinction occurs when there is not enough time available for chemical reactions compared to the time required to generate enough heat to ignite the fresh mixture. Zukoski & Marble

[1956] suggested the idea that ignition of fresh mixture occurs in the flame-air shear layer, and that flame extinction happens when the time during which the fresh gas mixes with the hot recirculation zone along the shear layer is too short for ignition to be accomplished. When it came to predicting the equivalence ratio corresponding to flame extinction, both of these ideas boiled down to correlations dependent on bluff body diameter, incoming flow velocity, pressure, and temperature. Plee & Mellor [1979] produced a quantitative application of the Zukoski & Marble [1956] theory for predicting lean blow-off limits in turbulent bluff body stabilised flames using a characteristic-time model.

Studies of blow-off of premixed gaseous and pre-vaporised flames were undertaken to further develop empirical correlations to predict blow-off events based on combustor and bluff body geometry, and the pressure, temperature, velocity, turbulence properties, and equivalence ratio of the incoming fresh mixture [Ballal & Lefebvre, 1979, 1980; Lefebvre, 1985]. Stability was found to improve with increase in the bluff body diameter, which causes longer residence times for the reactants in the recirculation zone. Lean blow-off was improved (extended to lower, more lean operable values) by (i) reduction in approach velocity, causing increased residence time, and (ii) increase in pressure and temperature, which causes increase in chemical reactions. These LBO prediction correlations found that the weak extinction equivalence ratio ϕ_{WE} (a.k.a. ϕ_{LBO}) was affected primarily by temperature for gaseous flames [Lefebvre & Ballal, 2010]. The weak extinction equivalence ratio ϕ_{WE} for pre-vaporised sprays on the other hand was dependent on temperature, pressure, fuel volatility and droplet sizes. Blow-off limits of mixtures involving liquid fuels were found dependent primarily on fuel evaporation rates, rather than chemical reaction rates as for gaseous flames. Lefebvre & Ballal [2010] also proposed a theory for the physics of flame blow-off, suggesting flame blow-off occurs when the rate of heat liberation in the combustion zone becomes insufficient to heat the incoming fresh mixture up to a necessary reaction temperature. This is fairly similar to the notion supported in Gupta et al. [1984], that at high velocity, blow-off occurs if the heat received by the recirculating eddy from the hot combustion gases becomes insufficient to maintain a temperature high enough to cause ignition.

These studies did not emphasize the difference between gaseous premixed and non-premixed flames; both were termed “homogeneous” mixtures. Sprays, whether pre-vaporised or not, were referred to as “heterogeneous” mixtures. Correlations for prediction are useful when using conventional jet fuels, however as SAFs are increasingly introduced with chemical compositions potentially out of the bounds of typical kerosene blends, empirical correlations will no longer be as useful for predicting

new fuel behaviour. Understanding the fundamental physics behind blow-off is necessary to streamline selection and certification of new fuels.

In more recent studies premixed flame blow-off was visualised using high speed imaging and laser sheets and has been observed to occur in various stages as the equivalence ratio is decreased [Muruganandam & Seitzman, 2005; Nair & Lieuwen, 2007; Shanbhogue et al., 2009]. In Muruganandam & Seitzman [2005], the dynamics of the blow-off phenomenon and potential blow-off precursors were investigated in premixed methane-air flames. Partial extinctions in the flame were observed, followed by reignition, which were triggered by cold pockets of reactants in the recirculation zone. The flame zone divided into upstream and downstream regions, stabilised by the walls of the chamber. After several partial extinction precursor events, the temperature was so reduced that the flame extinguished, with events occurring more frequently and for longer durations as blow-off was approached. Nair & Lieuwen [2007] studied the transient flame structure of a near-blow-off premixed methane-air flame and defined two distinct stages before blow-off: the occurrence of localised extinctions, or holes, in the flame sheet, and then violent flapping of the flame front and large straining of the flame as equivalence ratio was decreased further. In non-swirling premixed methane-air flames studied in Dawson et al. [2011]; Kariuki et al. [2012, 2015], the dominant location of extinction in premixed flames was found to occur not at the anchoring point of the flame near the bluff body, but rather downstream where the Karlovitz number is higher. This led to a build-up of unburnt gases on the downstream end of the recirculation zone and the presence of incomplete combustion markers such as CH_2O . Similar behaviour was observed recently in the same configuration but with pre-vaporised kerosene flames from the NJFCP in Pathania et al. [2020, 2021].

Although these studies of the blow-off transients of premixed gaseous and pre-vaporised flames are useful for understanding which blow-off precursors are more likely to occur during the process, they do not preclude the need for analogous experiments and simulations with non-premixed and multi-phase spray configurations, particularly in the context of understanding blow-off of practical fuels. This was acknowledged early on in Peters & Williams [1983], where the authors determined that the premixed flame rationale could not be used for predicting blow-off of lifted non-premixed flames; this is because insufficient premixing at the molecular scale occurs in non-premixed flames to use premixed assumptions. They instead suggested using extinction of laminar diffusion flamelets to predict extinction in turbulent diffusion (non-premixed) flames.

Experiments comparing swirl bluff body-stabilised premixed, non-premixed and liquid spray flames in Cavaliere et al. [2013] demonstrated that there are vast differences

in flame location, structure, and dynamics between the three regimes, particularly during the blow-off transient. Further experiments in the same configuration by Yuan et al. [2018] demonstrated that there are also significant differences between sprays with various fuel volatilities and evaporation characteristics. Considering these findings, the physics of spray flame blow-off requires further exploration through experiments and numerical simulations in order to provide a more general understanding of how spray flames of any fuel will behave at the lean limit.

2.2.3 LBO and local extinction in turbulent non-premixed flames

Non-premixed flames are useful and necessary for understanding spray flames, as the fuel vapour in the gaseous phase may follow similar trends in local extinction and lean blow-off. A large body of work has been completed in the study of extinction and blow-off for non-premixed swirl flames, with useful behavioural insights offered by experiments and physical understanding obtained from simulations.

Experiments

The limiting factor in non-premixed gaseous flames is the molecular mixing rate of the fuel and the air, hence the term “diffusion” flame commonly being applied to this configuration. Broadwell et al. [1985] suggested that lean blow-off in non-premixed flames occurs at conditions when the characteristic mixing time between hot combustion products entrained in the jet flame and unburnt reactants is small relative to the combustion time scale. Some of the first studies of blow-off in non-premixed swirling flames were reported in Feikema et al. [1991]. Excessive air velocity was used to measure the blow-off limit, and they made observations that there was a lack of flame lift-off at LBO; the flame would abruptly blow off instead. Feikema et al. [1991] studied blow-off events with and without swirl, and concluded that swirl creates local region of reduced velocity and local strain rate, which enhances the stability of flames compared to those without swirl.

Turbulent counterflow experiments in Mastorakos et al. [1992a] with non-premixed and partially premixed methane-air flames demonstrated that turbulent non-premixed flames extinguish at a critical total strain rate equal to the critical strain rate for extinction of laminar counterflow flames, confirming theory put forth by Peters & Williams [1983]. In an analysis using equations for the mean mixture fraction and its fluctuations along the stagnation streamline in a turbulent isothermal opposed

Literature review

jet flow, Mastorakos et al. [1992b] found that mean scalar dissipation rate increases with increase in bulk velocity and strain rates, and that high values of mean scalar dissipation rate are associated with flame extinction.

A large body of experimental non-premixed bluff body swirl flame work was completed at the University of Sydney to make a data repository [Masri et al., 2018] for combustion model validation. In these “Sydney swirl flames” [Dally et al., 1998; Masri & Bilger, 1984, 1986; Masri et al., 1988, 1994, 1996, 2004, 2007, 2000] finite rate kinetics and shear stresses from the coflow air were found to play a part in causing local extinctions. These findings were in agreement with piloted methane-air jet flame experiments in the Sandia flame D–F series [Barlow & Frank, 1998], which use an identical burner geometry to the Sydney flame series but with different fuel, pilot and air coflow settings. Sandia flames D and E exhibit low- to moderate-levels of local extinction, whereas Sandia flame F exhibits the highest levels of local extinction at a condition close to lean blow-off. The Sydney and Sandia flame experiments demonstrated in turbulent hydrocarbon flames that localized extinctions occurred increasingly as LBO was approached.

In the turbulent non-premixed experiments in Sutton & Driscoll [2007], combined laser-induced fluorescence (LIF) and Rayleigh scattering techniques were used to image local flame extinction that occurs when strong scalar dissipation layers overlap with the stoichiometric mixture fraction contour. These results provided visual evidence that scalar dissipation rate plays an important and direct role in local flame extinction.

The transient of flame blow-off in a swirling non-premixed flame was visualised for the first time in Cavaliere et al. [2013] using fast imaging (5 kHz) of OH* chemiluminescence in a lab-scale burner with methane, where the aim was to visualise the distinct processes which premixed, non-premixed, and spray flames undergo during lean blow-off. OH-Planar Laser Induced Fluorescence (PLIF) results showed that the non-premixed flame intermittently lifted off the bluff body with increasing likelihood as the air velocity was increased. The flame blow-off transient for the non-premixed flame, quantified using normalized area-integrated OH* signal, was similar in duration to the premixed flame. Local extinctions were identified in the non-premixed flame sheet, and the flame was observed to shorten and experience fragmentation during the blow-off event.

Recently, Ciardiello [2021]; Ciardiello et al. [2022] visualised blow-off of interacting flames in the context of annular combustors using non-premixed methane-air flames in both linear and annular configurations. High-speed OH* images showed localised extinctions of the flame above the bluff bodies in the linear-combustor configuration

(consisting of five bluff body swirl stabilised burners). These holes in the flame were reignited by convection of hot products from an adjacent burner. Ciardiello [2021] showed that a single burner cannot be used to predict lean blow-off in full annular combustors, as the flames were less stable due to strong flame-flame interactions and helped reignite blown-off neighbours. The beginning of the blow-off event however could be partially predicted in annular combustor set-ups with fewer burners, as they can resemble a set of individual burners.

Computational studies

DNS In the three-dimensional non-premixed turbulent combustion Direct Numerical Simulation (DNS) study by Sripakagorn et al. [2004], strong fluctuations of the scalar dissipation rate were shown to create local extinguished regions on the stoichiometric surface of the flame. The average scalar dissipation rate remained lower than the extinction threshold, accounting for why the flame did not fully extinguish and previously extinguished regions could reignite. Their study used a simple one-step chemistry model and did not account for density variation.

Non-premixed ethylene jet flames were studied in Lignell et al. [2011] with density-varying DNS and detailed chemistry to see the effects of Damköhler number on extinction and reignition. The scalar dissipation rate, stoichiometric mixture isosurface area and the heat release rate evolution were found to depend strongly on the amount of extinction.

DNS is useful for fundamental studies and model validation, however the computational intensity required to directly solve transport equations without any subgrid modelling makes DNS infeasible in more practical geometries with detailed chemistries for predicting transient phenomena.

Transported PDF Various advanced models have been used to try to predict the transient phenomena of local extinctions, with many using the Sydney [Masri et al., 2018] or Sandia flames [Barlow & Frank, 1998] to validate the capabilities of their approaches to capture extinction and lean blow-off phenomena. One promising approach has been the transported joint-probability density function (joint-PDF) approach [Pope, 1976, 1985]. The velocity–composition–turbulence frequency joint-PDF was applied in Xu & Pope [2000] to model the Sandia D–F flames. They used a reduced methane chemical mechanism which was computed by the *in situ* adaptive tabulation (ISAT) algorithm [Pope, 1997] to save computational costs, as the joint-PDF approach is very computationally intensive. The method was able to quantitatively predict extinction

and reignition to a very good degree against experiments using the flame burning index.

The transported PDF approach was used in Lindstedt & Louloudi [2002] to model the Sydney methanol flames M1–M4, which involve increasingly high Reynolds numbers approaching lean blow-off [Masri et al., 1992]. The transported joint-PDF method employed found similarly good agreement for the prediction of local extinction and reignition. The simulated flame blow-off velocity was 89.4% of the experimental value. Small variations in the scalar dissipation rate were determined to have a significant impact upon the burning characteristics of the flames close to extinction, and Lindstedt & Louloudi [2002] emphasized the importance of accurate closures for chemistry in turbulent reacting flames. Lindstedt et al. [2007] used the transported PDF approach with augmented reduced chemistry to model methane-hydrogen-air flames in a Sandia burner which found that an algebraic scalar dissipation rate closure was able to more accurately predict local extinctions.

The transported PDF with a hybrid Monte Carlo/finite volume algorithm and reduced chemistry was used in Gkagkas et al. [2009] and Tian & Lindstedt [2019] to model methane-hydrogen-air Sydney HM1–HM3 flames exhibiting local extinction with emphasis on closures of the scalar dissipation rate. The very different molecular mixing closures used were able to encompass the experimental data, although the extended modified Curl’s model (EMC) was considerably better at predicting local extinctions. Tian & Lindstedt [2019] also found that flame local extinction plays a crucial role in determining nitric oxide (NO) levels, emphasizing the importance of local extinction in affecting not only flame stability but also long-time scale pollutant formation.

The Sandia flames D–F were simulated in Jones & Prasad [2010] using the LES-subgrid-scale (LES-*sgs*) PDF evolution equation method in conjunction with the Eulerian Stochastic Field (ESF) solution technique with reduced chemistry. Qualitative extinctions in flame F were well-reproduced, however the degree of local extinctions was under-predicted. Chemical kinetics were suggested to strongly play a role in causing the extinctions in Sandia flame F, which were not well-captured by the reduced chemical mechanism in the simulation. The same model parameter set-up in Jones & Prasad [2010] was used in Prasad et al. [2013] for piloted turbulent methane-air jet Sydney flames L, B and M to assess experimental processing procedures. Local extinction flame holes and reignition were predicted well against experimental high speed OH-LIF visual and quantitative data on flame breakage and closure, which validated the experimental OH-LIF processing techniques.

Recently, the LES/PDF Eulerian Stochastic Fields framework in Yu et al. [2020] was applied to a co-centric conical non-premixed methane swirl burner [Elbaz et al., 2019] using a skeletal chemical mechanism to predict local extinctions and reignition. Local extinction was shown visibly along the stoichiometric mixture fraction contour in two-dimensional cut-planes. Flame holes/extinctions near the burner exit were quenched at scalar dissipation rates lower than the critical extinction value, and reignition was observed to occur due to turbulent flame folding. At the trailing edge of the flame the mechanism of extinction was similar to the quenching of a laminar flame, due to high scalar dissipation rates. Yu et al. [2020] also suggests that more accurate local extinction predictions can be made using more detailed chemical mechanisms, although due to the computational intensity of the transported PDF method using more detailed chemistry would be intractable without thousands of computer processors.

MMC models Ge et al. [2013] used the hybrid Eulerian LES/Sparse-Lagrangian Multiple Mapping Conditioning (MMC) method with a detailed chemical mechanism on the Sandia D–F flames and found the bimodal nature of local extinction in flame F was captured as well as the trend of increasing levels of local extinction from the increases in jet velocity from flame D to F, however there was difficulty in capturing the local extinction behaviour at distances more than fifteen jet diameters axially downstream.

Extinction has been modelled to a decent degree in the Sandia flames D and F [Vogiatzaki et al., 2011, 2015] using the MMC approach with the interaction by exchange with the mean (IEM) subgrid mixing model and the Curl’s subgrid model, however this was in a RANS context, making the transient process of extinction and blow-off more difficult to analyse in more qualitative terms of flame structure and dynamics.

Flamelet models The Sandia flames D and F were simulated using LES and non-premixed and premixed flamelet-generated manifolds (FGM) in Vreman et al. [2008]. Results for flame D were satisfactory, however the LES-FGM method was unable to adequately capture the extinctions in flame F. A thickened flame model was found to better predict extinctions to a limited extent, compared with using a presumed β -PDF for the subgrid chemistry.

The flamelet/progress variable (FPV) approach was developed by Pierce & Moin [2004], in which a flamelet parameter based on a reactive scalar is used instead of the scalar dissipation rate. Ihme et al. [2005] were the first to assess the ability of the

FPV approach to predict local extinction and reignition, which they compared against DNS studies [Sripakagorn et al., 2004]. They found that the steady flamelets with the flamelet progress parameter PDF modelled using a β -PDF conditioned on mixture fraction could predict local extinctions well even for high levels of extinction. The FPV model applied with LES for Sandia flames D and E in Ihme & Pitsch [2008a,b] aligned well with experiments for general flame characteristics, however the model considerably under-predicted the amount of local extinctions in the flames.

LES using the FPV approach and the dynamically thickened flame approach (TFLES) [Legier et al., 2000] was used in Ma et al. [2019] to predict the blow-off transient of the non-premixed methane flame from Cavaliere et al. [2013]. At stable conditions the FPV approach captured visual evidence of local extinctions, whereas the TFLES approach featured more connected OH regions along the flame front but did exhibit strong occurrences of flame lift-off which compared better with experiments than the FPV results. Ma et al. [2019] identified three stages of blow-off in the flame: initial increase in heat release rate, then large fluctuations of heat release rate, after which heat release rate fell monotonically to zero. The FPV predicted 100 ms for the duration of the blow-off event while TFLES predicted 30 ms; this difference was attributed to the large heat release rate fluctuations in the FPV case, which helped re-stabilise the flame for a longer period. Large amounts of local extinction were visible in the TFLES flame through lack of OH mass fraction along the stoichiometric mixture fraction isocontour, which contributed to the stronger and quicker reduction in heat release rate for that case. The FPV case also captured significant local extinctions as the flame neared global extinction. The FPV flame blew off at an air velocity 25% higher than the experimental value, whereas TFLES under-predicted blow-off by 20%. The TFLES approach was able to promote extinction through damping the chemical source term by the artificial thickening of the flame.

The same non-premixed methane configuration is studied with TFLES using a skeletal mechanism in Li & Ihme [2021] to examine blow-off mechanisms caused by changes in fuel and air mass flow rates. They found that inducing LBO through incremental step changes rather than large impulse caused the blow-off transient to last longer with greater fluctuations in heat release rate and OH mass fraction. Large fluctuations and high peaks of heat release rate were observed for blow-off via increase in the air flow rate and through reduction in the fuel flow rate, indicating that blow-off transients through the lean limit should behave similarly despite how they are induced. The results for LBO via increased air velocity confirmed previous findings; very intermittent flame shapes with strong lift-off events were observed, and local

extinctions grew in frequency and size along the stoichiometric isocontour, eventually causing the global extinction of the flame.

FPV combined with Eulerian Stochastic Fields was used to model both the Sandia flame D and a highly dilute oxy-methane flame in Mahmoud et al. [2019]. Extinction locations were reproduced numerically, although some extinctions could not be predicted in the centerline region of the flames.

These tabulated chemistry approaches use a laminar flame system or well-stirred reactor which has been pre-calculated, with the chemical reaction rate being stored in a table and subsequently accessed during simulation at relevant conditions [Giusti & Mastorakos, 2019]. Species present in the flow are unable to evolve independently in tabulated chemistry simulations. LES-FGM and LES-FPV methods are useful in that they are computationally relatively inexpensive, however they typically are applied to more stable non-premixed flame configuration. However with the recent advancements in LES-FPV in capturing extinction and blow-off shown in Li & Ihme [2021]; Ma et al. [2019] indicate that the approach has good potential at least for non-premixed gaseous flames.

Conditional Moment Closure Conditional Moment Closure, originally developed by Bilger [1993]; Klimenko [1990]; Klimenko & Bilger [1999], is a statistical and deterministic coupled turbulence-combustion model which requires fewer computational resources than joint-PDF methods, yet unlike flamelet approaches CMC still solves transport equations for chemical species as they develop in space and time. The studies in Roomina & Bilger [1999, 2001] applied CMC to the Sydney methanol flames and Sandia flame D respectively, with good predictions of flow field, temperature and species in fuel-lean regions, however there were discrepancies with experiments in more fuel-rich areas. First order chemical closure was used in the models, which was suggested as a potential reason for inaccuracies in the species trends. Singly-conditional CMC assumes that: (i) most fluctuations of quantities of interest can be associated with fluctuations of a single conditioning variable, typically the conserved scalar mixture fraction, and (ii) that the fluctuations around conditional averages are small. However non-negligible fluctuations around the conditional mean can occur due to local extinction, calling into question whether singly-conditioned CMC is completely appropriate for use to predict transient behaviour close to or during blow-off [Kronenburg & Papoutsakis, 2005].

Doubly-Conditional Moment Closure (DCMC, a.k.a. CMC2) was validated in Kronenburg & Papoutsakis [2005], with applications toward predicting local extinction and reignition, using two conditioning variables: one for the mixture fraction and

one for sensible enthalpy. The second conditioning variable can also be the reaction progress variable typically used in premixed combustion [Sitte & Mastorakos, 2017, 2019]. Results for DCMC in Kronenburg & Papoutsakis [2005] agreed very well with DNS species profiles accounting for local extinctions up through blow-off conditions. Kronenburg & Kostka [2005] used precomputed doubly-conditional reaction rates to close the chemical source term for singly-conditional CMC on the Sandia D–F flames with good results even for the Sandia F flame. This formulation of CMC enabled predictions to be qualitatively and quantitatively comparable to joint PDF simulations.

Nonetheless, singly-conditional CMC has been used in multiple configurations to predict various phenomena, with improvements in predictions observed when coupled with more advanced flow solvers. Singly conditional two-dimensional-CMC was applied to a turbulent lifted jet flame in Kim & Mastorakos [2005] which compared very well against experiments, with the scalar dissipation rate in the lifted region well below the quenched value. CMC was adapted to work with LES in Navarro-Martinez et al. [2005] with good results for the Sandia flame D. LES improved CMC as it was able to account for temporal and spatial variations of conditional scalar dissipation which were important for accuracy in turbulence–chemistry interactions. Kim & Pitsch [2005] derived an LES-CMC formulation simultaneously and found a similar improved performance of singly-conditional CMC with first order chemical closure. Large-scale fluctuations of reactive scalars on mixture fraction isosurfaces were resolved by the LES, making first-order closure more capable in predicting accurate levels of local extinctions.

Due to the promising results of the state-of-the-art LES-CMC methods in Triantafyllidis & Mastorakos [2010]; Triantafyllidis et al. [2009], LES-CMC using a fine-grained filtered PDF was applied to multiple non-premixed flame configurations to predict local extinctions and even global flame blow-off with reasonable success [El Helou et al., 2017; Garmory & Mastorakos, 2011, 2013, 2015; Zhang et al., 2015; Zhang & Mastorakos, 2016, 2017]. A useful feature of LES-CMC that reduces computational resource requirements is the separation of flow field modelling from the subgrid combustion modelling using two different meshes. The LES mesh should be appropriately refined for LES resolution and geometry constraints, however the CMC mesh in comparison can be very coarse, thus reducing the number of cells in which the CMC governing equations need to be solved. This allows for the use of detailed chemical mechanisms, which otherwise would be computationally intractable.

Garmory & Mastorakos [2011] applied LES-CMC to Sandia flames D and F. Local extinctions caused by fluctuations of the conditional scalar dissipation rates over the

quenching value were observed, and correct amounts of local extinctions were seen in most regions of the flame. Accuracy of the CMC predictions were dependent on the models used for the conditional scalar dissipation, the turbulent subgrid conditional flux, and the numerical diffusion associated with the CMC physical transport discretization schemes. In an LES-CMC sensitivity study Garmory & Mastorakos [2013] found that extinctions in CMC cells were caused by both high conditional scalar dissipation rates and spatial transport effects. By analysing the contribution of the individual CMC equation terms, the transport of scalars in the cross stream direction was determined to play a key role in extinguishing CMC cells. An oxy-fuel jet flame was simulated using LES-CMC in Garmory & Mastorakos [2015], and some over-prediction and under-prediction of local extinctions were noted in different regions of the flame, some of which were attributed to excess mixing and very high scalar dissipation rates near the fuel nozzle. Visual local extinctions along the flame isosurface were captured with excellent agreement with the experiment, as well as the trend of increasing extinction as hydrogen content in the jet was reduced.

Zhang et al. [2015] used LES-CMC with detailed chemistry to model the non-premixed methane flame in the work of Cavaliere et al. [2013]. Local extinctions and flame lift-off heights were well-predicted against the experiment. In the simulation, local extinction occurred when heat release rate, temperature, and OH mass fraction were low while simultaneously scalar dissipation rate was relatively high. This work was extended in Zhang & Mastorakos [2016] to simulate the blow-off curve of the flame at several fuel flow rates as in experiments, shown in Fig. 2.1. This was the first instance of combustion LES being used for prediction of a whole blow-off curve in a complex geometry. Blow-off velocities were within 25% of experimental values. During the blow-off transient, total heat release decreased gradually over a similar time duration as in the experiment. As flames approached blow-off, the conditional scalar dissipation rate experienced high-frequency and high magnitude fluctuations, which caused increasing areas of local extinction along the stoichiometric mixture fraction isosurface. This was shown with the “extinguished fraction” metric introduced in this work.

LES-CMC was also applied to Sydney flames using reduced methane chemistry in Zhang & Mastorakos [2017], where trends of increasing local extinctions in the flames were well-predicted, however the OH radical profiles were not as well-predicted which may be attributable to the use of the reduced chemical mechanism. The LES-CMC approach was used to model a non-premixed strongly swirling methane flame in a novel combustor designed for ultra-low NO_x emissions in El Helou et al. [2017] using

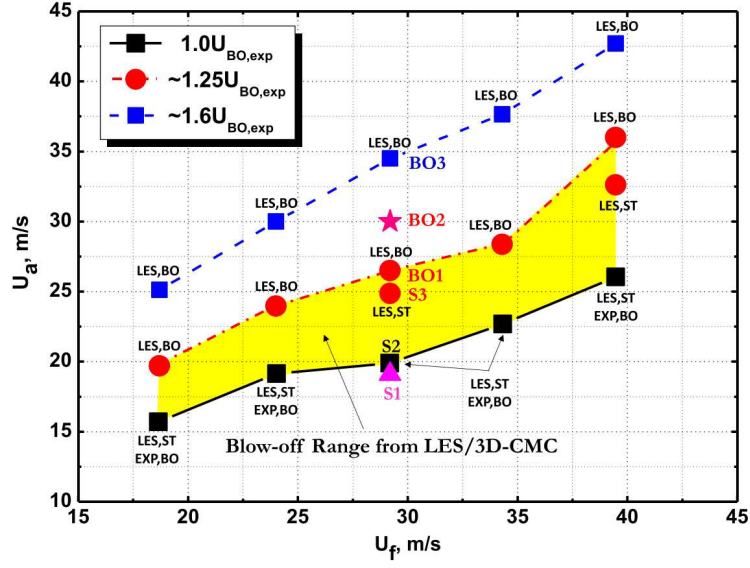


Fig. 2.1 Blow-off curve with fuel jet velocity along the x-axis and axial air bulk velocity along the y-axis based on the non-premixed methane experiment in Cavaliere et al. [2013]. LES-CMC simulation results are compared against the experimental blow-off velocities. The simulations blow-off within 25% of experimental values. Figure is reproduced with permission from Zhang & Mastorakos [2016].

reduced chemistry. The simulation showed that the flame was detached from the fuel jets around the injection points, as there were negligible amounts of OH mass fraction along stoichiometric mixture fraction isocontours near the jets. This was caused by the very large swirl induced by the eight angled air injection jets along the top of the combustor.

Summary of extinction and LBO in non-premixed flames

The most common understanding of non-premixed gaseous flame blow-off is that as flames are pushed toward lean blow-off by increasing the air flow rate, increasing frequency of local extinctions are observed. However unlike premixed flames, non-premixed flames do not exhibit much flame lift-off as they experience lean blow-off, and instead shrink downward and remain mostly attached to the bluff body edge. Local high scalar dissipation rate and large fluctuations of the scalar dissipation rate cause local extinctions to occur. Flames may recover from local extinctions and reignite if the scalar dissipation rate is not too high for too long a duration. Scalar transport and shear effects from the air-shear layer have also been shown to influence the occurrence of local extinctions.

2.2.4 LBO and local extinction in spray flames

Combustion of liquid fuels is a significantly more complex process than that of non-premixed gaseous flames. It is a multiphase problem with liquid and gaseous components, and combustion is limited by fuel evaporation rather than chemical reaction rate. Spray combustion is a challenge for modellers, however liquid fuels offer many practical benefits as they are much more energy dense, easier to transport, and generally safer than their gaseous counterparts. This is particularly important in long-haul aviation, where weight and energy density are of critical importance in safe and efficient operation of an aircraft.

The use of liquid hydrocarbon fuels and the presence of swirling flows, typically used for flame stabilization, make the blow-off event a very challenging phenomenon to predict due to the strong interaction between chemistry and turbulence. Spray flames are typically characterized by a wide range of scales and physical processes [Jenny et al., 2012; Masri, 2016] where both flame-turbulence interaction and spray evaporation play an important role in determining the local flame structure [Olguin & Gutheil, 2014] and extinction behaviour. In this section the focus is on primarily non-premixed liquid spray combustion, rather than pre-vaporised sprays which behave much more similarly to gaseous flames (see for example Refs. Pathania et al. [2020, 2021]).

Experiments

Non-premixed kerosene spray flames were studied in a disk-stabilised burner with varying disk sizes and coflow air in Hardalupas et al. [1994]. The lean extinction limit of the burner was sensitive to the disk diameter, as increased air velocity from the constricted annulus area caused larger amounts of colder air to be present in the recirculation zone and higher strain rates along the air shear layer, resulting in a lower equivalence ratio inside the recirculation zone. Several causes for global flame extinction were identified. One was decreased temperature in the recirculation zone, which was induced by high fuel entrainment and a large presence of cold air in the recirculation zone. Another was the turbulent strain rate, which reduced stability of the flame beyond a critical scalar dissipation rate. Finally, increase in the mixture fraction variance fluctuations resulted in reduced stability of the flame, as it corresponded with an increase in scalar dissipation rate beyond the quenching value. In Hardalupas et al. [1998] acoustic oscillations were applied to a kerosene-air swirl bluff body stabilised burner, where vortices induced by the oscillations were observed to increase the strain rate which contributed to local extinctions and flame lift-off.

Muruganandam et al. [2004] studied non-premixed Jet-A spray flames in both non-premixed and premixed regimes with the objective to sense the approach to LBO and develop an actuation approach to stabilise the combustor near blow-off. They described the transition of flames from a stable to blow-off transient regime as being characterised by large-scale unsteadiness with local loss of stabilisation and the occurrence of local extinction and reignition events. These transitional events were considered precursors to LBO. Muruganandam et al. [2004] made the distinction that LBO in premixed flames is governed by $\phi_{overall}$ and local fluid mechanics, whereas in non-premixed liquid fuel flames LBO dynamics are governed by fuel evaporation and nonuniform mixing of fuel and air. They observed greater intermittency in the stable non-premixed Jet-A flame, compared to the premixed configuration. As the equivalence ratio was decreased toward the lean blow-off limit ϕ_{BO} , the average number of extinction events increased, as did the duration of the extinction events.

A confined non-premixed swirl-stabilised kerosene-air flame at stable and near-blow-off conditions was investigated in Marinov et al. [2010, 2012]. Compared with a non-premixed methane flame studied in the same burner, flow fields at stable conditions were similar for the two fuels, however significant differences in the shape of the recirculation zone, the temperature and the species distributions in the chamber were observed at near-blow-off conditions. The kerosene flame experienced much larger regions of high air-to-fuel ratio and high reaction progress than the methane flame.

Local extinctions and flame structure during the lean blow-off transient were captured using OH* chemiluminescence and OH-PLIF for an n-heptane flame in Cavaliere et al. [2013]. As blow-off was approached the flame height decreased and the OH* intensity decreased along the inner flame zone along the spray, but along the flame-air shear layer the OH* intensity increased. The outer edges of the flame connecting to the bluff body were far from visible spray Mie scattering, indicating that along the flame-air shear layer only fuel vapour combustion occurs. Significant fragmentation and local extinctions in the flame were observed close to blow-off along with some small lift-off events. During the blow-off transient, the flame progressively diminished in size while remaining anchored along the edge of the bluff body. At the end of the transient, the last flame fragments visualized with OH* remained aligned with the spray cone. The spray blow-off transient was significantly shorter than those of the gaseous flames. *Fuel starvation* was suggested as a reason for the faster spray flame blow-off. Cold air in the recirculation zone reduces the temperature and lengthens evaporation times, decreasing fuel vapour availability to sustain the flame fragments.

A similar study on characterising LBO for spray flames with different volatilities was conducted in the same burner in Yuan et al. [2018]. The high-volatility fuels were n-heptane and ethanol, and the low-volatility fuels were n-decane and n-dodecane. Low-volatility fuels are of particular interest as their fuel properties should be more similar to kerosene. At unstable near-blow-off conditions the flames were all observed to shrink downward to become more firmly attached to the bluff body edge, with noted decrease in heat release along the inner flame near the spray and widening of strong heat release along the flame-air shear layer. OH was noted to be well-aligned with the spray cone and more attached to the bluff body surface close to blow-off. For low-volatility fuels, heat release regions (determined from OH* chemiluminescence) were non-axisymmetric, such that half of the flame was occasionally missing. This half-flame or “wedge-like” flame would slowly rotate around the bluff body edge. Yuan et al. [2018] suggested the missing flame was quenched in the inner recirculation zone at blow-off. During the blow-off transient, the inner and outer flame branches (along the spray and the shear layer respectively) appeared disconnected, and the flame branches experienced local extinction fragmentations before the OH presence disappeared entirely. The blow-off transient duration was between 10–30 ms for all the fuels. These results support the notion of fuel starvation causing the mechanisms for blow-off particularly in the low-volatility fuels. Spray penetration through the flame due to local quenching would contribute to reduced temperatures and too-rich fuel vapour regions, disrupting the flammability and causing these uneven half-flames before blow-off.

Sidey et al. [2017] and Allison et al. [2018], using the same bluff-body swirl burner studied in Cavaliere et al. [2013]; Yuan et al. [2018], looked at the blow-off behaviour of three kerosenes from the NJFCP (A2, C1, and C5) as well as several reference fuels to determine the effect of properties such as the derived cetane number (DCN) and unusual chemical compositions on lean blow-off. The blow-off curve of these results is reproduced in Fig. 2.2. Comparisons between flame structure and behaviour were made using OH* chemiluminescence, OH-PLIF and Mie scattering, with significant differences between the conventional Jet-A (a.k.a. A2) and the alcohol-to-jet fuel C1 [Sidey et al., 2017]. The A2 flame showed considerably larger sooting tendency but was more stable, whereas the C1 flame tended to exhibit more local extinctions and lift-off events and experienced LBO at a richer equivalence ratio.

Allison et al. [2018] found that synthetic kerosene fuels with unusual characteristics (C1 with low DCN and C5 with low viscosity and a flat boiling temperature) blow out at richer equivalence ratio than conventional petroleum fuel Jet-A. The DCN was

found to loosely correlate with blow-off equivalence ratio, however the correlation was not as strong as previously suggested in Heyne et al. [2017].

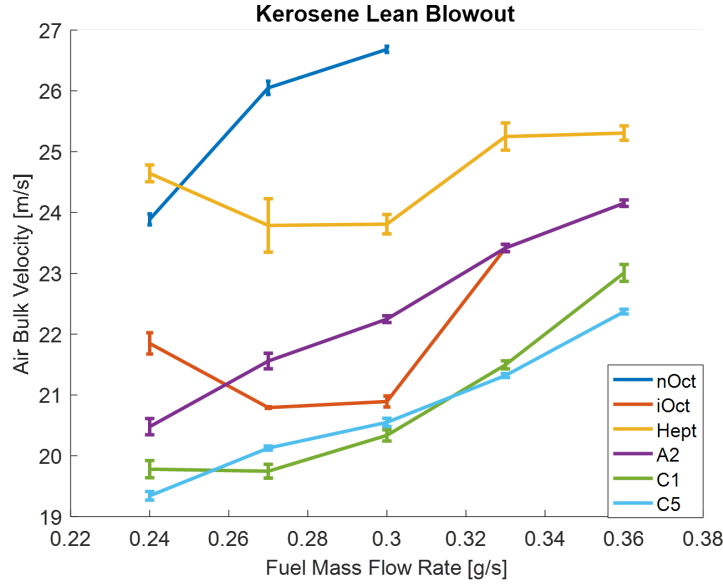


Fig. 2.2 Experimental blow-off curve of various fuels, including multi-component Jet-A (denoted as A2) and synthetic fuels C1 and C5 from the NJFCP, as well as single-component fuels n-octane, iso-octane, and n-heptane. The synthetic fuels consistently blow-off at lower air bulk velocity and higher equivalence ratio than conventional Jet-A. Figure is reproduced with permission from Allison et al. [2018].

Verdier et al. [2018] analysed turbulence–droplet–chemistry interaction events and local extinctions in an n-heptane spray flame in the Rouen lifted spray flame burner using Particle Image Velocimetry (PIV), Phase Doppler Anemometry (PDA) and OH-PLIF. Flame/droplet extinctions were observed along the flame front as large ballistic droplets broke through the flame, acting as heat sinks strong enough to extinguish the flame locally. Intense local strain rate induced by the shear layer in the inner recirculation zone caused flame/turbulence extinctions along the inner flame front, occurring mostly in the gas phase in a primarily premixed, pre-vaporised region. Large droplets evaporating near the outer flame also acted as fuel-rich sinks which decreased flammability locally, observed by strong decreases in OH around the droplet. This work highlights the complexity of spray flames, where various regions of the flame can experience local extinctions driven by entirely different physical mechanisms.

Fuel starvation was also noted as a likely reason for difficulties in igniting Jet-A droplets during an ignitability study of the three NJFCP fuels in de Oliveira et al. [2017], as fuel starvation was suggested as a cause in the discussion of long mode ignition

failure in Mastorakos [2017]. Laser ignition experiments on liquid fuel dispersions in turbulent air using line-of sight OH^* chemiluminescence showed that due to its low volatility, Jet-A was the most difficult to ignite of the three fuels, whereas the more volatile C5 was the only fuel that could ignite at an overall lean equivalence ratio at the experimental conditions. The ignitability of Jet-A and C1 was explored in more depth in de Oliveira & Mastorakos [2019], where large droplets were observed to break through the flame front and continue evaporating amongst burnt gases. This behaviour was linked to the slow evaporation time caused by low volatility compared to the flame front speed.

Bell et al. [2018] studied fuels from the NJFCP to understand the impact of preferential vaporisation on LBO using evaporative, chemical and chemical-evaporative time scales. They found that no single time scale analysis was sufficient to characterize experimental observations of the loose relation between DCN and lean blow-off. The composition of the distillation curve for each fuel was suggested to offer a stronger correlation between derived cetane number and LBO. Using results from the Referee Rig at the U.S. Air Force Research Laboratory (AFRL), Bell et al. [2018] found that the first 34% of the fuel liquid volume distillation curve to vaporise were the species which drove when LBO would occur. Thus the DCN number of the lightest third of the species composing the kerosene could be more strongly predictive of how a fuel would blow-off. This correlation of preferential vaporisation with the DCN of the light end of the distillation curve for fuels was explored further in Won et al. [2019], where instead the first 20% of the species in the distillation curve was determined adequate for correlation of DCN with the blow-off equivalence ratio. This suggests that the equivalence ratio at LBO is controlled by both vaporisation potential (lower initial distillation boiling temperatures) and chemical reactivity potential (DCN) of the initially vaporised species.

Rock et al. [2020] endeavoured to more fully characterise the physics causing local extinctions and lean blow-off in spray flames in experiments using the main fuels of interest from the NJFCP, including A2, C1, C5, n-dodecane and a surrogate fuel at a pressure of 345 kPa and two air temperatures: 300 K and 450 K. Extinction and reignition events at near-blow-off conditions for n-dodecane and Jet-A were visualised using CH^* chemiluminescence images. Analogous to premixed flame blow-off, they showed that spray flames show events of extinction, reignition, and recovery of the flame. The majority of flame recovery events were associated with convection of hot products back upstream, rather than reignition. Fuel composition had more influence at 300 K compared to 450 K, and a strong correlation was found between the boiling

temperature of a fuel and the duration of its extinction history prior to LBO. Fuels with high boiling temperatures were more likely to experience reignition recoveries. Rock et al. [2020] suggest this was caused by droplets with high boiling temperatures slowly vaporising, which allowed the flame to cool and caused longer extinction durations. This fresh fuel vapour was then finally able to reignite with fresh air, re-establishing a stable flame, while the hot gas products were swept downstream in the meantime. High DCN fuels were able to resist blow-off better through delay of local extinction and LBO precursor events, and were more capable of recovery through reignition.

Simulations

Three-dimensional compressible DNS was applied with a fine monodisperse spray of n-heptane to study ignition in Wandel et al. [2009]. They found that the flame kernel may quench due to fuel starvation in the vapour phase. A hot region could be created, however without enough fuel vapour available there was not enough energy to overcome the heat loss due to evaporation and diffusion in the flame front, and the flame would quench after a time on the order of a flame time scale. Wandel et al. [2009] determined the cause of the fuel starvation could be linked to either too large droplets or insufficient quantity of droplets.

Giusti et al. [2018] studied quiescent single kerosene droplets at high altitude relight conditions ($p = 0.3$ bar, $T_{air} = 250$ K) with the Dagaut detailed kerosene surrogate mechanism, using the methodology developed in Borghesi & Mastorakos [2015]; Giusti et al. [2017] to improve understanding of ignition phenomena. The lean flammable limit was observed to move away from the droplet immediately following ignition, but it returned back to the droplet surface in the last stages of the droplet's evaporation. At this point of the droplet's life, extinction was observed via high scalar dissipation rates causing low OH and temperature despite stoichiometric mixture being available.

Earlier studies of spray flames in more practical configurations have focused more on capturing the spray and evaporation characteristics of kerosene using the PDF approach with Eulerian Stochastic Fields, which takes into account evaporation from the liquid to the gaseous phase on subgrid scales [Jones et al., 2010, 2012, 2014]. In Jones et al. [2012], temperature and velocity measurements were compared with experiments at stable and rich near-blow-off conditions with reasonable accuracy. A simple 4-step chemical mechanism for kerosene was used, but it was suggested that a more detailed chemical mechanism would be necessary to get accurate intermediate species concentrations. In Jones et al. [2014] the subgrid-scale combustion model closure sensitivity was explored by varying the number of stochastic fields used, which

highlighted the closure of mixing model as a considerable challenge in using transported PDF approaches.

LES-CMC has demonstrated success in modelling extinction and blow-off in high-volatility spray flames. The same Cambridge bluff body swirl burner investigated in Cavaliere et al. [2013] was investigated numerically with LES-CMC and a one-step n-heptane chemical mechanism in Tyliczszak et al. [2014] to try to predict lean blow-off of a spray flame. Local extinctions were captured visually and in mixture fraction conditional space with significant drops of temperature associated with high quenching values of scalar dissipation rate. Full blow-off of the flame was achieved at the experimental blow-off velocity, with the flame structure strongly matching the visualisations from the experiments. The one-step chemistry allowed for good prediction of local and global extinction behaviour, however more detailed mechanisms could offer increased insight into the chemistry during blow-off with intermediate species behaviour included.

Using the same numerical configuration with the addition of including subgrid effects of spray in the mixture fraction variance equations, LES-CMC predicted local extinction and blow-off in ethanol spray flames [Giusti & Mastorakos, 2016, 2017] based on the experiments by Yuan [2015]; Yuan et al. [2018] using detailed ethanol chemistry. Local extinctions were observed to increase both along the air shear layer and the spray cone during the blow-off transient, and the flame structure followed that of experiments, shrinking downward toward the bluff body just before blow-off. In Giusti & Mastorakos [2016] the role of evaporation in causing extinction was discussed—through both the increase of local mixing caused by increased scalar dissipation rate and the decrease of the availability of fuel vapour as the extinction transient progressed. More local extinctions in the spray region led to a lower evaporation rate. As evaporation reduced during the blow-off transient the temperature of the mixture was reduced and the volume integrated heat release rate was also significantly reduced to almost nothing, corresponding to the disappearance of stoichiometric mixture fraction. This behaviour indicates that fuel starvation probably contributed to the extinction process. This work demonstrated the importance of including subgrid scale effects of the spray on the mixture fraction variance.

A realistic gas-turbine combustor was studied using the LES-FPV approach with detailed HyChem mechanisms for the three fuels under investigation in the NJFCP (A2, C1, and C5) to determine fuel effects on lean blow-out [Esclapez et al., 2017]. The LBO-limits were found to be very close for both the Jet-A and the two alternative fuels and marginal fuel effects were observed on the LBO-limits, contrary to predictions

from empirical correlations. The tabulated LES-FPV combustion model was suggested to be one of the limiting factors contributing to lack of sensitivity of the resulting flame behaviour to chemistry or fuel effects, despite being used with detailed chemical mechanisms.

Hasti et al. [2018] simulated LBO of the NJFCP fuels in a referee combustor using LES with automatic meshing and adaptive mesh refinement and finite-rate chemistry (FRC) with “compact” chemical models for A2 and C1 [Dooley et al., 2010]. LBO occurred at richer global equivalence ratio in the simulations compared to the experiments, however flame structure, temperature and species trends were well-captured by the simulations compared to experiments. Lower temperatures were noted in the recirculation zone of the C1 flame compared to the A2 flame, with C1 blowing off at a richer equivalence ratio as seen previously in experiments. A similar study using the same fuels and numerical set-up but with HyChem skeletal mechanisms for A2 and C1 was done in Piehl et al. [2018]. The relative blow-off behaviour between A2 and C1 was captured and blow-off was captured within 1% of experimental data, however the simulations predicted blow-off at leaner equivalence ratio than experiments. Due to the limited nature of the chemical mechanisms, a detailed analysis on the physics and chemistry of these flames during blow-off would be difficult. These studies also made no attempt at describing local extinction behaviour or understanding the physics of spray flame LBO in general. Rather, they looked only at large-scale global blow-off phenomena between A2 and C1.

Local extinction in n-heptane non-swirling lifted flames in the Rouen spray burner was studied in Benajes et al. [2021] using LES and a tabulated chemistry method based on steady and unsteady extinguishing diffusion flamelets at different enthalpy levels, and a presumed shape PDF. A 188-species skeletal n-heptane mechanism was used to generate the tabulated chemistry manifold. Extinction was predicted in various parts of the flame. Extinction caused by droplet interaction was observed along the flame leading edge; OH and temperature were observed to decrease near stoichiometric mixture fractions as droplets crossed the flame front, which coincided with regions of high localised evaporation source term. Little to no OH mass fraction was found at the mid-range to highest evaporation rates which correspond to more rich mixture fractions, whereas CH₂O was observed to peak around the high-mid-range evaporation rates. Benajes et al. [2021] suggest the concentration of CH₂O can be used to indicate extinction events. These results suggest droplets which are experiencing strong evaporation locally quench the flame with too-rich mixtures and low temperature. The simulation also captured extinction caused by turbulence-flame interactions due to

increased levels of scalar dissipation rate, and extinction events for scalar dissipation rates lower than the laminar flamelet quench value were observed.

2.3 Literature Summary

Important factors involved in spray flame phenomena are the chemical composition of real fuels and the chemistry modelling methodology. Recent experimental studies have demonstrated how various blends of heavy hydrocarbon fuels like those in the NJFCP can have widely varying ignition [de Oliveira et al., 2017] and blow-off [Allison et al., 2018] characteristics. The surrogate method of chemistry modelling for aviation fuels is a well-established approach [Dagaut, 2002], but alternative methods for specific fuels have been developed – such as the Hybrid Chemistry “HyChem” high-temperature lumped pyrolysis method to simplify chemistry modelling of real fuels [Wang et al., 2018a,b; Xu et al., 2018] – and have been applied in LES chemistry sensitivity studies of lean blow-off of different kerosene blends in realistic combustors [Esclapez et al., 2017].

A numerical approach capable of capturing the finite rate chemistry effects, with all the physical processes leading to the extinction transient included, is required to reliably predict extinction behaviour. Developing numerical tools capable of such predictions is one of the major challenges of current generation turbulent combustion models [Giusti & Mastorakos, 2019].

There are various turbulent combustion models currently used in attempts to capture transient phenomena like extinction and blow-off. These turbulent combustion models involve different approaches, one of which being the tabulated chemistry method commonly used in the FPV and FGM approaches. The FPV method has shown some success in predicting local extinctions and LBO [Benajes et al., 2021; Esclapez et al., 2017; Ma et al., 2019]. Benajes et al. [2021] showed good success in capturing local extinctions in spray flames using tabulation, however this was in a single-component n-heptane spray flame, rather than with a real aviation fuel. Esclapez et al. [2017] had mixed success in predicting the global LBO behaviour of the NJFCP kerosene fuels using tabulation, and they suggested that this may have been the limiting factor in their blow-off predictions. Tabulated chemistry approaches use a laminar flame system or well-stirred reactor which has been pre-calculated, with the chemical reaction rate being stored in a table and subsequently accessed during simulation at relevant conditions [Giusti & Mastorakos, 2019]. Tabulation speeds simulations up considerably, however through linking all species behaviour to a single variable (i.e., the progress variable) the solution can be more limited and less general than the methods which

employ independent transport equations for species and other quantities of interest. This is especially important for transient phenomena like LBO and local extinctions.

The untabulated, or “online” solution of chemistry approach in contrast appears to be the most appropriate for prediction of extinctions/blow-off of real fuels as it solves time-varying transport equations for the coupled interaction between turbulence and flame structure, where turbulence directly affects the transient evolution of species [Giusti & Mastorakos, 2019]. This is particularly important when modelling sprays, as evaporation directly interacts with local flame structures [Olguin & Gutheil, 2014]. The online method of the transported PDF has shown great accuracy in its predictions of extinction, as demonstrated in Yu et al. [2020] for a gaseous flame, however its large computational resource requirements limit it to use with skeletal and reduced chemical mechanisms [Jones et al., 2012, 2014], especially when sprays are involved.

LES-CMC has shown very promising ability to predict local extinction and blow-off in spray flames [Giusti & Mastorakos, 2016, 2017; Tyliczszak et al., 2014] with more volatile fuels like n-heptane and ethanol. However, the modelling of heavy hydrocarbons like kerosene, which are generally characterized by lower volatility and a more complex chemical behaviour, introduces new challenges that may affect the local and global extinction behaviour through the evaporation process and turbulence-chemistry interactions.

Recent computational studies of kerosene spray flames besides that of Esclapez et al. [2017] include those by Felden et al. [2018] and Eckel et al. [2019], although these studies emphasised emission predictions, such as nitric oxide and soot precursors, rather than local extinctions or LBO. In Felden et al. [2018], LES of a lean direct-injection combustor using the Dynamically Thickened Flame (DTF) combustion model and the HyChem Jet-A mechanism with a NO_x mechanism, reduced using the Analytically Reduced Chemistry (ARC) approach, they investigated spray characteristics and pollutant formation. The study benefited from increasing the number of transported species to twenty-nine, compared to previously using empirically fitted global schemes or tabulation for the chemistry. This suggests that greater detail in the chemical mechanism may lend deeper insight into the physics of heavy hydrocarbon flames.

A lab-scale swirl burner configuration in Eckel et al. [2019] was modelled using a multi-component vaporization model with a detailed kerosene surrogate chemistry and direct solution of chemical reactions using the finite-rate chemistry (FRC) approach with a focus on capturing soot precursors and other pollutants. Spray parameters and the reaction zone location were well-reproduced compared to experiments, however

temperature profiles were not as accurate. The results indicated that detailed chemistry and effective spray vaporization modelling were necessary in order correctly predict soot emissions.

The state of the art suggests that several key elements are necessary for accurate modelling of kerosene spray flames:

- Detailed chemistry is necessary for accurate intermediate and soot precursor species concentrations.
- Online combustion solvers, as opposed to tabulated solvers, are needed to capture nuances in chemical differences between different fuels especially during local extinction and blow-off.
- Spray models taking evaporation effects and liquid fuel properties into account are of high importance for accuracy in simulations.
- Comprehensive analysis of detailed chemistry in laminar counterflow flamelet simulations up to and through the extinction transient is lacking for real fuels and SAFs.

These points highlight a definite need for continued numerical study of kerosene spray flames. The research in this thesis utilizes the HyChem detailed kerosene mechanisms used in some of the previous studies, as it has shown good potential for prediction of key intermediate species and important soot precursors for both Jet-A and alternative jet fuels. Detailed mechanisms offer a wealth of data in species behaviour to understand which chemical processes are involved in extinctions and LBO.

This work attempts to predict the LBO curve of Jet-A in the context of the experiments in Allison et al. [2018]; Sidey et al. [2017]. Very few such attempts at modelling LBO of jet fuel sprays currently exist in literature, due to the complexity of the models and the computational power required. The LES-CMC method for online solution of the chemical reaction step, which prior to this doctoral research was untested with multi-component heavy hydrocarbon fuels like kerosene, is used to evaluate its capabilities in replicating the flame structure and blow-off duration during the LBO transient observed in experiments and to gain further insight for the physical reasons for spray flame blow-off. 0D-CMC is also evaluated in its ability to replicate experimental blow-off trends between the different NJFCP fuels in the laminar counterflow flamelet context, which isolates chemical behaviour from physical behaviour. The speciation and extinction trends give insights into understanding the causes for the contrasts in behaviour between different jet fuels.

Literature review

This thesis endeavours to provide a stronger understanding of the chemical and physical processes involved at the lean limit of operability for conventional and alternative jet fuels, and emphasizes the role of fuel starvation as a driving cause of LBO and extinction in spray flames.

Chapter 3

Methodology

Key concepts in combustion and turbulent fluid modelling in the context of non-premixed flames are introduced in this section. Non-premixed flames and relevant concepts such as the mixture fraction, scalar dissipation rate, and laminar flamelets are presented. Flame stabilisation techniques relevant for preventing flame lean blow-off are outlined and liquid fuel spray modelling is discussed. The computational fluid dynamics technique of Large Eddy Simulation (LES) and the turbulence-combustion model Conditional Moment Closure are introduced, with focus on their coupling to perform transient simulations capable of capturing finite-rate phenomena. The major concepts, equations and closure methods are discussed. Then the detailed chemical mechanisms used to solve for the reaction rates are presented, including the Dagaut surrogate mechanism and the HyChem lumped pyrolysis mechanism for Jet-A. Finally, the solver implementation, case set-up, and solution strategies are detailed.

3.1 Non-premixed flames

Non-premixed flames (also sometimes referred to as diffusion flames) are a basic flame configuration where fuel and oxidizer are injected separately and react as they mix. Examples of non-premixed flames are in jet engines, Diesel engines, steam boilers, and hydrogen-oxygen rocket motors [Warnatz et al., 1999]. Non-premixed flames, contrary to premixed flames, are fixed to the mixing interface between fuel and oxidizer and cannot propagate. This makes non-premixed flames safer to handle than premixed flames, as premixed flames can move at high speeds in the direction of the unburnt gases into regions not designed for the flame temperatures (e.g., flashback [Lefebvre & Ballal, 2010]). Non-premixed flames are sustained by diffusion on both the fuel and oxidant sides, and only move as the fuel and air are convected in turbulent fluid motion.

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Fuel and oxidizer diffuse to the flame zone, where they are converted into products by chemical kinetics with corresponding exothermic heat release. After this the products and heat diffuse and are convected away from the flame zone.

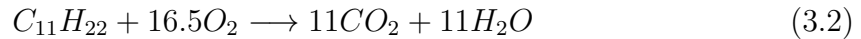
Non-premixed flows exist in both laminar and turbulent flow regimes. The theoretical backgrounds presented in Sections 3.1 to 3.4 and Sections 3.8.5 and 3.9 are relevant for both laminar and turbulent flame modelling, whereas the other sections apply primarily to turbulent flame modelling background.

Stoichiometry and equivalence ratio

In a simple form of a reaction equation, Eq. 3.1 shows fuel (F) and oxidant (O), the reactants, reacting to make products, where ν_F and ν_O are the molar stoichiometric coefficients corresponding to complete reaction.



A more specific example of a reaction equation is the global combustion equation for an approximate single-component formulation of Jet-A, shown in Eq. 3.2, where the coefficients ν_F and ν_O are 1 and 16.5 respectively for the balanced equation.



These coefficients are important as they provide information on the stoichiometric ratio or stoichiometry of the mixture: the condition at which the most complete and efficient combustion occurs, such that the proportions of fuel and oxidizer molecules are at the exact ratio to create only carbon dioxide and water with the same proportion of elements as in the reactants. The value of stoichiometry can be determined using Eq. 3.3 with the molecular weights of the reactants W and the stoichiometric coefficients, which corresponds to the ratio of the chemical species mass fractions of the mixture Y_F and Y_O at stoichiometry.

$$s = \frac{\nu_O W_O}{\nu_F W_F} = \left(\frac{Y_O}{Y_F} \right)_{st} \quad (3.3)$$

Mass fractions, expressed using Y_α , are used to denote the mass of species α compared to the total mass in the system, such that $Y_\alpha = m_\alpha / m_{total}$.

3.2 Conserved Scalar: The mixture fraction

Knowledge of stoichiometry can then provide the local equivalence ratio, ϕ , when multiplied by the ratio of fuel mass fraction Y_F to oxidant mass fraction Y_O in Eq. 3.4.

$$\phi = s \frac{Y_F}{Y_O} \quad (3.4)$$

In non-premixed flames the global or overall equivalence ratio in Eq. 3.5 is different from the local in Eq. 3.4, and is determined using the inlet fuel mass flow rate and air mass flow rate, $\dot{m}_F$ and $\dot{m}_O$.

$$\phi_{overall} = s \frac{\dot{m}_F}{\dot{m}_O} \quad (3.5)$$

ϕ is a useful parameter in characterising whether a flame is operating in either rich combustion or lean combustion regimes. $\phi = 1$ indicates the fuel/air proportions are stoichiometric, where the flame should burn nearly at its strongest. When $\phi > 1$, the system is in the rich combustion regime. In rich combustion there is an excess of fuel, resulting in some of it not being burnt. When $\phi < 1$, the system is in the lean combustion regime. In lean combustion there is too little fuel, thus some of the oxidizer remains unburnt. For every flame, there are rich and lean *flammability limits* which can be characterised with ϕ or $\phi_{overall}$. Flammability limits are discussed further in Section 3.10.

3.2 Conserved Scalar: The mixture fraction

In order to simply characterize non-premixed flames mathematically, one can look to the element mass fractions Z_i of the system, where Z denotes the ratio between the mass of an element i and the total mass. The element mass fractions are special in that they cannot be changed or converted through reactions. They are only transformed through mixing [Warnatz et al., 1999], unlike species mass fractions Y_i , which are changed by both reactions and mixing. In a simple non-premixed flame, which can be treated as a fuel inlet and oxidizer inlet opposite each other (counterflow configuration), the *mixture fraction*, ξ , can be defined using element mass fractions (where indices 1 and 2 are the fuel stream and oxidizer stream):

$$\xi = \frac{Z_i - Z_{i2}}{Z_{i1} - Z_{i2}} \quad (3.6)$$

Using this formulation for ξ is advantageous due to its linear relation to the mass fractions, and if diffusivity of the elements are considered equal, then the mixture

Methodology

fraction is independent of the elements used for its definition [Warnatz et al., 1999]. This linear relationship only holds with fast chemistry (infinite rate/mixed equals burnt).

By solving for the mixing of ξ , the mixing of everything else can be computed. Using normalized boundary conditions such that $\xi = 1$ in the fuel stream and $\xi = 0$ in the oxidizer stream, ξ signifies the mass fraction of substance that originally came from the fuel stream, at any point in the flow [Cant & Mastorakos, 2008]. When using finite-rate chemistry there will be overlap between fuel and oxidizer at the stoichiometric mixture fraction ξ_{st} , however the linear relations are useful as an initial solution in numerical simulations. Reaction rates are highest in regions of stoichiometric proportions, thus ξ_{st} is a useful parameter for approximating the location of the reaction zone in both laminar and turbulent simulations [Cant & Mastorakos, 2008]. The stoichiometric mixture fraction can be solved for using the stoichiometric ratio s and initial fuel and oxidizer mass fractions via:

$$\xi_{st} = \frac{1}{1 + sY_F^0/Y_O^0} = \frac{1}{1 + \phi} \quad (3.7)$$

where $Y_F^0 = Y_F(\xi = 1)$ and $Y_O^0 = Y_O(\xi = 0)$.

The mixture fraction is an example of a conserved, nonreactive scalar governed by a transport equation that does not have a chemical source term. The concept assumes unity Lewis number ($Le = \lambda/D\rho c_p = 1$), where λ is thermal conductivity and c_p is heat capacity, and that the diffusivity D is governed by Fick's Law (and is the same for all species). The equation for the mixture fraction distribution in a turbulent flow is as follows:

$$\frac{\partial \rho \xi}{\partial t} + \frac{\partial (\rho \mathbf{u}_i \xi)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial \xi}{\partial x_i} \right) \quad (3.8)$$

where ρ is density, t is time, $\mathbf{u}_i$ is the velocity vector, and x_i is the spatial dimension. Modelling turbulent non-premixed flames is reduced to tracking the turbulent mixing of ξ [Warnatz et al., 1999]. Knowledge of the mixture fraction value can be used to solve for critical quantities like temperature and species mass fraction. This however necessitates knowledge of the probability density function (PDF) of the mixture fraction. Rather than solving conservation equations for the PDF, much simplification can be achieved if the shape of the PDF $P(\xi)$ is presumed. A generic shape, such as the β -function, can be described by just two parameters—the mean and variance of the resolved mixture fraction, $\tilde{\xi}$ and $\widetilde{\xi'^2}$ [Bilger, 1980; Devaud et al., 2004; Girimaji, 1991].

3.3 Micro-mixing: The scalar dissipation rate

Thus instead of conservation equations for the PDF, only conservation equations of $\tilde{\xi}$ and $\widetilde{\xi''^2}$ are necessary.

The transport equation for the mixture fraction $\tilde{\xi}$ (resolved in the flow solver) is [Triantafyllidis & Mastorakos, 2010]:

$$\frac{\partial(\bar{\rho}\tilde{\xi})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{\mathbf{u}}_i\tilde{\xi})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho}(D + D_t) \frac{\partial \tilde{\xi}}{\partial x_i} \right) \quad (3.9)$$

and the Favre subgrid scale variance of the mixture fraction $\widetilde{\xi''^2}$ (where $\widetilde{\xi''^2} = \rho\xi''^2/\bar{\rho}$) is [Jiménez et al., 2001]:

$$\frac{\partial(\bar{\rho}\widetilde{\xi''^2})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{\mathbf{u}}_i\widetilde{\xi''^2})}{\partial x_i} = \frac{\partial}{\partial x_i} (\bar{\rho}(D + D_t) \frac{\partial \widetilde{\xi''^2}}{\partial x_i}) - 2\bar{\rho}\widetilde{N} + 2\bar{\rho}(D + D_t) \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}}{\partial x_i} \quad (3.10)$$

where $D = \mu/Sc$, μ is the laminar viscosity, Sc is the laminar Schmidt number, $D_t = \mu_t/Sc_t$, μ_t is turbulent viscosity, and Sc_t is the turbulent Schmidt number. Both Schmidt numbers are set to constant values. With Equations 3.9 and 3.10 the Favre-averaged (density-weighted) PDF of ξ is generated:

$$\tilde{P}(\xi) = \frac{1}{\bar{\rho}} \int_0^1 \rho P(\rho, \xi) d\rho. \quad (3.11)$$

$\tilde{P}(\xi)$ can also be referred to as a filtered probability density function, or FDF. The $\widetilde{N}$ term in (3.10) is a very important parameter which acts as a sink term for fluctuations, known as the scalar dissipation rate (see Eq. 3.12). This term is filtered and resolved directly using the flow solver. This term is discussed in more detail in Section 3.3.

3.3 Micro-mixing: The scalar dissipation rate

The scalar dissipation rate (SDR) is a fundamental parameter that describes how quickly scalar fluctuations decay. It is related to strain, has dimensions of inverse time (s^{-1}), and it measures the gradients of ξ and the molecular flux of species toward the flame [Poinsot & Veynante, 2005]. When there is little to no fluctuation of a scalar, it indicates the flow is in the state of being a “well-mixed” fluid, which makes scalar dissipation a measure of the rate of molecular mixing [Cant & Mastorakos, 2008]. SDR,

denoted as N in Eq. 3.12, dampens scalar fluctuations just as viscosity dampens fluctuations in velocity [Warnatz et al., 1999]:

$$N = D \left(\frac{\partial \xi}{\partial x_i} \right)^2 \quad (3.12)$$

where D is diffusivity, ξ is the mixture fraction and x_i is the spatial dimension. SDR is based on the gradients of the fluctuations of the mixture fraction ξ' . In the case of finite-rate chemistry, a flame with low N experiences little micro-mixing; the flow can become heterogeneous, experiencing fuel-rich regions and high temperatures. As mixing rates increase, some chemical processes more sensitive to mixing will begin to depart from equilibrium. As N increases further, more chemical species will depart from equilibrium until primary energy releasing reactions are competing directly with the mixing rate [Warnatz et al., 1999]. When scalar dissipation rates are increased, micro-mixing is increased along with homogeneity of the flow, and the overall temperature of the system decreases. Then, if the rate of mixing becomes too high it can result in local extinction or even global flame blow-off, which is marked by a dramatic drop in temperature as combustion reactions cease to occur.

Increase in the scalar dissipation rate can be related to increase in air jet velocity in practical systems. Higher flow velocity tends to produce greater amounts of turbulence, which is desirable in combustion as turbulence enhances mixing and chemical reactions. However there is a limit to the rate of scalar dissipation a flame can endure before it is extinguished, just as turbulent flames in experiments are limited by their blow-off velocity U_{BO} . Before U_{BO} is reached, a flame can sustain itself, although holes in the flame known as local extinctions may appear due to the large amounts strain imparted onto the flame by high SDR, especially in regions where fresh fuel and oxidants meet [Peters, 2000]. The cause of lift-off of turbulent flames is also ascribed to extinction via high scalar dissipation [Peters & Williams, 1983]. The SDR is highest near the point of fuel/air injection, where the mixture fraction occurs at its highest and lowest values, thus causing local flame extinction [Warnatz et al., 1999]. Unburnt hydrocarbons are another consequence of local flame extinction [Warnatz et al., 1999]. High strain of the flame front, where the flame is stretched by intense turbulence, can lead to local extinctions. In rich or lean mixtures the effects of flame extinction are more important, as reduced temperatures cause longer reaction times and reduced oxidation of pollutants, resulting in increased quantities of harmful flame emissions like unburnt hydrocarbons.

In the case of laminar non-premixed flame simulations a stable solution of the flame can persist up to the critical N , with decreasing values of maximum temperature. The temperature drops because the reaction rates are reduced, as well as residence time in the flame zone, while simultaneously the convective-diffusive heat removal rate is increasing [Warnatz et al., 1999]. When N is increased above the critical value, referred to as $N_{0,ext}$ in this work, the flamelet extinguishes, or blows off [Peters & Williams, 1983].

Solving for the scalar dissipation rate in multi-dimensional turbulent flame simulations can be approached in a number of ways. The SDR is most commonly calculated using algebraic relations [Devaud et al., 2004; Kolla et al., 2009; Sitte et al., 2021]. Some solve a separate transport equation for the scalar dissipation rate to increase accuracy [Knudsen et al., 2012], although with the potential trade-off of additional complexity and computational cost.

More on the SDR, its conditional counterpart $N|\eta$, and its implementation in laminar counterflow diffusion flames and in LES-CMC can be seen in Sections 3.8.4 and 3.8.5.

3.4 Transient flamelet concept

In order to simplify understanding and modelling, a turbulent non-premixed flame can be approximated as an ensemble or aggregate of many thin, instantaneous laminar non-premixed flame structures [Williams, 1975]. These reactive-diffusive laminar flames ($Re < 2000$) are called *flamelets*. Non-premixed flamelets are typically described in the context of a counterflow diffusion flame configuration [Williams, 2000], where fuel and oxidizer are injected axisymmetrically opposing one another and the flame is spatially fixed along the stagnation point at the surface of stoichiometric mixture, as shown in Fig. 3.1.

These flamelets describe the instantaneous local mixture state and whether it is burning or inert/extinguished, and can provide information on the species and temperature using the mixture fraction and the scalar dissipation rate [Liew et al., 1981]. The laminar flamelet concept was developed by Peters [1983, 1984, 1986], based on the conserved scalar concept and the linking of relationship between scalar dissipation rate N and the chemical reaction rate ω by Bilger [1976, 1979]. The

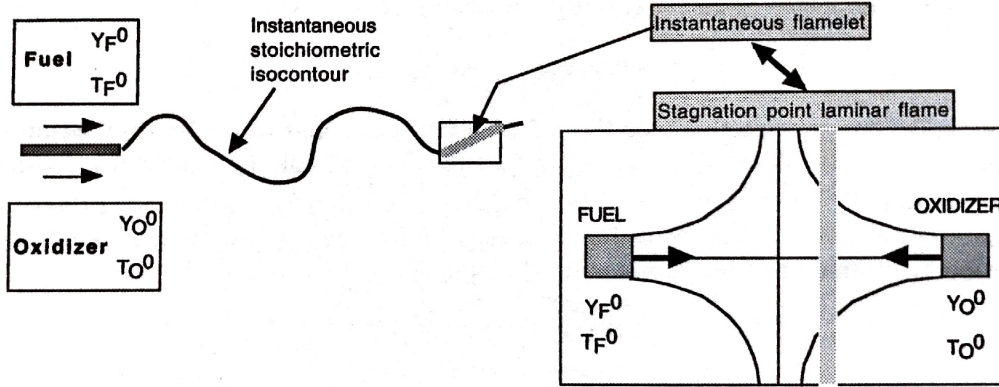


Fig. 3.1 Flamelet concept for a turbulent non-premixed flame and an example of the counterflow diffusion flame configuration. Figure is reproduced with permission from Poinot & Veynante [2012].

unsteady or transient laminar flamelet equations are provided for temperature and species mass fraction [Cant & Mastorakos, 2008]:

$$\rho \frac{\partial T}{\partial t} = \rho N(\eta) \frac{\partial^2 T}{\partial \eta^2} + \omega_T(Y_1, Y_2, \dots, Y_N, T) \quad (3.13)$$

$$\rho \frac{\partial Y_\alpha}{\partial t} = \rho N(\eta) \frac{\partial^2 Y_\alpha}{\partial \eta^2} + \omega_\alpha(Y_1, Y_2, \dots, Y_N, T) \quad (3.14)$$

where η is the mixture fraction which replaces physical space dependence in a non-dimensional sample space, and Y_α is the mass fraction of the α -th species. In this version of the equations unity Lewis number is assumed and the diffusivity of the species is assumed to be the same. In this simplified model the boundary conditions for T and N are fixed with a prescribed value (Dirichlet boundary conditions). Depending on the boundary temperatures and a low value of N , the unsteady flamelet can ignite to a range of fully burning high temperature states. As N is increased, the temperature will decrease and the flame will remain in a burning state, but once the critical extinction N value is applied a burning flame will extinguish. The response of species can be calculated over time during sudden events like ignition and extinction, and their behaviour will depend on the nature of the chemical mechanism used to solve for the reaction rate ω .

The flamelet model allows simplified calculations for turbulent non-premixed flames in η -space and the use of any type of chemistry, from one-step mechanisms to detailed mechanisms with hundreds of species. This model is useful for understanding the CMC

turbulence-combustion model used in this work, which is discussed later in the chapter, as well as its simplified form 0D-CMC, which is based on the laminar flamelet concept.

3.5 Large Eddy Simulation

Large Eddy Simulation, or LES, is a Computational Fluid Dynamics (CFD) tool which is well-adapted for many numerical turbulent combustion studies. CFD typically involves using a mesh or grid (2D or 3D) representing discretised physical space and system geometry, where at every cell or element in the mesh the Navier-Stokes equations for fluid dynamics are solved iteratively to approximate the fluid velocity, density, and pressure in space and time. LES has become increasingly viable in academia and industry in the last decade as computational power has increased exponentially, while previously computers were not able to handle the grid sizes needed for LES within a reasonable amount of computing time. LES lies at the crossroad between Direct Numerical Simulation (DNS) and Reynolds-Averaged Navier-Stokes (RANS), as it combines solving the time-varying Navier-Stokes equations on an intermediate size grid, resolving most large turbulence structures directly, while eddy structures smaller than the grid are statistically modelled. A comparison between DNS, LES and RANS approaches is shown in Fig. 3.2. DNS solves the Navier-Stokes equations on extremely

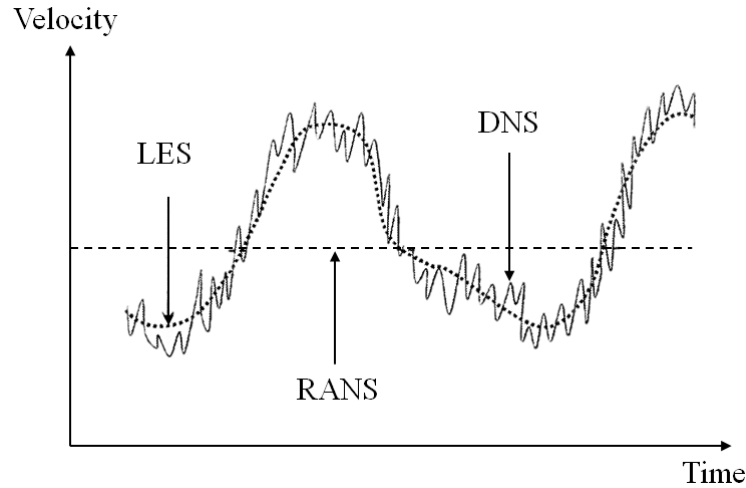


Fig. 3.2 Flow resolved by DNS, LES, and RANS. Figure is reproduced with permission of Andersson et al. [2011] through PLSclear.

fine, high resolution grids. This allows for the equations to be solved without any statistical modelling, however the computational cost on such grids can be enormous, and thus greatly limits the applications of DNS to fundamental and small-scale studies.

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RANS on the other hand solves the Navier-Stokes equations without the unsteady term, removing time-dependence, although modelling is still required to close the Reynolds stresses. The Reynolds decomposition of an instantaneous flow parameter (e.g., velocity) into its mean and fluctuations around the mean, $\Phi = \bar{\Phi} + \Phi'$, is employed in RANS. RANS is computationally much cheaper and faster than LES and is still used in many contexts, particularly when transient phenomena are not the focus. However, LES offers a computationally feasible way to solve fluid dynamics as it varies through time, which is especially important when studying highly transient phenomena like ignition, local extinctions and LBO.

For turbulent flows in general, large eddy structures and vortices depend more on the system geometry whereas small eddies are usually assumed to have more universal attributes. Thus, subgrid turbulence-viscosity models are well-suited to describe small eddies/flow structures [Poinsot & Veynante, 2005]. These subgrid models are typically based on similarity assumptions between the large and small scales, following the Kolmogorov energy cascade of energy flows from large (resolved) structures to small (unresolved) scales [Poinsot & Veynante, 2005]. The historical origins of LES lie in atmospheric science with meteorology applications in the work of Smagorinsky [1963], and subsequently the most popular subgrid scale model is the Smagorinsky model, which will be discussed later.

Large Eddy Simulation resolves the Navier-Stokes equations directly for the large fluid eddies present in the instantaneous turbulent flow field, while the small eddies are filtered out and modelled using subgrid scale (SGS) models [Andersson et al., 2011]. This is accomplished by means of low-pass Favre filtering the instantaneous governing equations to separate the large scales from the small. A spatially filtered physical space variable is defined as [Poinsot & Veynante, 2005; Pope, 2000]:

$$\bar{f}(\mathbf{x}, t) = \int_V f(\mathbf{x}', t) F(\mathbf{x} - \mathbf{x}') dV' \quad (3.15)$$

where F is the filter function (with filter size Δ) that determines the scale of the eddies to resolve, and the expression is integrated over the physical fluid domain volume V . The LES filter F must satisfy the normalisation condition:

$$\int_V f(\mathbf{x}', t) F(\mathbf{x} - \mathbf{x}') dV' = 1 \quad (3.16)$$

When applied to the governing equations, the filtering operation generates the LES mathematical model. Some example filter functions are the box, Gaussian and

sharp spectral filters [Andersson et al., 2011]. In finite-volume flow solvers, such as OpenFOAM, the computational grid itself can act as a filter for LES.

For variable density flows such as those in combustion, density-weighted Favre filtering [Favre, 1969] is employed:

$$\tilde{f}(\mathbf{x}, \mathbf{t}) = \frac{\overline{\rho f}}{\bar{\rho}} \quad (3.17)$$

The spatially-filtered and Favre-filtered variable (denoted with a tilde $\tilde{}$) instantaneous Navier-Stokes equations used in general turbulent reacting LES are shown for mass, momentum, chemical species, and sensible enthalpy [Poinso & Veynante, 2005]:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho} \tilde{\mathbf{u}}_i) = 0 \quad (3.18)$$

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{\mathbf{u}}_i) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j) + \frac{\partial \bar{p}}{\partial x_j} = \frac{\partial}{\partial x_i}[\bar{\tau}_{ij} - \bar{\rho}(\tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j - \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j)] \quad (3.19)$$

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{Y}_\alpha) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{\mathbf{u}}_j \tilde{Y}_\alpha) = \frac{\partial}{\partial x_i}[\overline{V_{\alpha,i} Y_\alpha} - \bar{\rho}(\tilde{\mathbf{u}}_i \tilde{Y}_\alpha - \tilde{\mathbf{u}}_i \tilde{Y}_\alpha)] + \bar{\omega}_\alpha \quad \alpha = 1, N \quad (3.20)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\bar{\rho} \tilde{h}_s) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{\mathbf{u}}_j \tilde{h}_s) = & \frac{\partial \bar{p}}{\partial t} + \overline{\mathbf{u}_i \frac{\partial p}{\partial x_i}} + \frac{\partial}{\partial x_i} \left[\lambda \frac{\partial T}{\partial x_i} - \bar{\rho}(\tilde{\mathbf{u}}_i \tilde{h}_s - \tilde{\mathbf{u}}_i \tilde{h}_s) \right] + \overline{\tau_{ij} \frac{\partial \mathbf{u}_i}{\partial x_j}} \\ & - \frac{\partial}{\partial x_i} \left(\overline{\rho \sum_{\alpha=1}^N V_{\alpha,i} Y_\alpha h_{s,\alpha}} \right) + \bar{\omega}_T \end{aligned} \quad (3.21)$$

The following unresolved quantities must be determined with SGS models: the Reynolds stresses: $\tau_{ij} = (\tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j - \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j)$, species fluxes: $(\tilde{\mathbf{u}}_i \tilde{Y}_\alpha - \tilde{\mathbf{u}}_i \tilde{Y}_\alpha)$, enthalpy fluxes: $(\tilde{\mathbf{u}}_i \tilde{h}_s - \tilde{\mathbf{u}}_i \tilde{h}_s)$, filtered laminar diffusion fluxes: $\overline{V_{\alpha,i} Y_\alpha}$, and filtered mean chemical reaction rate: $\bar{\omega}_\alpha$.

The main challenge in using LES for reacting flows is the modelling of the spatially filtered reaction rate term $\bar{\omega}$ [Bray, 1996; Pope, 1991], which appears in the chemical species and enthalpy balance equations. As chemical reactions occur at the small subgrid scales, combustion modelling has to be adjusted to interface with the LES subgrid models. DesJardin & Frankel [1998] showed closure of $\bar{\omega}$ without a SGS model gave poor results compared to DNS, and Meneveau & Katz [2000] showed scale-similarity used in the case of LES-turbulence closure modelling could not be applied to combustion processes originating from unresolved scales [Pitsch, 2006]. This makes subgrid scale combustion models necessary.

The equation system for solving the flow of a multi-dimensional turbulent flame in LES in this work involves conservation equations for the velocity field, and the pressure, as well as the filtered conservation equations for the mixture fraction and its variance, which generate the mixture fraction PDF. Details on the LES filtered transport equations including source terms are in Section 3.8.1. As the CMC subgrid scale turbulence-combustion model is used to solve for chemical species and enthalpy transport, Eqs. 3.20 and 3.21 are not required for LES in this work.

3.6 Liquid fuel sprays

Liquid fuels are typically used in engines for aircraft and automobiles. Liquid fuel has advantages over gaseous fuels in that it is compact and energy dense, making it easier to store in small containers, which is particularly important in highly weight- and space-sensitive applications like aviation. Liquid fuels such as kerosene have also been developed to be safer than gasoline, for example, by reducing volatility [Maurice et al., 2001], which makes it difficult to ignite kerosene spontaneously at atmospheric conditions. However, using liquid fuels turns combustion into a multi-phase liquid-gas problem, which leads to many additional challenges to engineers and modellers. Some processes in the liquid phase, gaseous phase, and the exchange at the interface of these phases must be represented, although depending on the application the accuracy can be increased or decreased as necessary. Liquid droplet modelling requires the use of numerous interacting submodels [Warnatz et al., 1999], although the more models used with increasing accuracy will rapidly compound the required computational time. Submodels can account for liquid sheet breakup, atomization, droplet dispersion, spray film deposition, and stochastic collisions, to name a few [Jenny et al., 2012], and then there is the strongly coupled evaporation and combustion process of the droplets to be considered [Pera et al., 2006].

In combustion contexts, fuel is typically injected through an orifice and the emerging liquid streams break up into ropey strands and then into a cloud of droplets that becomes increasingly dilute as distance from the injection point increases. This process is illustrated in Fig. 3.3. These ballistic droplets pass through the gaseous field into the reaction zone, where heat transfer increases the vapour pressure and ensuing fuel evaporation into the gas phase until gas-phase ignition occurs [Warnatz et al., 1999].

Sprays can be separated into two areas of research: (i) single droplet combustion, and (ii) spray combustion. Single droplet combustion is analogous to spray combustion

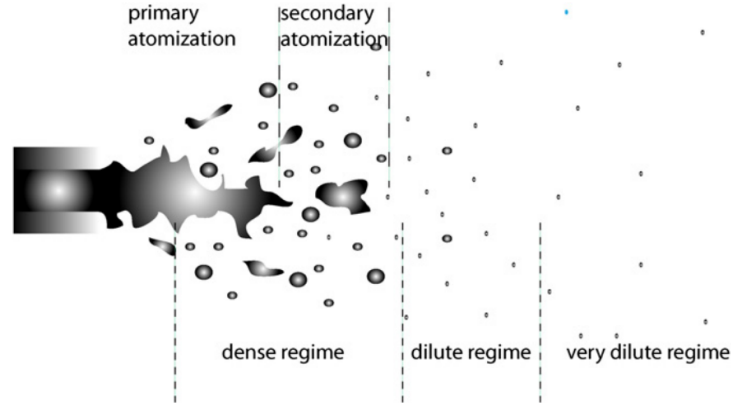


Fig. 3.3 An illustration of the different regimes of an injected liquid spray, reproduced from Jenny et al. [2012] with permission from Elsevier.

in the same manner that laminar flamelet models are embedded within turbulent flame combustion approaches [Warnatz et al., 1999].

In this work single droplet combustion concepts are utilized to account for droplet motion and evaporation. This is implemented in the context of a dilute polydisperse regime, where the burning spray is assumed to be an ensemble of single, non-interacting, spherical burning droplets of varying size which are sufficiently far from one another [Jenny et al., 2012]. Details on the single droplet modelling are in Section 3.6.1, and a brief description of the dilute polydisperse spray modelling technique is in Section 3.6.2.

3.6.1 Single droplet combustion model

The three phases of single droplet combustion are: the heating phase, the fuel evaporation stage, and the combustion phase [Warnatz et al., 1999]. In the heating phase, heat from the gas phase causes the surface of the droplet to heat up toward the boiling point. Then during the fuel evaporation stage, where the boiling temperature is reached, the fuel evaporates and the droplet loses mass. A combustible mixture is formed around the droplet. Finally in the third phase, the mixture around the droplet ignites from the higher surrounding gas temperature and burns as a spherically symmetric, laminar non-premixed flame, and the diameter of the droplet reduces at a quicker rate until there is no liquid fuel left to burn.

The ensuing models for single droplet motion and evaporation are implemented in the flow solver, OpenFOAM, as a part of the Lagrangian-Eulerian approach for LES.

Equations of motion for a single droplet

The methodology in this section is the same as the spray modelling described in Sitte [2019]. The position and velocity of a droplet are described by the following equations of motion:

$$\frac{d\mathbf{X}_d}{dt} = \mathbf{U}_d \quad \frac{d\mathbf{U}_d}{dt} = \frac{1}{m_d} \mathbf{F}_d \quad (3.22)$$

where the mass of the droplet $m_d = \rho_L(\pi/6)d_d^3$ and $\mathbf{F}_d$ is the sum of forces on the droplet. The particle forces in this case only consists of the drag force $\mathbf{F}_d = \mathbf{F}_D$ [Sitte, 2019]. The drag force is modelled as sphere drag using the Schiller & Naumann [1933] correlation for the drag coefficient C_D :

$$C_D = \begin{cases} \frac{24}{\text{Re}} (1 + 0.15 \text{Re}^{0.687}) & \text{if } \text{Re} \leq 1000 \\ 0.44 & \text{otherwise} \end{cases} \quad (3.23)$$

The droplet Reynolds number Re and subsequent drag force $\mathbf{F}_D$ can then be computed:

$$\text{Re} = \frac{\|\tilde{\mathbf{u}} - \mathbf{U}_d\| d_d}{\nu_G} \quad (3.24)$$

$$\mathbf{F}_D = \frac{1}{2} A_d \rho_G C_D \|\tilde{\mathbf{u}} - \mathbf{U}_d\| (\tilde{\mathbf{u}} - \mathbf{U}_d) \quad (3.25)$$

where A_d is the cross-section of a sphere, i.e., $A_d = \pi d_d^2/4$, and ρ_G and ν_G are the density and kinematic viscosity of the gas phase around the droplet. The temperature and species mass fraction of the gas phase around the droplet are evaluated using the one-third rule:

$$T_G = T_s + \frac{1}{3}(\tilde{T} - T_s), \quad Y_G = Y_s + \frac{1}{3}(\tilde{Y}_F - Y_s) \quad (3.26)$$

where the s subscript for temperature T_s and mass fraction Y_s denotes the surface of the droplet in the gaseous phase. $\tilde{T}$ and $\tilde{Y}_F$ are the local mean LES-filtered temperature and fuel species mass fraction of the gas phase around the droplet, representative of the mixture far from the droplet surface [Sitte, 2019].

Evaporation model

The overall rate of evaporation depends on numerous factors: pressure, temperature, gas transport properties, the volatility and diameter of the droplets in the spray, and the velocity of the droplets relative to the surrounding gas [Lefebvre & Ballal, 2010].

The evaporation model code was executed in the work of Sitte [2019] using the single-droplet evaporation model developed by Abramzon & Sirignano [1989], and the same version is used in this thesis. Stefan flow correction, non-unity Lewis number in the film and infinite conductivity of the liquid are applied. The key equations for the Abramzon & Sirignano model are presented here. The droplet mass m_d and temperature T_d are solved via the following equations:

$$\frac{dm_d}{dt} = -\pi d_d \rho_G D_G \text{Sh}^* \ln(1 + B_M) = -\dot{m}_d \quad (3.27)$$

$$\frac{dT_d}{dt} = -\frac{1}{m_d C_{p,L}} \frac{\dot{m}_d C_{p,V}}{B_T} (\tilde{T} - T_d) + \frac{1}{m_d C_{p,L}} \dot{m}_d LHV \quad (3.28)$$

where d_d is the droplet diameter, calculated as $d_d = (\frac{m_d}{\rho_L} \frac{6}{\pi})^{1/3}$, D_G is the average diffusivity of the gas phase of the droplet film, $C_{p,L}$ is the heat capacity of the liquid, $C_{p,V}$ is the heat capacity of the fuel vapour, $\tilde{T}$ is as described for Eq. 3.26, and LHV is the latent heat of vaporisation of the fuel. B_M and B_T are the Spalding mass (subscript M) and heat transfer (subscript T) numbers, evaluated using the following equations:

$$B_M = \frac{Y_{Fs} - \tilde{Y}_F}{1 - Y_{Fs}} \quad B_T = (1 + B_M)^\varphi - 1 \quad (3.29)$$

where $\tilde{Y}_F$ is the gas phase LES-filtered mean fuel mass fraction at the droplet location and Y_{Fs} is the fuel mass fraction at the surface of the droplet. This surface fuel vapour mass fraction is computed from the vapour saturation pressure evaluated at the droplet temperature T_d :

$$Y_{Fs} = x_{Fs} W_F / \sum_{\alpha} (x_{\alpha} W_{\alpha}) \quad x_{Fs} = \frac{p_{sat}(T_d)}{\bar{p}} \quad (3.30)$$

where x_{α} is the vapour molar fraction of the α -th species in the gaseous phase, x_{Fs} is the vapour molar fraction at the droplet surface, the saturation pressure p_{sat} is given by the Clausius-Clapeyron relation, and $\bar{p}$ is the average local pressure of the gaseous field. The flow field solver requires average droplet properties, thus the average fuel

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mass fraction at the surface of the droplet can be computed by taking an average over all the droplets in a computational cell:

$$\langle Y_{Fs} \rangle = \frac{\sum_i^{N_d} \dot{m}_{d,i} Y_{Fs,i}(T_{d,i})}{\sum_i^{N_d} \dot{m}_{d,i}} \quad (3.31)$$

where it is weighted with the evaporation rate of the droplet $\dot{m}_d$. N_d refers to the number of droplets in the cell.

The φ term for the Spalding heat transfer calculation in Eq. 3.29 is computed using the following relation:

$$\varphi = \frac{C_{p,V} \text{Sh}^*}{C_{p,G} \text{Nu}^* \text{Le}} \quad (3.32)$$

in which the non-dimensional Lewis number Le appears (the ratio of thermal diffusivity to mass diffusivity), and is defined by the Schmidt and Prandtl numbers:

$$\text{Le} = \frac{\text{Sc}}{\text{Pr}}, \quad \text{where} \quad \text{Sc} = \frac{\nu_G}{D_G}, \quad \text{Pr} = \frac{\nu_G C_{p,G}}{\lambda_G}. \quad (3.33)$$

In these relations, $C_{p,G}$ is the heat capacity of the gaseous carrier phase, ν_G is the kinematic viscosity and λ_G is the thermal conductivity. These values are evaluated for the gaseous field near the droplet surface.

The non-dimensional Sh^* and Nu^* are the modified Sherwood and Nusselt numbers, which take into account the thickening of the diffusion and thermal layer around the droplets due to surface blowing (Stefan flow correction):

$$\text{Sh}^* = 2 + (\text{Sh}_0 - 2)/F_M, \quad \text{Nu}^* = 2 + (\text{Nu}_0 - 2)/F_T \quad (3.34)$$

where Nu_0 and Sh_0 are the Nusselt and Sherwood numbers respectively, representing the heat and mass transfer between the droplet and the gaseous fluid. These values are calculated by the Frössling [1938] correlation:

$$\text{Sh}_0 = 2 + 0.552 \text{Re}^{1/2} \text{Sc}^{1/3}, \quad \text{Nu}_0 = 2 + 0.552 \text{Re}^{1/2} \text{Pr}^{1/3}. \quad (3.35)$$

Re is calculated using Eq. 3.24. F_M and F_T are the diffusion and thermal film correction factors, which are given as functions of the respective mass and heat transfer numbers, such that:

$$F_M = F(B_M), \quad F_T = F(B_T), \quad \text{where} \quad F(B) = (1 + B)^{0.7} \frac{\ln(1 + B)}{B}. \quad (3.36)$$

The quantities ρ_L , $C_{p,L}$, p_{sat} , and LHV are calculated at the droplet temperature T_d , whereas the gaseous properties ρ_G , ν_G , λ_G , D_G , $C_{p,G}$ and $C_{p,V}$ are computed at average reference conditions using the one-third rule in Eq. 3.26. Additionally, the non-dimensional numbers are solved at these average reference conditions. Liquid droplet property relations for ρ_L , $C_{p,L}$, p_{sat} and LHV are fits based on those reported in Esclapez et al. [2017] and are shown in the Appendix in Fig. A.1.

3.6.2 Spray combustion model

The single droplet model is applied in a polydisperse (meaning droplets are of varying size), dilute spray in which all droplets are spherical. This avoids the need for breakup or coalescence submodels [Pera et al., 2006]. The droplets, also referred to as the disperse phase, are unaware of each other and only interact with the gaseous phase.

The Eulerian-Lagrangian computational approach for two-phase flow is used. In this method, the gaseous Eulerian phase is modelled as a continuum, whereas the dispersed phase is modelled using Lagrangian point sources of mass, momentum, and energy [Pera et al., 2006]. The system is two-way coupled, which means the dispersed phase is aware of the continuous (gaseous) phase and the continuous phase is aware of the disperse phase [Andersson et al., 2011]. This requires the presence of spray source terms in the gaseous fluid governing equations, including the subgrid variance of the mixture fraction [Réveillon & Vervisch, 2000], which is detailed in Section 3.8. This approach requires the droplets to be much smaller than the gaseous-phase grid cells. The number of particles is limited as it requires solving for an ordinary differential equation (ODE) (see Eq. 3.22) for every single particle. To counter this limitation, tens to thousands of particles which behave similarly can be bundled into “parcels” with a representative ODE, reducing the computational requirements while still providing correct spray source terms for the continuous gaseous phase [Andersson et al., 2011]. The Euler-Lagrange model tracks the centre of gravity of the parcels, and the parcel size limit is based on the notion that the particles within the parcel should exist within one computational cell [Andersson et al., 2011]. This condition is met by the LES mesh, with the only exception in the narrow region just above the bluff body surface. The spray modelling in OpenFOAM, which is utilized for its LES flow solver in this work, is implemented using dispersed phase parcels of droplets.

Although sprays are known to contain both premixed and non-premixed regimes, the work of this thesis utilizes singly conditional CMC, which explicitly accounts for non-premixed dilute spray regimes only. The spray model implementation is described in further detail in Section 3.11.3.

3.7 Conditional Moment Closure

Conditional Moment Closure (CMC) is an advanced subgrid turbulence-combustion model for non-premixed flows developed independently by Klimenko [1990] and Bilger [1993] and jointly reviewed in Klimenko & Bilger [1999]. The model is of an inherently statistical nature and is able to decouple the large-scale macromixing fluid flow from the chemical kinetics, while preserving the micromixing and scalar dissipation effects [Bilger, 1993]. This allows for flexibility in the chemistry which can be used with the model, from simple one-step models to large detailed chemical mechanisms. This gives CMC an advantage in capability to predict highly transient phenomena such as ignition or extinction which are dependent on finite-rate chemistry.

The underlying hypothesis of CMC is that most fluctuations of scalar quantities of interest (species mass fractions, temperature, etc.) can be associated with the fluctuations of one key quantity [Klimenko & Bilger, 1999]. To do this, the passive scalar mixture fraction concept is utilised, as it is more convenient to solve only for transport of the mixture fraction, which has no source term, as opposed to transport of every single reacting species dependent on highly non-linear reaction rates [Cant & Mastorakos, 2008]. This adds dimensionality to the turbulent combustion problem by dividing it into two problems: a mixing problem to determine the mixture fraction $\xi(\mathbf{x}, t)$, and a time-varying local flame structure problem to determine species mass fractions $Y_\alpha(\mathbf{x}, t)$ and temperature $T(\mathbf{x}, t)$ as a function of ξ [Sitte, 2019].

Conditional means or averages of the mixture fraction are then used to reduce non-linearity and obtain more accurate closure for the reaction rate term ω_α [Bilger, 1993]. Conditional moments are averages or variances of those scalars in a system ensemble which meet a certain, specified condition [Bilger, 1993] and are indicated with a vertical bar $|$. In conditional averaging, moments become functions conditioned on a prescribing variable, such as the mixture fraction. Then statistical values like the averages and variances (the first and second moments) of a reacting scalar conditioned on the mixture fraction can be generated.

The conditional mean of a reacting scalar, denoted as Q_α in CMC, is defined as an ensemble average of $Y_\alpha(\mathbf{x}, t)$ that is conditional on the condition $\xi(\mathbf{x}, t) = \eta$ [Bilger, 1993]:

$$Q_\alpha(\eta, \mathbf{x}, t) \equiv \langle Y_\alpha(\mathbf{x}, t) | \xi(\mathbf{x}, t) = \eta \rangle \equiv \langle Y | \eta \rangle \quad (3.37)$$

where angle brackets $\langle \star | \star \rangle$ signifies the conditional ensemble average of a variable over an ensemble of realisations of the flow, such that only those members of the entire

ensemble that meet this condition are used in the average [Bilger, 1993]. η is defined as a sample space variable (the prescribing variable) corresponding to the continuous random function $\xi = \xi(\mathbf{x}, t)$, which exists in the range $0 \leq \eta \leq 1$. $Q_\alpha(\eta, \mathbf{x}, t)$ is a non-random function of independent variables $\eta, \mathbf{x}$, and t with a specific value at each point of the five-dimensional space. Using this averaging procedure the instantaneous value of a reactive scalar can be decomposed (as in Reynolds decomposition) into the conditional mean and a fluctuation around the conditional mean [Bilger, 1993]:

$$Y_\alpha(\mathbf{x}, t) = Q_\alpha(\xi[\mathbf{x}, t], \mathbf{x}, t) + Y_\alpha''(\mathbf{x}, t) = Q_\alpha(\xi) + Y_\alpha''(\mathbf{x}, t) \quad (3.38)$$

This is where the underlying CMC hypothesis is implemented; if the fluctuations of Y_α are primarily associated with fluctuations of ξ , then the fluctuations around the conditional mean $\langle Y_\alpha | \eta \rangle = Q_\alpha(\xi)$ will be small compared to fluctuations around the conventional mean, $Y_\alpha'' \ll Y_\alpha'$, where $Y_\alpha' = Y_\alpha - \langle Y_\alpha \rangle$ [Sitte, 2019]. This hypothesis is proved visibly in the comparison with experiments made by Klimenko & Bilger [1999] in Fig. 3.4, where the conditional average points on the right match the mean of the experimental data with minimal fluctuations around the mean, thus making an improvement in scalar predictions compared to the laminar counterflow diffusion flame prediction portrayed as a solid line.

To obtain unconditional values of the reactive scalars such as those that exist in physical space, Q is integrated with the PDF of the mixture fraction $P(\eta)$ using the well-known statistical identity [Cant & Mastorakos, 2008]:

$$\langle Y_\alpha \rangle = \int_0^1 \langle Y_\alpha | \eta \rangle P(\eta) d\eta \quad (3.39)$$

The purpose of CMC is to provide closed transport equations for the conditional averages Q of reactive scalars in order to link the spatial dependence of unconditional averages to both the spatial variation of the presumed PDF of the mixture fraction $P(\eta)$ and to the spatial variation of the reacting scalars [Cant & Mastorakos, 2008]. This provides additional accuracy in predicting flame structure. The transport equation for conditional moments Q , assuming high Reynolds number, Fickian molecular mass diffusion, and unity Lewis number gives the following CMC governing equation for gaseous flames:

$$\frac{\partial Q_\alpha}{\partial t} + \langle \mathbf{u}_i | \eta \rangle \frac{\partial Q_\alpha}{\partial x_i} = \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \langle \omega_\alpha | \eta \rangle - \frac{1}{\bar{\rho} P(\eta)} \frac{\partial}{\partial x_i} (\langle \mathbf{u}_i'' Y_\alpha'' | \eta \rangle \bar{\rho} P(\eta)). \quad (3.40)$$

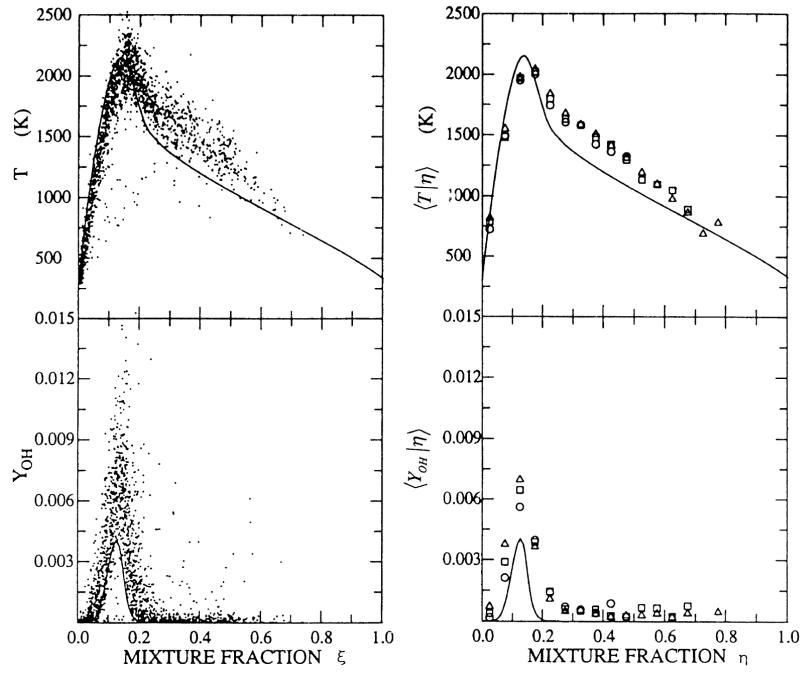


Fig. 3.4 Left: scatter plots of temperature and mass fraction of OH, measured by advanced laser diagnostic methods, as a function of the simultaneously made measurement of the mixture fraction from Masri et al. [1992]. Right: conditional average values of temperature, T , and hydroxyl radical mass fraction, Y_{OH} , conditional on the mixture fraction, ξ , with a prescribed value, η , made at various radial positions (hence the various marker shapes). Lines are a laminar counterflow diffusion flame simulation at low strain rate. The figure is reproduced from Klimenko & Bilger [1999] with permission from Elsevier.

Similar transport equations are solved for temperature and enthalpy. The conditional mean of the density is calculated using the system equation of state. CMC being inherently a statistical model lends flexibility to its application, as it does not require *a priori* knowledge of the flame structure or combustion mode [Kronenburg & Mastorakos, 2011], and it produces Q 's that respond to spatial and temporal variations of $\langle N|\eta \rangle$ and hence can capture a wide range of non-premixed reacting flow problems, including extinction and ignition.

Closure is necessary for the terms $\langle \mathbf{u}_i|\eta \rangle$, $\langle N|\eta \rangle$, $\langle \mathbf{u}_i'' Y_\alpha''|\eta \rangle$ and $\langle \omega_\alpha|\eta \rangle$. The first three terms are closed using various models incorporating information from the physical fluid and mixing fields, which is discussed in the next section. The motivation for developing CMC was to provide more accurate closure of the reaction rate term $\langle \omega_\alpha|\eta \rangle$ and to make the model work flexibly with various types of chemistry. Using the same assumption as before that fluctuations around the conditional means are small, a very simple first order closure can be employed for the reaction rate:

$$\langle \omega_\alpha(Y_1, Y_2, \dots, Y_{N_\alpha}, T)|\eta \rangle \approx \omega_\alpha(Q_1, Q_2, \dots, Q_{N_\alpha}, Q_T) \quad (3.41)$$

This is the closure used in *first-order CMC*, signifying that the conditional averages are used to calculate the reaction rate directly, which is employed for the research undertaken in this thesis.

CMC was originally developed for use in experimental and DNS studies of non-premixed gaseous flames, however its application has been broadened considerably over the years. In Navarro-Martinez et al. [2005] and Kim & Pitsch [2005] the CMC model was integrated into an LES framework for the first time and in the work of Navarro-Martinez & Kronenburg [2007] LES-CMC was applied to a turbulent bluff body stabilised methane/hydrogen flame. Triantafyllidis & Mastorakos [2010]; Triantafyllidis et al. [2009] discusses more recent methods for using LES and CMC in tandem. Often times in gaseous flames the subgrid scale mixture fraction variance $\widetilde{\xi''^2}$ in LES is modelled using gradient type models [Triantafyllidis & Mastorakos, 2010]. However Jiménez et al. [2001] developed a transport equation for the mixture fraction variance, which has since been utilised in more recent implementations of LES-CMC especially in spray flame applications, as spray evaporation has significant effects on the subgrid mixture fraction variance [Giusti & Mastorakos, 2016; Pera et al., 2006].

CMC equations were first modified to include spray terms in Mortensen & Bilger [2009] and have since been utilised in n-heptane [Tyliczszak et al., 2014] and ethanol [Giusti & Mastorakos, 2016] spray flames. The LES-CMC equations were modified further by Pera et al. [2006] and implemented in Giusti & Mastorakos [2017]; Sitte &

Mastorakos [2019] to incorporate spray terms in the mixture fraction variance equation for LES. The version of LES-CMC utilised in this work includes spray terms in both the LES mixture fraction and mixture fraction variance transport equations and in the CMC governing equations for reacting scalars and enthalpy.

3.8 LES-CMC Theory

The kerosene flames in this thesis are modelled using the LES-CMC approach in conjunction with an Eulerian-Lagrangian approach for dilute sprays using the methods discussed in Garmory & Mastorakos [2015]; Giusti & Mastorakos [2017]; Sitte & Mastorakos [2019]; Tyliczszak et al. [2014]; Zhang & Mastorakos [2016]. CMC is a finite-rate conserved scalar turbulence-combustion model used to solve for conditionally filtered scalars derived from unconditional values acquired from the solution of the transport equations in a flow solver. The CMC model solves exact balance equations for conditional values ($Q_\alpha|\eta = Y|\eta, T|\eta, \rho|\eta$, etc.) in mixture fraction η space, accounting for the subgrid scale chemical behaviour too small to be solved at the resolution of the LES grid. Advantages of CMC are that conditional mass fractions can be compared directly with experimental measurements [Poinot & Veynante, 2012], and certain combustion phenomena (such as auto-ignition and extinction) are strongly tied to mixture fraction isosurfaces [Mastorakos et al., 1997]. The CMC equations are coupled with LES, and a PDF of the mixture fraction is used to get unconditional values from the CMC computed quantities. This model is shown in Equation 3.42:

$$\tilde{Y}_\alpha(x, t) = \int_0^1 Q_\alpha(\eta, x, t) \tilde{P}(\eta, x, t) d\eta \quad (3.42)$$

where the Favre-averaged LES-filtered species mass fraction $\tilde{Y}_\alpha$ for example is being determined. In CMC terms, η is used to represent the sample space variable for ξ . ξ typically refers to unconditional mixture fraction solved in LES.

The left factor in the integral, Q_α , represents the reacting scalar solved for in CMC (i.e., temperature, density, enthalpy, or chemical species mass fractions). The α subscript denotes the α -th species index when solving for species mass fractions. This equation relates the reacting scalar Q_α to the non-reacting scalar, η , which is solved for in LES. The LES code solves for the flow (velocity $\mathbf{u}_i$) and mixing field (mixture fraction ξ) at every time step, and then passes these quantities to the CMC code which solves the species mass fractions Y_α , enthalpy H , temperature T , and density ρ , the

latter of which is then passed back to the LES for the next time step. This coupling makes the equation set quite stiff and requires a significant amount of time to solve.

The second term in the integral in (3.42), $\tilde{P}$, is the filtered PDF of the mixture fraction, which is used to obtain unconditional quantities from the conditional quantities solved for in the CMC equations. One can imagine it as a converter of scalars from conditional subgrid η -space into unconditional physical space. A presumed shape for the PDF is supplied, such as the β -function, and then scaled to fit the required mean $\tilde{\xi}$ and variance $\widetilde{\xi'^2}$ of the mixture fraction [Klimenko & Bilger, 1999]. Both are resolved by transport equations in LES, which are presented later in (3.49) and (3.51).

The β -PDF used in (3.42) as defined in Poinso & Veynante [2005] is modelled using the filtered mean $\tilde{\xi}$ and variance $\widetilde{\xi'^2}$:

$$\tilde{P}(\eta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \eta^{\alpha-1} (1 - \eta)^{\beta-1} \quad (3.43)$$

where $\Gamma(x)$ is the Gamma function. α is defined as $\alpha = \tilde{\xi}(\tilde{\xi}(1 - \tilde{\xi})/\widetilde{\xi'^2} - 1)$ and β is defined as $\beta = \alpha(1 - \tilde{\xi})/\tilde{\xi}$ [Sitte, 2019]. The β -function in particular provides a good statistical shape distribution of the mixture fraction due to its ability to change continuously from PDF shapes with one to two peaks to Gaussian shapes [Poinso & Veynante, 2012].

3.8.1 LES-filtered Navier-Stokes equations

The gas phase LES spatially filtered Navier-Stokes equations for two-phase flow are introduced based on those for single-phase flow described in Section 3.5. The equations for continuity and momentum are:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{\mathbf{u}}_j) = \bar{\rho} \tilde{\Pi} \quad (3.44)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{\mathbf{u}}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j) = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \bar{\rho} \tilde{\Pi}_{NS} \quad (3.45)$$

where $\tilde{\mathbf{u}}$ are the velocity vectors and p is the pressure. The resolved field viscous stress tensor τ_{ij} , and the unresolved subgrid scale viscous stress tensor τ_{ij}^{sgs} , resulting from the filtering of the non-linear advection terms [Tyliszczak et al., 2014], are defined as the following:

$$\tau_{ij} = \mu \left[\left(\frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \frac{\partial \tilde{\mathbf{u}}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{\mathbf{u}}_k}{\partial x_k} \right], \quad \tau_{ij}^{sgs} = \bar{\rho} (\tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j - \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j) \quad (3.46)$$

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where μ is the molecular viscosity defined by Sutherland's law and δ_{ij} is the Kronecker delta (essentially an identity matrix $\mathbf{I}$).

The subgrid Reynolds stress τ_{ij}^{sgs} is modelled using the constant Smagorinsky model [Smagorinsky, 1963], which is an eddy viscosity model based on the assumption that the smallest scales with turbulent viscosity μ_{sgs} (or μ_t) fully dissipate the energy received from the large scales through the energy cascade. Rather than solving the τ_{ij}^{sgs} equation in (3.46), this subgrid scale Reynolds stress term is modelled using the Boussinesq [1877] turbulent viscosity assumption:

$$\tau_{ij}^{sgs} = 2\mu_{sgs}\tilde{S}_{ij} - \frac{2}{3}\bar{\rho}k_{sgs}\mathbf{I}. \quad (3.47)$$

$\tilde{S}_{ij}$ is the resolved strain rate tensor, defined as $\tilde{S}_{ij} = \frac{1}{2}(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i})$ and k_{sgs} is the subgrid scale turbulent kinetic energy. The Smagorinsky model is used to solve for k_{sgs} and μ_{sgs} . μ_{sgs} is proportional to the square root of the subgrid scale turbulent kinetic energy, the LES filter width Δ (evaluated as $\Delta = \sqrt[3]{V_{LES}}$), $\bar{\rho}$, and model constant C_k , such that $\mu_{sgs} = C_k\bar{\rho}\Delta k_{sgs}^{1/2}$. The same constant Smagorinsky coefficients as in Sitte [2019] based on Fureby [1996] are used: $C_k = 0.02$ and $C_\epsilon = 1.048$.

Two-way coupling of the gas phase with the dispersed spray phase is implemented using the methodology in Sitte [2019]. The spray source terms are calculated by summing over all droplets in a LES cell. The source term for the momentum equation $\bar{\rho}\tilde{\Pi}_{NS}$, which represents transfer of momentum from the liquid phase to the gas phase, is evaluated using:

$$\bar{\rho}\tilde{\Pi}_{NS} = -\frac{1}{V_{LES}} \sum_i^{N_d} \frac{dm_{d,i}\mathbf{U}_{d,i}}{dt}. \quad (3.48)$$

V_{LES} is the volume of the LES cell in which the droplet is located, N_d is the total number of droplets in the LES cell, $m_{d,i}$ is the mass of droplet i , and $\mathbf{U}_{d,i}$ is the velocity vector of droplet i . Gravitational force is neglected and drag is the only force on the droplet, thus the momentum transfer is the same as the change of momentum of the droplet. Closure for the volumetric evaporation rate term $\bar{\rho}\tilde{\Pi}$ in the continuity equation (3.44) is nearly the same as for the momentum equation source term (3.48), except it is without the droplet velocity term. $\bar{\rho}\tilde{\Pi}$ closure is shown in Eq. 3.50.

3.8.2 LES-filtered $\tilde{\xi}$ and $\tilde{\xi}^{m2}$ equations with source terms

The spray flame simulations in this work are modelled using Lagrangian spray parcels which are coupled with the gaseous Eulerian field, thus to account for the spray the

mixture fraction equation introduced in (3.9) must contain a corresponding evaporation mass source term $\bar{\rho}\tilde{\Pi}$, as shown in Eq. 3.49:

$$\frac{\partial(\bar{\rho}\tilde{\xi})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{\mathbf{u}}_i\tilde{\xi})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho}(D + D_t) \frac{\partial \tilde{\xi}}{\partial x_i} \right) + \bar{\rho}\tilde{\Pi} \quad (3.49)$$

where $\bar{\rho}\tilde{\Pi}$ is exact and provided directly by the evaporation model implemented in LES as in Sitte [2019]:

$$\bar{\rho}\tilde{\Pi} = -\frac{1}{V_{LES}} \sum_i^{N_d} \frac{dm_{d,i}}{dt}. \quad (3.50)$$

V_{LES} is the volume of the LES cell in which the droplet is located, N_d is the total number of droplets in the LES cell, and $m_{d,i}$ is the mass of droplet i . The molecular and turbulent diffusivities are $D = \mu/(\bar{\rho}Sc)$ and $D_t = \mu_{sgs}/(\bar{\rho}Sc_t)$ with $Sc = 0.7$ and $Sc_t = 0.4$. The turbulent Schmidt number is taken from the work of Pitsch & Steiner [2000]. μ_{sgs} is solved using the constant Smagorinsky model. The evaporation mass source term $\bar{\rho}\tilde{\Pi}$ is related to the volumetric rate of phase change per unit volume $\tilde{\Pi}$.

The subgrid scale mixture fraction variance $\widetilde{\xi'^2}$ introduced in (3.10) is computed with an additional set of spray terms included, as presented in Pera et al. [2006]:

$$\begin{aligned} \frac{\partial(\bar{\rho}\widetilde{\xi'^2})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{\mathbf{u}}_i\widetilde{\xi'^2})}{\partial x_i} = & \frac{\partial}{\partial x_i} (\bar{\rho}(D + D_t) \frac{\partial \widetilde{\xi'^2}}{\partial x_i}) - 2\bar{\rho}\widetilde{N} + 2\bar{\rho}(D + D_t) \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}}{\partial x_i} \\ & + 2\bar{\rho}(\widetilde{\xi\Pi} - \tilde{\xi}\tilde{\Pi}) - \bar{\rho}(\widetilde{\xi^2\Pi} - \tilde{\xi}^2\tilde{\Pi}). \end{aligned} \quad (3.51)$$

The $\widetilde{\xi'^2}$ equation includes unclosed evaporation terms $\widetilde{\xi\Pi}$ and $\widetilde{\xi^2\Pi}$. These spray terms are closed using the methods described in Section 3.8.4 which are based on the work of Sitte [2019] and Giusti & Mastorakos [2017]. The scalar dissipation rate $\widetilde{N}$ in this equation includes subgrid evaporation effects and is limited using gradients of mixture fraction from the surface of a droplet to maintain stability [Sitte, 2020].

3.8.3 CMC governing equations

LES-CMC allows for direct computation of time-varying local flame structure in mixture fraction space. The method accounts for turbulence effects, micro-mixing/diffusion, and effects of spray evaporation. The three-dimensional CMC formulation solving for a

conditionally-filtered reactive scalar Q_α is expressed as the following [Tyliszczak et al., 2014]:

$$\begin{aligned} \frac{\partial Q_\alpha}{\partial t} + \widetilde{\mathbf{u}_i|\eta} \frac{\partial Q_\alpha}{\partial x_i} = & \widetilde{N|\eta} \frac{\partial^2 Q_\alpha}{\partial \eta^2} + e_\alpha + \widetilde{\omega_\alpha|\eta} + \delta_{\alpha,f} \widetilde{\Pi|\eta} \\ & - \left(Q_\alpha + (1 - \eta) \frac{\partial Q_\alpha}{\partial \eta} \right) \widetilde{\Pi|\eta} \end{aligned} \quad (3.52)$$

and a governing CMC equation similar to (3.52) without the chemical source term $\widetilde{\omega_\alpha|\eta}$ is solved for conditionally filtered enthalpy $Q_h = \widetilde{h|\eta}$ [Tyliszczak et al., 2014]:

$$\frac{\partial Q_h}{\partial t} + \widetilde{\mathbf{u}_i|\eta} \frac{\partial Q_h}{\partial x_i} = \widetilde{N|\eta} \frac{\partial^2 Q_h}{\partial \eta^2} + e_h + \widetilde{\Pi_h|\eta} - \left(Q_h + (1 - \eta) \frac{\partial Q_h}{\partial \eta} \right) \widetilde{\Pi|\eta}. \quad (3.53)$$

$Q_\alpha = \widetilde{Y_\alpha|\eta}$ is the conditionally filtered mass fraction of the α -th species. Temperature $\widetilde{T|\eta}$ is solved similarly. The overbar tilde indicates Favre-averaged (density-weighted) LES-filtered terms and $(\cdot|\eta)$ indicates a quantity conditioned on the mixture fraction. These equations are discretised on a very coarse mesh, independently of the fine LES mesh, as Q 's generally change slowly in space [Zhang et al., 2015].

The first term in Eqn. 3.52 is the unsteady term, the second term is convection, the third is the micro-mixing term including conditional scalar dissipation rate $\widetilde{N|\eta}$, the fourth is the subgrid scale conditional flux e_α and the fifth is the chemical production rate $\widetilde{\omega_\alpha|\eta}$. The last two terms involving $\widetilde{\Pi|\eta}$ on the right hand side are the conditional source terms for spray evaporation, and are modelled following the strategies discussed in Giusti & Mastorakos [2017] and Sitte & Mastorakos [2019], which are based on the models in Tyliszczak et al. [2014]. The Kronecker delta $\delta_{\alpha,f}$ is set to equal one for the fuel and zero for every other species. Evaporation is solved using the Abramzon & Sirignano [1989] single droplet method with Stefan flow correction, non-unity Lewis number in the film and infinite conductivity assumption for the liquid [Sitte & Mastorakos, 2019]. The LES filtered spray source terms are computed by summing over all droplets in a cell.

3.8.4 Closure of the CMC governing equations

The unclosed quantities in (3.52) and (3.53) are $\widetilde{\mathbf{u}_i|\eta}$, e_α , e_h , $\widetilde{N|\eta}$, $\widetilde{\Pi|\eta}$, $\widetilde{\Pi_h|\eta}$, and $\widetilde{\omega_\alpha|\eta}$. They are the conditionally filtered velocity, subgrid scale conditional species flux, subgrid scale conditional enthalpy flux, scalar dissipation rate, species volumetric

evaporation rate, enthalpy volumetric evaporation rate, and chemical source terms respectively.

Velocity

The velocity $\widetilde{\mathbf{u}_i|\eta}$ is modelled in the same manner as in Tyliszczak et al. [2014]. The conditional velocity is assumed to be uniform in η -space and equal to the local filtered velocity from LES, i.e., $\widetilde{\mathbf{u}_i|\eta} = \widetilde{\mathbf{u}_i}$.

Subgrid scale conditional flux

The subgrid scale conditional species flux e_α and the corresponding flux e_h for the enthalpy equation account for conditional species transport and fluctuations in physical space and in mixture fraction space. In the presence of spray, e_α is defined as [Tyliszczak et al., 2014]:

$$e_\alpha = -\frac{1}{\widetilde{\rho\tilde{P}}(\eta)}\frac{\partial}{\partial x_i}[\widetilde{\rho\tilde{P}}(\eta)(\widetilde{u_i Y_\alpha|\eta} - \widetilde{\mathbf{u}_i|\eta}Q_\alpha)] \quad (3.54)$$

where the joint conditional fluctuations of the velocity and species are modelled with a gradient model [Navarro-Martinez et al., 2005; Triantafyllidis & Mastorakos, 2010]:

$$(\widetilde{\mathbf{u}_i Y_\alpha|\eta} - \widetilde{\mathbf{u}_i|\eta}Q_\alpha) \approx -\widetilde{D_t|\eta}\frac{\partial Q_\alpha}{\partial x_i}. \quad (3.55)$$

Conditionally filtered turbulent diffusivity is modelled as $\widetilde{D_t|\eta} \approx D_t$ as in Triantafyllidis & Mastorakos [2010]. A similar expression is assumed for the enthalpy-velocity fluctuations e_h appearing in the enthalpy equation (3.53).

Conditional scalar dissipation rate

The conditional scalar dissipation rate $\widetilde{N|\eta}$ is closed using the Amplitude Mapping Closure (AMC) model described in O'Brien & Jiang [1991]:

$$\widetilde{N|\eta} = N_0 G(\eta), \quad (3.56)$$

where

$$G(\eta) = \exp(-2[erf^{-1}(2\eta - 1)]^2), \quad (3.57)$$

and

$$N_0 = \widetilde{N} / \int_0^1 G(\eta) \widetilde{P}(\eta) d\eta. \quad (3.58)$$

Methodology

N_0 is known as the maximum scalar dissipation rate and is the highest value of micro-mixing in the system. The $G(\eta)$ error function distribution is shown in Fig. 3.5. The end points of the distribution are fixed at $\eta = 0$ and $\eta = 1$. The filtered scalar dissipation rate $\widetilde{N}$ is calculated in the LES using resolved scales, $\widetilde{N}_{res}$, and subgrid scales, $\widetilde{N}_{sgs}$, using the following model:

$$\widetilde{N} = \widetilde{N}_{res} + \widetilde{N}_{sgs} = D \left(\frac{\partial \widetilde{\xi}}{\partial x_i} \right)^2 + \frac{C_N \mu_t \widetilde{\xi}''^2}{2\bar{\rho}\Delta^2} \quad (3.59)$$

The first term $\widetilde{N}_{res}$ is evaluated directly from the LES, where $D = \mu/(\bar{\rho}Sc)$ and the laminar Schmidt number $Sc = 0.7$. The second term $\widetilde{N}_{sgs}$ includes the subgrid scale mixture fraction variance $\widetilde{\xi}''^2$, which is solved via transport equation (3.51). In this subgrid term, $C_N = 42$ (a constant from calibration against the experimental results in Sandia flame D) [Garmory & Mastorakos, 2011], Δ is the LES filter width, and μ_t is the subgrid turbulent viscosity solved using the constant Smagorinsky model. The scalar dissipation rate $\widetilde{N}$ takes into account subgrid scale effects from spray evaporation through the $\widetilde{\xi}''^2$ term in $\widetilde{N}_{sgs}$.

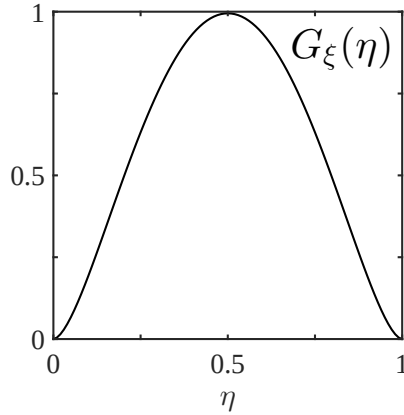


Fig. 3.5 The AMC model [O'Brien & Jiang, 1991] of conditional scalar dissipation rate for $N_0 = 1 \text{ s}^{-1}$. This model for $\widetilde{N}|\eta$ is used in both LES-CMC and 0D-CMC combustion models to describe the micro-mixing which affects quantities such as chemical species and temperature. Figure is reproduced with permission from Sitte [2019].

The AMC approach, despite being a fairly simple model, approximates the distribution of $\widetilde{N}|\eta$ reasonably well. Its distribution generally captures those observed in experiments, although occasionally the peak is more offset, in Triantafyllidis & Mastorakos [2010]; Tyliszczak [2013]. Scalar dissipation rate distributions in experiments conducted by Sutton & Driscoll [2013] were noted to not vary much in shape despite increases in jet velocity from a stable to a near-blow-off flame.

Other options than AMC for modelling the conditional scalar dissipation rate in the context of CMC have been discussed in Devaud et al. [2004]; Kim & Mastorakos [2006]; Sitte et al. [2021]. Kim & Mastorakos [2006] found that of three models tested to close the $\widetilde{N|\eta}$ term (including the Girimaji [1992] model and the Bilger [1993] model), the AMC model was the most accurate against experiments, as the other two were valid primarily for homogeneous flows. Recently Sitte et al. [2021] confirmed that the AMC model used in conjunction with a β -PDF is able to satisfactorily model the scalar dissipation rate against DNS data.

Spray source terms

The volumetric conditional evaporation rate $\widetilde{\Pi|\eta}$ in (3.52) is based on a FDF-weighted cell-mean saturation mixture value provided from each LES cell, where evaporation $\widetilde{\Pi}$ is computed by averaging over all the droplets within a particular cell. A similar method to the computation of $\widetilde{N|\eta}$ is implemented to compute the evaporation at CMC resolution, utilizing the AMC model with a presumed shape $G_{\Pi}(\eta) = G(\eta)$, the same as in Fig. 3.5 and Eq. 3.57. Using this method described in Sitte [2019]:

$$\widetilde{\Pi|\eta} = \Pi_0 G_{\Pi}(\eta) \quad (3.60)$$

where Π_0 is the scaling factor:

$$\Pi_0 = \frac{\widetilde{\Pi}}{\int_0^1 G_{\Pi}(\eta) \widetilde{P}(\eta) d\eta}. \quad (3.61)$$

Enthalpy spray source terms $\widetilde{\Pi}_h$ are solved analogously to those in (3.50), such that:

$$\bar{\rho} \widetilde{\Pi}_h = -\frac{1}{V_{LES}} \sum_i^{N_d} \frac{d(m_{d,i} C_{p,L} T_{d,i})}{dt} \quad (3.62)$$

where $T_{d,i}$ is the temperature of the i -th droplet and $C_{p,L}$ is the heat capacity of the liquid fuel. Conditional enthalpy evaporation source term $\widetilde{\Pi_h|\eta}$ is subsequently solved using:

$$\widetilde{\Pi_h|\eta} = \frac{\widetilde{\Pi_h}}{\widetilde{\Pi}} \widetilde{\Pi|\eta} \quad (3.63)$$

where $\widetilde{\Pi}$ is solved using Eq. 3.50.

Closure for the evaporation term $\widetilde{\xi\Pi}$ in the mixture fraction variance in (3.51) can be provided by the CMC model [Tyliszczak et al., 2014]:

$$\widetilde{\xi\Pi} = \int_0^1 \eta \widetilde{\Pi} | \eta \tilde{P}(\eta) d\eta = \langle \xi_s \rangle \tilde{\Pi} \quad (3.64)$$

Similar closure to (3.64) is adopted for the term $\widetilde{\xi^2\Pi}$, resulting in $\widetilde{\xi^2\Pi} = \langle \xi_s \rangle^2 \tilde{\Pi}$ [Giusti & Mastorakos, 2017], where average droplet surface mixture fraction $\langle \xi_s \rangle$, which can be approximated by the fuel mass fraction at the droplet surface.

Conditional reaction rate

First order closure is used for the conditionally filtered chemical source term $\widetilde{\omega_\alpha| \eta}$. Conditional fluctuations at subgrid scale are neglected and conditionally filtered reacting scalars Q_α are used to solve for the conditionally filtered reaction rate [Klimenko & Bilger, 1999]:

$$\widetilde{\omega_\alpha| \eta} = \omega_\alpha(Q_1, Q_2, \dots, Q_n) \quad (3.65)$$

where n is the number of reacting scalars. The reaction rate is evaluated using the chemical mechanisms described in Section 3.9.

3.8.5 0D-CMC

A less computationally intensive version of the LES-CMC model, called 0D-CMC, is solved first (the name 0D-CMC implying a lack in spatial diffusion) to use as an initial input for LES-CMC. 0D-CMC is basically the unsteady laminar flamelet concept discussed in Section 3.4 and involves the same model assumptions. The 0D-CMC equation is a transient, imposed solution of CMC— without spray source terms or terms representing physical transport —for a prescribed constant maximum scalar dissipation rate N_0 . This equation solves for reacting scalars Q_α conditioned in η -space and only includes unsteady, micro-mixing and chemical reaction rate terms:

$$\frac{\partial Q_\alpha}{\partial t} = N | \eta \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \omega_\alpha | \eta \quad (3.66)$$

0D-CMC can solve for the conditional temperature $T| \eta$, species mass fraction $Y_\alpha| \eta$, and density $\rho| \eta$ of the reacting field by integrating the fixed solution through a β -function PDF of the mixture fraction (see Eq. 3.43). $N| \eta$ is solved using Eq. 3.56 with

prescribed N_0 and $\omega_\alpha|\eta$ is solved as in (3.65) using the detailed chemical mechanisms described in Section 3.9.

3.9 Chemical reaction mechanisms

Chemical or kinetic mechanisms are optimised lists of species, reaction equations, and their corresponding reaction rates, which are expressed through coefficients for the empirical Arrhenius rate law:

$$k = AT^b \exp\left(-\frac{E_a}{RT}\right) \quad (3.67)$$

where k is the forward or backward reaction rate for a particular equation, A is the pre-exponential factor, T^b is temperature dependence, which is typically small compared to the exponential dependence, R is the universal gas constant, T is temperature, and E_a is the activation energy, i.e., the energy barrier which must be overcome to initiate chemical reaction. Chemical mechanisms list reaction equations with the relevant A , b , and E_a terms to the side to compute the reaction rate for every equation.

The reaction rate k (k_f and k_r indicating forward and reverse reaction rates) for a reaction j and species α multiplied with species molar concentrations $[X_\alpha]$ to the power of their molar stoichiometric coefficients ν_α , then multiplied by the summation of species atomic weight W_α multiplied by corresponding stoichiometric coefficients produces the chemical source term ω_α :

$$\sum_{\alpha=1}^N \omega_\alpha = \sum_{j=1}^M \left(\left(k_{fj} \prod_{\alpha=1}^N [X_\alpha]^{\nu_{\alpha,fj}} - k_{rj} \prod_{\alpha=1}^N [X_\alpha]^{\nu_{\alpha,rj}} \right) \sum_{\alpha=1}^N W_\alpha \nu_{\alpha j} \right) = 0 \quad (3.68)$$

which summed over all reactions comes to zero, showing that total mass is conserved. Kinetic rates are expressed using molar concentrations $[X_\alpha] = \rho Y_\alpha / W_\alpha$ [Poinsot & Veynante, 2005].

When coupled with species thermodynamic data, species mass fractions at different temperatures and pressures in time can be modelled. Key principles for designing chemical mechanisms, particularly for hydrocarbons, are understanding the driving forces for fast chemical reactions, i.e., radical formation, and understanding how the fuel is consumed to yield final combustion products [Maas, 2016]. Chemical mechanisms are formulated with particular criteria in mind for a specific fuel and generally have wide applicability; they are tested and validated against experiments studying laminar

flames, ignition phenomena and/or perfectly stirred reactors, shock tubes, and jet stirred reactors [Maas, 2016]. It is common to implement reduced or skeletal mechanisms for complex three-dimensional burner geometries or to use simplified combustion models to save computational costs. However these simplifications can severely limit a model’s ability to capture finite-rate kinetics— for example, slow transient behaviour like pollutant formation or complex chemical phenomena like extinction and blow-off [Maas, 2016]. The need for modelling finite-rate chemical kinetics is why detailed mechanisms are still necessary, despite large computational costs compared to reduced mechanisms.

Reliable detailed mechanisms exist for the combustion of lighter hydrocarbons, like the widely-used GRI-Mech for methane [Smith et al., 1999]; however heavy hydrocarbon fuel mixtures like gasoline or kerosene require much larger and more complicated models [Maas, 2016]. Various sub-mechanisms exist for NO_x chemistry and formation through numerous pathways such as thermal NO, prompt NO, and formation via N_2O , some of which are mentioned or used in Refs. [Dagaut et al., 2008; Felden et al., 2018; Maas, 2016; Moesl et al., 2012; Smith et al., 1999]. Another consideration is whether to include a polyaromatic hydrocarbon and soot sub-mechanism. A soot mechanism can increase the size and complexity of a mechanism considerably if a detailed mechanism is used [Eckel et al., 2019]. This approach was taken in the recent work of Gkantonas et al. [2020] where a detailed mechanism for kerosene was combined with a soot model developed for ethylene. Implementing a soot model on top of a detailed kerosene mechanism is currently beyond the scope of this thesis, but soot precursors like ethylene, acetylene, benzene and toluene are discussed.

The surrogate method of chemistry modelling for aviation fuels is a well-established approach [Dagaut, 2002; Dagaut & Cathonnet, 2006], but alternative methods are now being developed — such as the Hybrid Chemistry “HyChem” lumped pyrolysis approach [Wang et al., 2018a; Xu et al., 2018] to simplify chemistry modelling for real jet fuels. The next two sections discuss these chemical mechanisms in more depth.

3.9.1 Dagaut surrogate mechanism

As the nature of kerosene is that of complex hydrocarbon mixtures, it is common to represent kerosene with simpler mixture of better-understood hydrocarbons— these simplified mixtures are referred to as “model-fuels” or “surrogates” [Dagaut, 2002; Dagaut & Cathonnet, 2006]. Surrogates are generally mixtures of a limited number of hydrocarbons (between one and twelve) and should be well-defined in composition and exhibit behaviour similar to the commercial fuel. Surrogate fuels can be designed to

model either the physical or the chemical characteristics of a real fuel, or both (known as a comprehensive surrogate).

In order to model fuel ignition, general thermal-oxidation behaviour, and emissions, it is crucial that the necessary chemical classes are replicated by the surrogate fuel [Dagaut & Cathonnet, 2006; Edwards & Maurice, 2001]. For example, n-decane (an alkane/paraffin) has been used as a single-component model-fuel as it has similar oxidation rates to kerosene [Dagaut, 2002]. This model-fuel is not useful for soot modelling however, as aromatic molecules are not included. This led to many surrogate fuel studies adding aromatic molecules like toluene or n-propylbenzene to the mixture with n-decane, and after several studies a multi-component mixture with good agreement for kerosene oxidation was found [Dagaut, 2002, 2006]: n-decane (76.7%), n-propylbenzene (13.2%) and n-propylcyclohexane (10.1%). For this surrogate, n-propylbenzene represents monocyclic aromatics in kerosene, and n-propylcyclohexane represents the polycyclic aromatics. Other notable kerosene and alternative jet fuel surrogates using n-decane, iso-octane and toluene among other blends have been developed by Dooley et al. [2010, 2012].

The detailed Dagaut surrogate mechanism, formulated on the French military aviation fuel TR0 (very similar to Jet A-1) uses jet-stirred reactor data over a wide range of conditions: pressure ranging from 1-40 atm, equivalence ratios of 0.2-2, and temperatures from 500-1300 K; it was found to capture benzene quantities among other soot precursors very well against experiments [Dagaut, 2006]. This mechanism, consisting of 209 species and 1673 reactions, is implemented for modelling the Jet A-1 surrogate fuel which will be used as a reference for comparison for the HyChem lumped-pyrolysis detail mechanism developed for Jet-A, discussed in the next section.

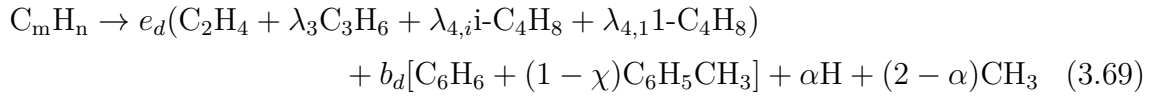
3.9.2 Hybrid Chemistry “HyChem” mechanisms

One of the main limitations of detailed surrogate models is the difficulty to capture both the key chemical and physical fuel properties (such as viscosity, the distillation curve, etc.). Surrogate mechanisms also generally very large, computationally expensive and difficult to validate experimentally [Wang et al., 2018a]. To address some of these limitations, the hybrid chemistry “HyChem” method proposes a different way to characterise complex jet and rocket fuels.

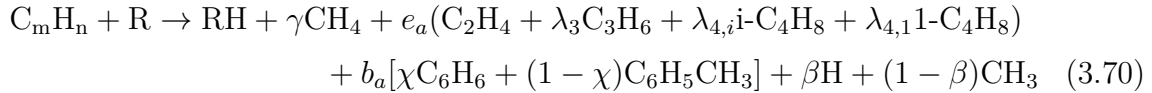
The HyChem approach is based on the assumption that fuel pyrolysis, or cracking, is very fast at high-temperature conditions compared with the subsequent oxidation of the smaller molecular fragments, and that the fuel decomposes entirely into a handful of components in the reaction zone [Wang et al., 2018a,b; Xu et al., 2018]. This is very

Methodology

similar to the approach described in the work of Gu  ret et al. [1990] which was also applied to kerosene (TR0). This approach is also referred to as the lumped pyrolysis method, as the fuel cracking step is approximated as quasi-steady state and is lumped into a few semi-global reaction steps. The fuel is modelled as a single-component lumped species C_mH_n , with m and n representing the average number of carbon and hydrogen elements respectively. The first irreversible reaction (of seven) in the lumped pyrolysis model is the fuel cracking by beta-scission:



where the eight products (ethylene, propene, iso-butene, 1-butene, benzene, toluene, hydrogen and the methyl radical) are the same for all conventional petroleum fuels. The other six reactions in the lumped pyrolysis set of equations go through H-abstraction and then fuel radical breakdown, via the formula:



where R species are: H, CH₃, OH, O₂, HO₂, and O. Coefficients λ_3 , $\lambda_{4,i}$, $\lambda_{4,1}$, χ , α , and β are stoichiometric parameters determined experimentally in Stanford shock tubes and flow reactors as described in Xu et al. [2018] and Wang et al. [2018a]. The coefficients e_a , e_d , b_a , and b_d are variables determined by λ_3 , $\lambda_{4,i}$, $\lambda_{4,1}$, χ , α , and β by elemental conservation. Combined with the seven lumped pyrolysis reactions is a detailed kinetic mechanism to model the oxidation of the reaction products seen above—USC Mech-II is used with modified reactions for iso-butene (i-C₄H₈) [Wang et al., 2007]. The mechanism includes the Stanford Research Institute (SRI) chemiluminescence mechanism for OH* and CH*.

Each fuel studied in this thesis from the NJFCP is modelled using the HyChem method. The molar proportions for the species in reaction Equations 3.69 and 3.70 were found using shock tube and flow reactor experiments for each real fuel [Wang et al., 2018a,b; Xu et al., 2018]. The high-temperature lumped pyrolysis method has been investigated using auto-ignition studies, perfectly stirred reactors (PSRs), 1-D laminar flames and turbulent premixed flames, and was found valid in these set-ups [Gao & Lu, 2017]. The resulting three detailed high-temperature HyChem mechanisms for A2, C1 and C5 contain 119 species and 843 reactions each. These mechanisms have

been used already by several groups [Esclapez et al., 2017; Felden et al., 2018; Zhang, 2018] for premixed gas turbine applications. This report utilises the new HyChem mechanisms in the yet to be explored non-premixed combustion context.

3.9.3 Jet-A (A2)

The A2 fuel from the NJFCP is specifically a Jet-A fuel obtained from the Shell Mobile refinery and is also known by its batch number POSF10325 [Colket et al., 2017]. Tables 3.1 and 3.2 show key properties and fuel composition of A2 [Colket et al., 2017; Wang, 2018].

Table 3.1 A2 key properties

Property	Value
Model formula	$C_{11}H_{22}$
LHV (MJ/kg)	43.1
Molec. wt. (g/mol)	154.3
DCN	48.3
Viscosity (cS, -20°)	4.5

Table 3.2 A2 composition

Type	Mass %
n-paraffins	20.0
iso-paraffins	29.4
cycloparaffins	31.9
aromatics	18.7

This fuel is a standard reference jet fuel with average properties, falling under Category A because it is a conventional distillate kerosene [Colket et al., 2017]. A2 is in the middle of three petrochemical reference fuels, each ranging in three combustion-related properties: flash point, viscosity and aromatics content [Colket et al., 2017]. This nominal fuel has a relatively wide boiling range and a wide range of hydrocarbon types evenly distributed between several carbon numbers [Colket et al., 2017]. This is in contrast to the Category C fuels, where research targets were aimed at fuels with narrow boiling range and narrow carbon number distribution.

3.9.4 C5

This Category C synthetic test fuel was designed to be a fully formulated jet fuel, but has a very flat boiling range (boiling at basically one temperature) [Colket et al., 2017]. It was created to evaluate the effect of a highly limited vaporization range of the fuel on LBO, relight and cold start [Colket et al., 2017; Edwards, 2017]. C5 also features an unusually low viscosity (seen in Table 3.3), which could have a significant impact on interpreting results [Edwards, 2017]. C5 is also known by batch number POSF12345.

Table 3.3 C5 key properties

Property	Value
Model formula	$C_{10}H_{19}$
LHV (MJ/kg)	43.0
Molec. wt. (g/mol)	135.4
DCN	39.6
Viscosity (cS, -20°)	1.9

Table 3.4 C5 composition

Type	Mass %
n-paraffins	17.7
iso-paraffins	51.6
cycloparaffins	0.0
aromatics	30.7

A2 and C5 have a similar H to C ratio of about 1.9 [Wang, 2018], so it is expected that their production of soot precursors (acetylene, ethylene, methane, benzene, toluene, etc.) should be similar.

3.9.5 C1

The Category C fuels are test fuels with particular properties, with a main purpose to identify hydrocarbon blends with properties outside of typical experience [Colket et al., 2017]. C1 is an alcohol-to-jet synthetic fuel developed by GEVO. The fuel consists of only C_{12} and C_{16} highly branched paraffins and has an extremely low derived cetane number at 17.1, compared to A2 at 48.3 and C5 at 39.6. This lower DCN for C1 corresponds to a longer autoignition delay time. C1 was created to determine the effect of low DCN on LBO, relight, and cold start [Colket et al., 2017]. More properties of C1 can be seen in Tables 3.5 and 3.6 [Colket et al., 2017; Wang, 2018]. C1 is also known by batch number POSF11498.

Table 3.5 C1 key properties

Property	Value
Model formula	$C_{13}H_{28}$
LHV (MJ/kg)	43.9
Molec. wt. (g/mol)	178.0
DCN	17.1
Viscosity (cS, -20°)	4.9

Table 3.6 C1 composition

Type	Mass %
n-paraffins	0.0
iso-paraffins	99.6
cycloparaffins	0.0
aromatics	0.4

Table 3.6 in particular shows how C1 has a composition very unlike the average kerosene, being almost entirely composed of isoparaffins. C1 has a higher H to C ratio (2.2) and hardly any aromatics, indicating that it should burn considerably cleaner than the conventional A2 fuel [Bonifazi et al., 1983].

3.9.6 Kinetic mechanism summary

A summary of the chemical mechanisms employed in the simulations discussed in this thesis is tabulated in Table 3.7, comparing the number of species and reactions for the various surrogate and HyChem fuels. The high-temperature lumped pyrolysis method, in which pyrolysis is assumed to be very fast at temperatures of 1500 K and above, is utilized in the HyChem mechanisms, which were developed for particular conventional and synthetic jet fuels formulated in the NJFCP. Three fuel mechanisms using the HyChem method are employed: the A2 (Jet-A), C5 and C1 mechanisms. The “A” denotes a conventional petroleum jet fuel, whereas “C” denotes a synthetic or alternative-sourced jet fuel with unusual properties. These fuels behaviour in 0D-CMC simulations are explored in comparison against the Dagaut surrogate mechanism for Jet A-1.

Table 3.7 Chemical mechanisms used for simulations, including the number of species and number of reactions per mechanism. The high-temperature version of the HyChem mechanisms are used. The Dagaut mechanism is a surrogate blend for jet fuel, consisting of: n-decane (76.7%), n-propylbenzene (13.2%), and n-propylcyclohexane (10.1%).

Fuel	Mechanism	Species Reactions	Reference
Jet A-1	Dagaut	209 1673	Dagaut [2002]
A2/Jet-A	HyChem	119 843	Wang et al. [2018a]; Xu et al. [2018]
C5	HyChem	119 843	Wang & Egolfopoulos [2016]
C1	HyChem	119 843	Wang et al. [2018b]

3.10 Flame stabilisation

3.10.1 Swirl stabilisation

Adding swirl to injected air is a very common stabilization technique for combustion-related applications, such as: automotive engines, gas turbines, industrial furnaces and utility boilers [Gupta et al., 1984]. Flame shape, size, stability and intensity are all affected by swirled flows, which can be generated using guided swirl vanes, axial-and-tangential entry swirl generators, or by direct tangential entry into the chamber. An example of a swirl stabilized set-up is shown in Fig. 3.6.

Swirled air widens flame stability and operation limits by providing a central toroidal recirculation zone, depicted in Fig. 3.6 by the grey curves. The central recirculation

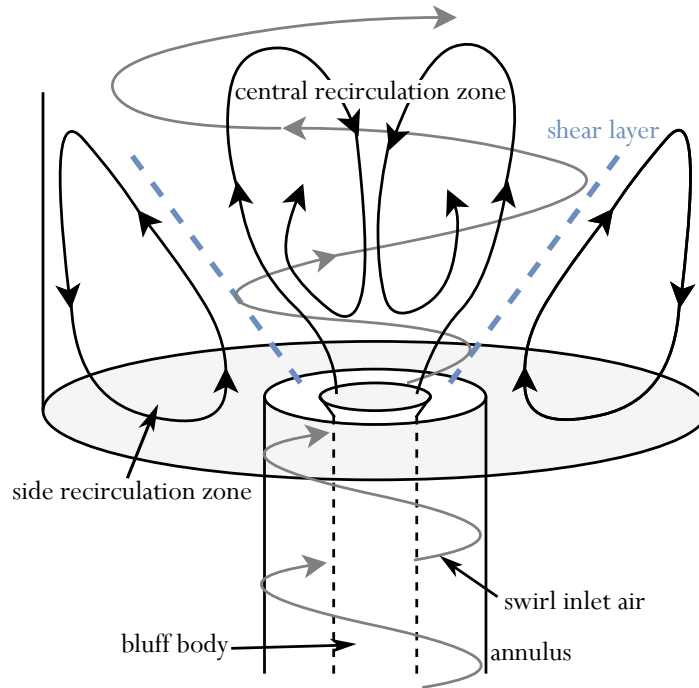


Fig. 3.6 Depiction of typical stabilization features in the context of a generic axisymmetric walled combustor: swirling inlet air, central and side recirculation zones (a.k.a. outer recirculation zones), and a bluff body. Figure is adapted from Hedman et al. [2002], which is based on the swirl schematic in Gupta et al. [1984].

zone (CRZ) is associated with high levels of shear and turbulence intensity in the flow, which promote cleaner and more efficient combustion [Gupta et al., 1984]. A reduced-velocity region containing hot burnt products from the combustion reaction is formed in the CRZ, redistributing heat and mass from downstream in the combustor to the flame zone upstream. This is imperative to sustain continuous ignition of fresh air and fuel reactants. In the case of sprays, the recirculation zone even aids droplet vaporization by bringing droplets which escaped downstream back toward the hot combustion zone.

By creating a region with reduced velocity and local strain rate, swirl flows lead to a compact flame with increased rates of molecular mixing, thus enhancing stability and efficiency. Swirl is critically necessary to generate overall lean flames over a wide range of conditions [Feikema et al., 1991].

3.10.2 Bluff body stabilisation

A blunt object, referred to as a bluff body, can be placed in a flow stream as another method of flame stabilization. Its presence in the flow creates recirculating eddies

downstream and a negative velocity in its wake, with a stabilizing effect very similar to swirl flows by increasing heat and mass transfer back into the combustion zone [Gupta et al., 1984]. The bluff body generates a vortex boundary-layer flow and provides a physical anchor point to which flames can attach. This allows the flame to stabilize near the shear layer of the high velocity air swirl flow exiting the annulus, shown in Fig. 3.6, by attaching itself to the bluff body edge. In this region the flame has access to increased availability of oxidation reactants and proximity to high-intensity turbulence, enhancing the efficiency of the flame and enabling the flame to exist over a large range of inlet velocities and air/fuel mixture ratios.

3.10.3 Flammability/stability limits

Not all fuel-air mixtures will result in combustion. Flames exist in a range between the flammability limits. The lower flammability limit, weak extinction limit or lean limit is at the maximum viable air to fuel ratio, where there is just enough fuel for the mixture to burn. Below this limit the flame will extinguish, or quench. This is shown in Fig. 3.7 as the lower part of the curve. The upper or rich flammability limit is at the minimum viable air to fuel ratio, where any more fuel in the mixture would cause the flame to extinguish. This corresponds to the upper part of the stability curve in Fig. 3.7. Lean equivalence ratio ($\phi < 1$) are closer to the lean flammability limit, whereas

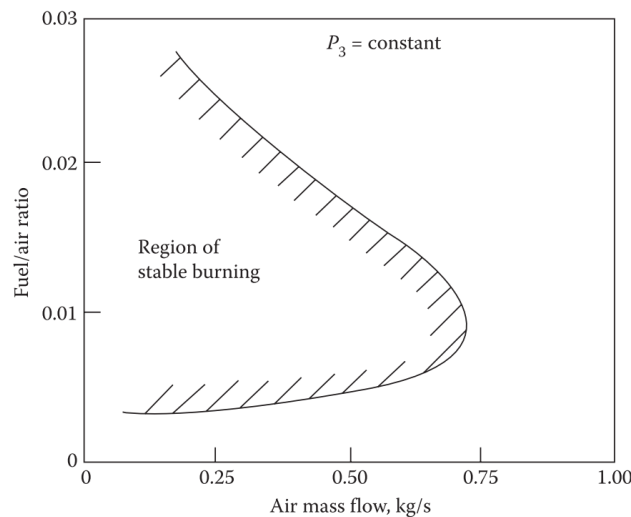


Fig. 3.7 The relationship between fuel/air ratio and air mass flow rate for a combustion chamber demonstrating flammability limits. Figure is reproduced from Lefebvre & Ballal [2010] with permission of the Taylor & Francis Group conveyed through Copyright Clearance Center, Inc.

rich equivalence ratio ($\phi > 1$) are closer to the rich limit. Then there are air mass flow rates beyond which no mixture of fuel or air is able to support a flame, corresponding to the region to the right of the peak in Fig. 3.7. The lean blow-off limit along the bottom and to the right of the stability curve that is of most interest and importance in gas turbine combustors [Lefebvre & Ballal, 2010].

Liquid fuels are also subject to temperature dependent flammability limits. The lower temperature limit is the minimum at which the vapour pressure of the fuel can form vapour in air, while upper limit is tied to the rich-limit of fuel concentration in the air [Lefebvre & Ballal, 2010]. Liquid fuel combustion stability is improved by increased fuel volatility, increased evaporation, and finer atomization (i.e., reduced mean droplet size) [Lefebvre & Ballal, 2010]. Increasing pressure widens the flammability limits and improves lean blow-off limits for spray flames, such that operation is possible at lower equivalence ratios [Ballal & Lefebvre, 1980]. This pressure effect is the reason why jet engines operate at pressures between 10 to 30 atm at cruising altitudes (and even higher pressures during power-intensive take-off).

3.11 Case Set-up and Solution Strategy

3.11.1 0D-CMC implementation

The zero-dimensional/0D-CMC equations are based on the laminar flamelet concept and provide the core of the combustion modelling approach for CMC. The 0D-CMC equation, described in Section 3.8.5, consists of unsteady, diffusion via scalar dissipation, and chemical source terms and uses the conserved scalar mixture fraction concept. Spray terms are not used in this version of 0D-CMC; it is assumed that fuel and oxidizer are in the gaseous phase.

Boundary conditions

Conditional mixture fraction space, denoted with η , is discretised into 51 nodes with clustering around stoichiometry ($\eta_{st} = 0.0637$), and boundaries of $\eta = 0$ for pure air and $\eta = 1$ for pure vaporized fuel. The simulations run at atmospheric pressure use boundary conditions $T_{fuel} = 475$ K, $T_{air} = 300$ K, whereas simulations run at a pressure of 10 atm use boundary conditions $T_{fuel} = 570$ K, $T_{air} = 300$ K. The increased fuel temperature in the high pressure case ensures that the fuel is represented in purely vapour form. The simulations are run with a time step of $1 \mu s$. The fuel streams are undiluted. Air consists of 23.2% O_2 and 76.7% N_2 .

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Simulations are computed at various values of user-prescribed constant N_0 , leading up to the critical scalar dissipation rate, above which no stable burning solution exists. The scalar dissipation rate $N|\eta$ is solved with the user-prescribed N_0 utilizing the AMC model, which is symmetric in η -space spanning from $\eta = 0$ to $\eta = 1$. The time-varying 0D-CMC simulations converge to a stable burning solution when N_0 is lower than the extinction value. When N_0 is higher than the extinction value, the solution undergoes an extinction transient, after which the simulation converges to an inert, extinct solution.

CMC

The 0D-CMC equation is solved using operator splitting and the SpeedCHEM package [Perini, 2013] is used for computation of the chemical reaction step. Operator splitting is a common technique employed for stiff transport equations [Kronenburg & Mastorakos, 2011], such as the governing equation for species mass fraction Y_α in (3.20). In the operator splitting method, partial differential equations (PDEs) can be transformed into several ordinary differential equations (ODEs) which are solved separately and sequentially. In the case of the 0D-CMC equation in Eq. 3.66, the micro-mixing term is solved first, then the chemical source term is solved using the intermediate solution obtained from the other term. The VODPK solver [Brown & Hindmarsh, 1989; Hindmarsh, 2006], which is used to solve sets of non-linear ODEs and is second-order accurate, is employed to solve for the scalar diffusion in mixture fraction space term $\frac{\partial^2 Q_\alpha}{\partial \eta^2}$. Central-differencing schemes for non-uniform grids are used. The errors induced by operator splitting have been assessed to be negligible at time steps below $2 \mu\text{s}$ [Gkantonas, 2021; Wright et al., 2005].

The chemical source term $\omega_\alpha|\eta$ is solved last using the SpeedCHEM solver (a.k.a. LIBSC), which is based on a sparse Jacobian matrix formulation and tabulation of temperature-dependent properties [Perini et al., 2012]. The method allows for use of an analytical Jacobian to approximate the ODE Jacobian matrix. However in the case of the HyChem mechanisms, a numerically determined Jacobian is required, as the analytical Jacobian method requires a limit of six species per reaction equation. The SpeedCHEM package utilizes LSODES solvers [Radhakrishnan & Hindmarsh, 1993] to evaluate the chemical fractional step with a numerical Jacobian matrix. The detailed mechanisms for the three HyChem jet fuels (A2, C1 and C5) and the Dagaut surrogate for jet fuel are used to close the reaction step. Very tight relative and absolute solver tolerances (10^{-14} and 10^{-21} respectively) were required to evaluate the chemical reaction step with the HyChem mechanisms

3.11.2 Experimental burner details for LES-CMC simulations

The non-premixed bluff body spray swirl burner geometry used in this study, shown schematically in Fig. 3.8 was studied previously experimentally [Allison et al., 2018; Cavaliere et al., 2013; Sidey et al., 2017; Yuan et al., 2018] and numerically [Foale et al., 2019, 2021; Giusti & Mastorakos, 2016, 2017; Tyliczszak et al., 2014] with different fuels. These fuels include n-heptane, ethanol, n-decane, n-dodecane, and the kerosenes studied by the NJFCP.

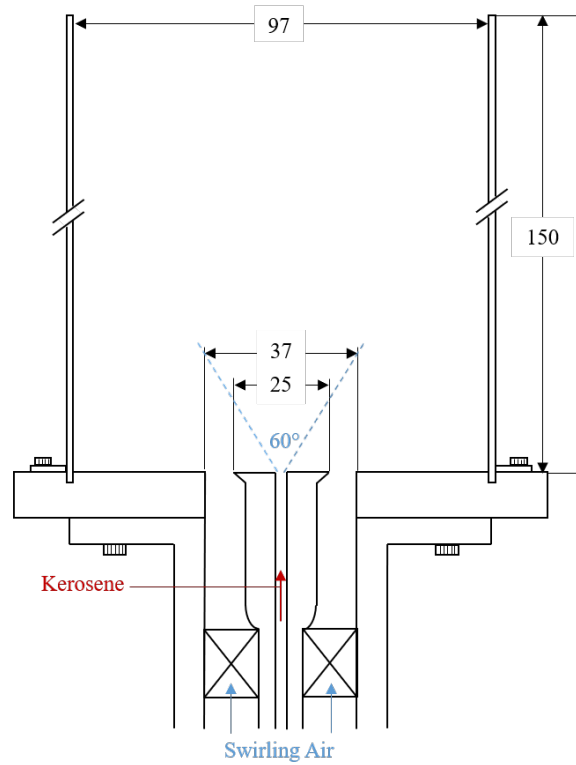


Fig. 3.8 Experimental burner schematic, dimensions in mm.

The fuel spray is injected at a constant mass flow rate as a hollow cone via a pressure atomizer. The spray is injected with a 60° spreading angle from the centre of the 25 mm diameter bluff body. Air is swirled clockwise through a 60° swirler in the annular duct with outer diameter of 37 mm, which is surrounding the bluff body. The swirl number is 1.2 [Allison et al., 2018]. The flame region is enclosed in a quartz rectangular enclosure that is open at the top, exposed to atmospheric pressure at the outlet. The stable fuel and air mass flow rates used in the simulation are indicated in Table 3.8, based on the the experimental blow-off curve for Jet-A in Fig. 2.2. From

3.11 Case Set-up and Solution Strategy

these conditions the bulk air velocity is increased to $U_{BO,exp}$ values or higher to induce blow-off.

Table 3.8 Stable simulation fuel mass flow rates ($\dot{m}_f$), bulk velocities (U_b), overall equivalence ratio ($\phi_{overall}$), and comparison with experimental blow-off velocities.

$\dot{m}_f$ (g/s)	Condition	U_b (m/s)	$\phi_{overall}$	$U_b/U_{BO,exp}$
0.27	Stable	15.9	0.37	74%
0.30	Stable	18.6	0.35	83%
0.33	Stable	22.1	0.32	93%

3.11.3 Spray modelling for LES-CMC

Polydisperse distribution

The polydisperse spray size distribution is modelled using a binned Rosin-Rammler distribution with Sauter Mean Diameter (SMD) D_{32} of $60 \mu\text{m}$ reported from previous experiments [Cavaliere et al., 2013]. The Rosin-Rammler distribution is shown in Fig. 3.9. The same size distribution is used for all the cases, only the number of droplets is increased via increase in fuel mass flow rate.

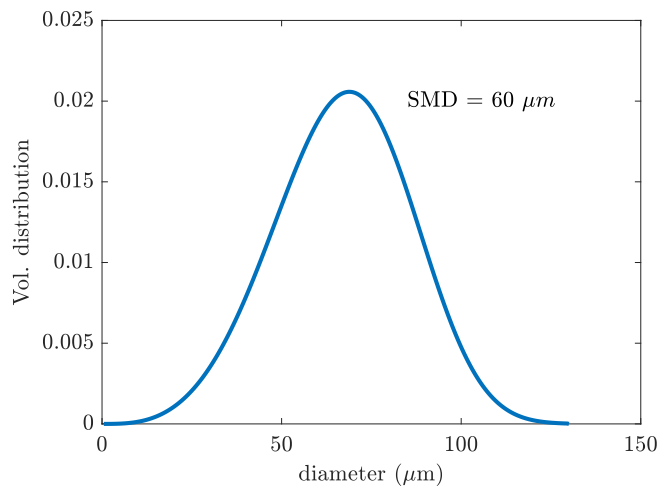


Fig. 3.9 The Rosin-Rammler distribution is used for the spray injection. The volume distribution of the droplet diameters is shown, with SMD equal to $60 \mu\text{m}$.

Methodology

The Rosin-Rammler distribution is modelled using the standard form:

$$Q = 1 - (\exp - (d_d/X)^q). \quad (3.71)$$

Droplet diameter d_d ranges between 1 μm and 130 μm with a volume distribution Q weighted toward smaller droplets to improve vaporisation. Estimates for the X and q terms are used (74 and 4 respectively) based on measurements from dodecane [Yuan et al., 2018]. q gives a measure of the spread of the drop sizes, such that the higher the value, the more uniform the spray will be. X is the drop diameter such that 63.2% of the total liquid volume is contained in droplets of diameter $d_d < X$.

Single droplet behaviour

The Abramzon & Sirignano [1989] single droplet evaporation model with infinite conductivity between the droplet centre and surface is utilised. An example of the single droplet evaporation behaviour for a droplet of Jet-A is shown in Fig. 3.10, where a droplet of initial temperature $T_d = 300$ K is injected into gaseous air at a temperature of $T_G = 1000$ K. The initial droplet diameter d_d is 60 μm and initial fuel and air mass flow rates correspond to those used in the stable LES-CMC flame conditions, $\dot{m}_f = 0.27$ g/s, $\dot{m}_{air} = 10.853$ g/s. These fuel and air mass flow rates correspond to the stable case in the first row of Table 3.8. The heating and steady state phases of the droplet are shown in Fig. 3.10a. The steady-state phase indicates the droplet's boiling temperature is approximately 440 K.

The droplet change in mass is shown in Fig. 3.10b. During the initial part of the heating stage the droplet hardly changes in mass, however once the droplet reaches a temperature over 400 K the mass begins to reduce at a steep rate. The instantaneous vaporisation rate curve in Fig. 3.10c reaches peak vaporisation about 3 ms into the process, after which the rate slows due to the significant reduction in mass and diameter of the droplet. For a droplet with d_d equal to 60 μm , it takes about 8 ms to heat up and vaporise completely in gaseous mixture of 1000 K. Similar results were obtained for fuels used in Abramzon & Sirignano [1989], indicating that model is working as expected using the liquid fuel properties for kerosene taken from Esclapez et al. [2017].

Spray implementation in LES

The spray models are implemented in the two-way coupled Eulerian-Lagrangian framework for LES using the existing libraries in OpenFOAM 2.3.1. The disperse phase is injected as mass-based parcels using a point source as a 60° dilute hollow cone spray

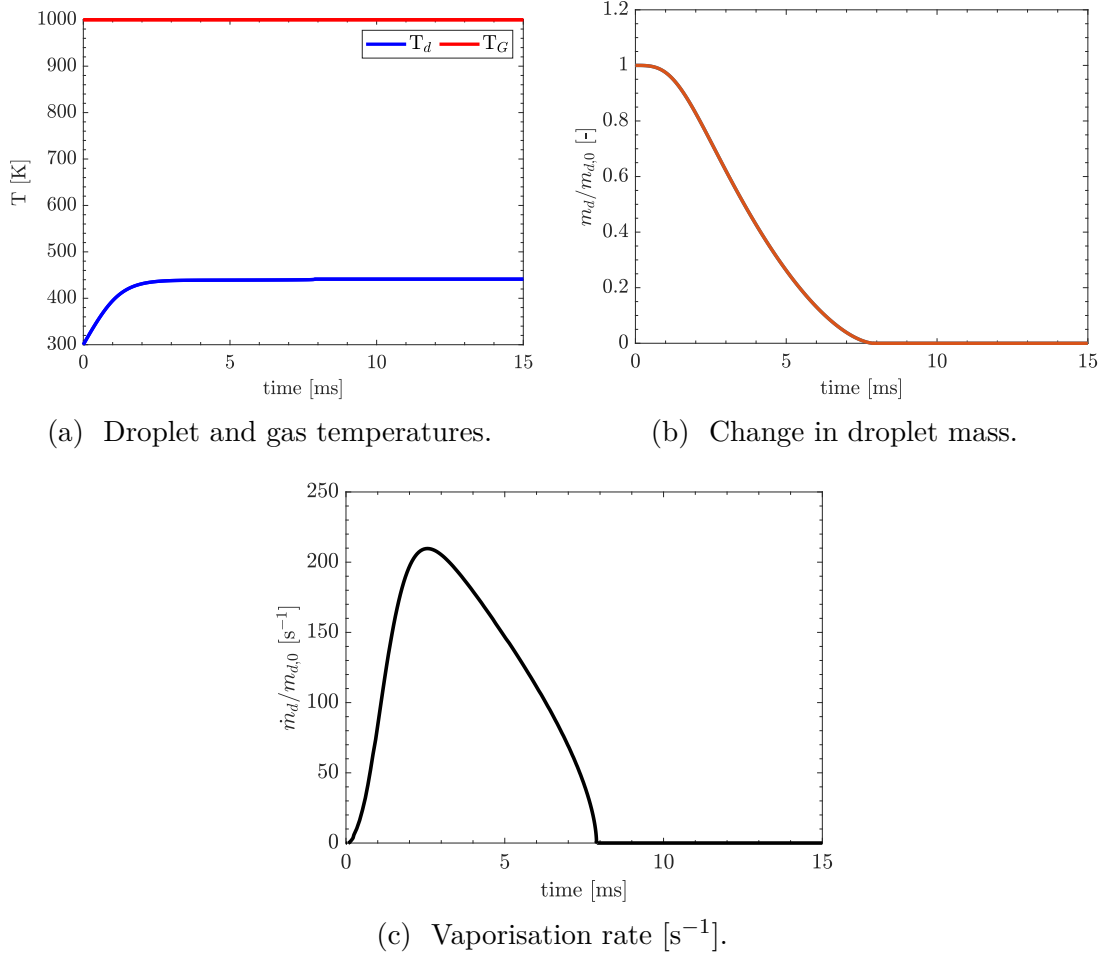


Fig. 3.10 Single droplet vaporisation behaviour over time for Jet-A using the Abramzon & Sirignano [1989] evaporation model and liquid fuel properties from Esclapez et al. [2017] for Jet-A, which are shown in Fig. A.1.

with a variation of $\pm 2.5^\circ$. Initial temperature of the droplets upon injection is set to $T_{d,i} = 300$ K. Spherical drag is exerted as a force on the droplets. Heat transfer is accounted for in the Abramzon & Sirignano [1989] evaporation model, which is implemented as described in Sitte [2019] and summarized in Section 3.6.1. No spray breakup or atomization is included and droplets are set to rebound against walls. Particle collisions, droplet dispersion, devolatilisation, and surface film models are also not used. These simplifications are necessary to reduce complexity, instability, and computational time.

A visualisation of the Lagrangian spray parcels in the computational domain is shown in Fig. 3.11. The magnitude of the injection velocity is assumed to be the same for all injected spray parcels at 25 m/s, based on the work of Sitte [2019] for the Rouen lifted heptane spray flame, as limited knowledge of the spray parameters for the kerosene flames were available. Liquid fuel property relations are obtained from Esclapez et al. [2017] for liquid density, liquid heat capacity, surface tension, liquid viscosity, heat of combustion (LHV), and saturation pressure. The relations of these properties against temperature are shown in the Appendix. Vapour diffusivity is calculated using the fuel's single-component approximation ($C_{11}H_{22}$ for A2). For other liquid and gaseous fuel properties, values for n-decane are used.

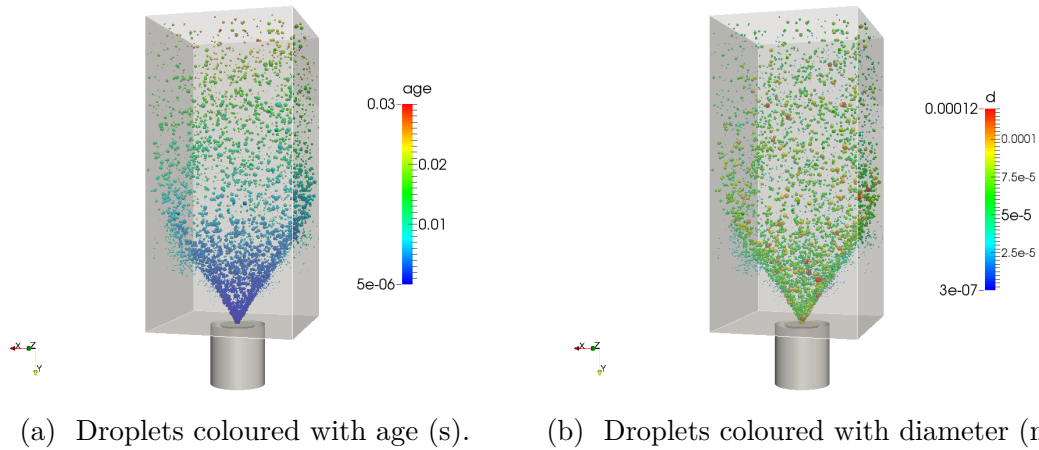


Fig. 3.11 An example of the Lagrangian droplet parcel cloud in the computational domain used for simulation, scaled by droplet diameter with size increased for visibility.

3.11.4 LES-CMC implementation

The LES-CMC equations are solved using an unstructured in-house code [Garmory & Mastorakos, 2015; Zhang, 2015; Zhang et al., 2015] interfaced with an Eulerian-

3.11 Case Set-up and Solution Strategy

Lagrangian solver for dilute sprays [Giusti & Mastorakos, 2017; Sitte & Mastorakos, 2019]. The open source CFD tool OpenFOAM 2.3.1 [OpenFOAM, 2014], which is based on the finite-volume approach, is used to solve the physical flow field LES and is coupled with the subgrid CMC code for the turbulent-combustion modelling.

LES

In the LES, the equation of state for a perfect gas is used. The flow field solver is based on the transient PIMPLE algorithm, which is a combination of the commonly used PISO and SIMPLE algorithms. PISO (Pressure Implicit with Splitting of Operators) [Issa, 1986] and SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) [Patankar, 1980] are iterative procedures for solving velocity and pressure equations, PISO used in transient problems and SIMPLE in steady-state applications. The PIMPLE method is used with two outer corrector steps, and two inner corrector steps (one of which is a non-orthogonal corrector). If one outer corrector step were employed, the method would be equivalent to the PISO solver.

Under-relaxation factors are used for the pressure and velocity, with 0.95 used for the first PIMPLE outer iteration, and 1.0 (no under-relaxation) used for the final PIMPLE iteration. Stronger relaxation was used when initializing the simulations in order to maintain numerical stability. Under-relaxation factors were increased toward 1.0 gradually, and the simulations were run for at least one flow through time with no under-relaxation before recording time-averages or changing the inlet air mass flow rate. The linear solver employed for solution of the transport equations is the generalized Geometric Algebraic MultiGrid (GAMG) solver. This solver is used to solve for the pressure, velocity, mixture fraction and mixture fraction variance equations. Final tolerances of 10^{-6} , 10^{-8} , 10^{-7} are used in the GAMG solvers for pressure, velocity, and mixture fraction/mixture fraction variance respectively.

An implicit first-order Euler scheme for time derivatives is used with a time step of $1 \mu\text{s}$. In the case of the LES-CMC simulations the maximum Courant–Friedrichs–Lewy (CFL) number values observed in individual LES cells are 0.5 or lower. The mean CFL number is below 0.015 for all simulations. Keeping the CFL number low using a small time step allows for the use of more stable time derivative schemes such as the Euler scheme. Bounded second-order numerical schemes are used for the divergence terms $(\nabla \cdot \rho \tilde{\mathbf{u}}_i \tilde{\mathbf{u}}_j, \nabla \cdot \rho \tilde{\mathbf{u}}_i \tilde{\xi}, \nabla \cdot \rho \tilde{\mathbf{u}}_i \tilde{\xi'^2})$. The *filteredLinear2V* scheme is used for the convection term in the momentum equation (3.45) and the *limitedLinear* scheme is used for the convection in the transport equations for mixture fraction (3.49) and mixture fraction

Methodology

variance (3.51). Unbounded second-order linear schemes are used for all other spatially discretised terms (e.g., diffusion).

Uniform axial and tangential swirl velocity components are imposed at the annulus inlet boundary with pure inert air ($T_{air} = 300$ K) at different air mass flow rates corresponding to stable and blow-off bulk air velocities used in the experiments of Allison et al. [2018]. The air bulk velocities and fuel mass flow rates for the initial LES-CMC stable conditions are shown in Table 3.8. A constant atmospheric pressure condition is used at the outlet. No-slip conditions are used for the walls and bluff body, and zero gradient is used on these boundaries for temperature, pressure, and mixture fraction. The constant Smagorinsky model is used to close the Reynolds stress and solve for the subgrid scale turbulent viscosity.

CMC

For every time step in LES, the CMC step is called after the Lagrangian solver and PIMPLE algorithm have solved for the spray evaporation and the flow field pressure, velocity, mixture fraction, and mixture fraction variance. The structure and implementation of the unstructured CMC code are same as in Sitte [2019] for singly-Conditional Moment Closure. The CMC equations are solved in a similar manner as the 0D-CMC equations in Section 3.11.1 using the operator splitting technique. Transport in physical space is solved first, followed by diffusion and the reaction source term in mixture fraction space.

Mixture fraction conditional space, denoted with η , is discretised with 51 nodes with clustering around stoichiometry ($\eta_{st} = 0.0637$), and boundaries of $\eta = 0$ for pure air and $\eta = 1$ for pure vaporized fuel. The pure fuel boundary $\eta = 1$ corresponds physically to the surface of a boiling droplet. An atmospheric stable 0D-CMC flamelet solution ($T_{fuel} = 475$ K, $T_{air} = 300$ K, $P = 1$ atm) with prescribed $N_0 = 30$ s⁻¹ is used to initialize the LES-CMC calculations.

To track conditional quantities Q in mixture fraction space over time, Q probes are used in several pre-determined CMC cells to track species mass fractions, temperature, scalar dissipation rate and heat release rate. CMC cells along the flame-air shear layer are analysed with Q probes to identify local extinctions and quantify their frequency and duration.

For terms in physical space (convection, subgrid scale conditional flux), a first order upwind scheme is used. The VODPK solver [Hindmarsh, 2006], a second-order central differencing scheme, is employed to solve for the scalar diffusion in mixture fraction space term $\frac{\partial^2 Q_\alpha}{\partial \eta^2}$. The SpeedCHEM package [Perini, 2013] which utilizes LSODES

3.11 Case Set-up and Solution Strategy

solvers [Radhakrishnan & Hindmarsh, 1993] is used in conjunction with CHEMKIN routines for the evaluation of the chemical source step. The evaluation of the chemical source term typically requires about 75% of the computation time per simulation time step, i.e. about 45 seconds of the 60 seconds total for each time step using 288 CPUs.

Meshes

In both LES and CMC, the equations are discretised using the finite-volume method [Zhang, 2015]. In the case of the CMC equations, common practice allows a significantly coarser grid to be used than the one for the flow field, resulting in numerous LES cells being contained by a single CMC cell. The LES structured mesh, shown in Fig. 3.12 as a 2D cut-plane, consists of 5.3 million cells, while the CMC structured mesh, shown in Fig. 3.13, consists of only 5,714 cells.

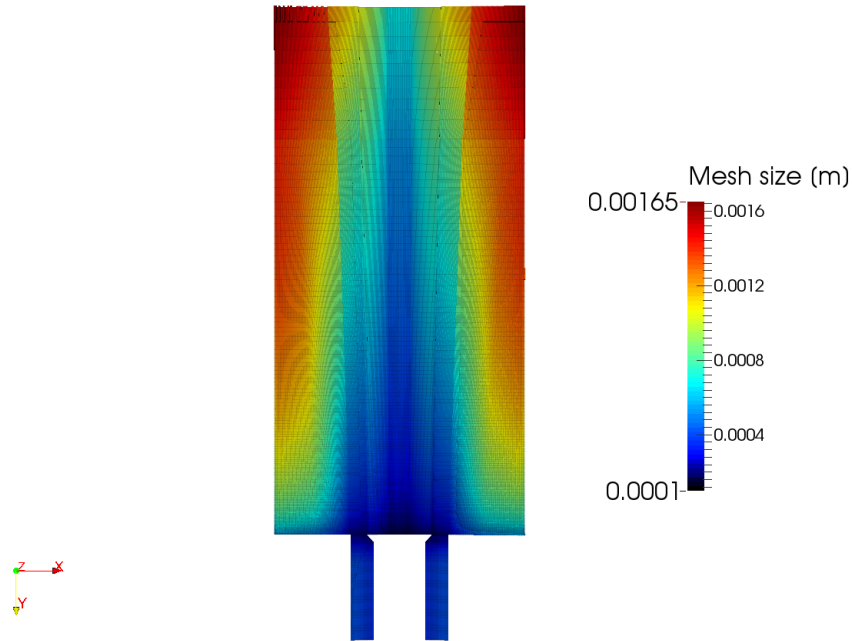


Fig. 3.12 Structured grid domain of the burner in the X-Y cut-plane for LES flow solver. The domain axial length was extended by 50 mm to reduce boundary condition instabilities, acting as a small plenum.

Both meshes are refined above the bluff body. The same meshes are used in all LES-CMC cases. The stable LES-CMC simulation was run initially using a CMC mesh containing fewer than 3,000 cells, however the resolution of the gradients along the air shear layer and spray injection region was insufficient. The CMC cell count was increased until gradients were adequately resolved, resulting in 5,714 cells total. In

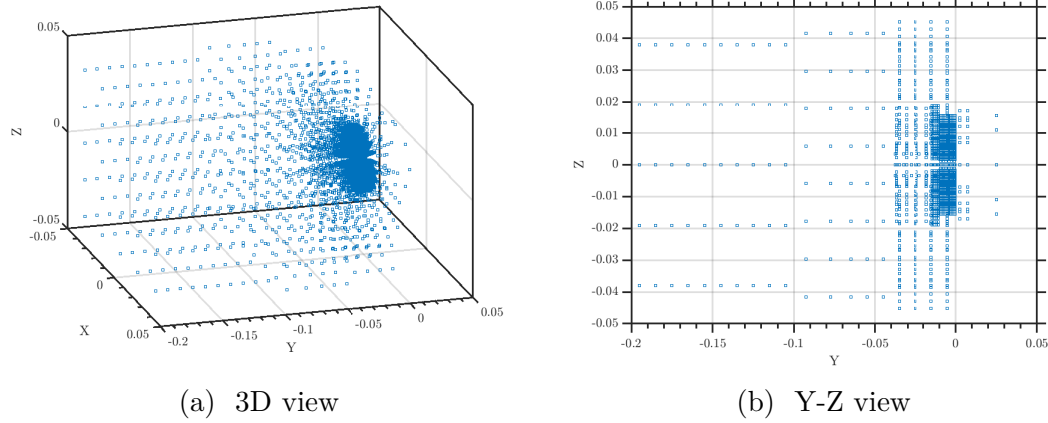


Fig. 3.13 Centroids of 5,714 cells used for computation of the CMC equations with refinement near the bluff body.

Giusti & Mastorakos [2017], the same 5.3 million cells LES mesh is used but with a 45,000 cells CMC mesh. The size of the CMC mesh in this thesis is very coarse to reduce the computational time required by the significantly larger detailed chemical mechanism.

Computational requirements

The computation of 1 ms of physical time requires 24 hours with 384 Cray XC30 system 2.7 GHz processors using the Archer UK National Supercomputer. Some of the simulations are also run on the Cambridge super-computing cluster CSD3 using 288 Intel Xeon Skylake system 2.6 GHz processors, where 1.5 ms in the simulation could be computed in 24 hours. Care was taken to ensure the spray injection location in the computational domain existed within a single processor, as domain decomposition for parallelization can split injection points between multiple processors, which causes errors in the evolution of the spray. LES-CMC solutions are saved at a frequency of 0.0001 s (10 kHz), whereas probes of conditional quantities Q (i.e., Q probes) in pre-determined CMC cells are saved at a frequency of 50 μ s (20 kHz). Q probes for each monitored CMC cell are text files containing conditional time-varying values of temperature, heat release rate, scalar dissipation rate, as well as species mass fractions at that particular location.

This research falls under the umbrella of “big data”, for each full time solution saved every millisecond of simulation time is approximately 3 GB, whereas solutions

saved between round milliseconds were saved in compressed forms with fewer variables, at approximately 1.5 GB each.

3.11.5 LBO solution strategy

In this study the flame is simulated at three fuel mass flow rates : 0.27 g/s, 0.30 g/s and 0.33 g/s. Stable air bulk velocities corresponding to the respective fuel mass flow rates are: 15.9 m/s, 18.6 m/s, and 22.1 m/s. These stable conditions are used as the initial solutions from which blow-off is initiated. The three stable cases and their conditions are shown in Table 3.8. The stable $\dot{m}_f = 0.27$ g/s case corresponding to $\phi_{overall} = 0.36$ is the original, from which the fuel and air mass flow rates were increased to generate the successive 0.30 g/s case. From this case the $\dot{m}_f = 0.33$ g/s case was similarly generated. The base case $\dot{m}_f = 0.27$ g/s was run for more than one flow through time without any numerical relaxation, after which the blow-off procedure was initiated. The $\dot{m}_f = 0.30$ g/s and 0.33 g/s simulations were run for 5 ms with no under-relaxation to adjust to the new fuel and air flow rates before commencing blow-off.

Experiments initiated blow-off by increasing the bulk air flow rate in steps of about 2% of the total, and the velocity where extinction occurred was recorded as the blow-off velocity $U_{BO,exp}$. Increasing the velocity at such an incremental rate would have been infeasible for simulations given the computational time requirements. To initiate blow-off in the simulations, the air mass flow rates were increased in steps by 10% until matching the blow-off air bulk velocities $U_{BO,exp}$ reported for Jet-A in Allison et al. [2018] (shown for reference in Fig. 2.2). Total simulation time reached 0.3 s when the $\dot{m}_f = 0.27$ g/s simulation bulk air velocity reached the corresponding $U_{BO,exp}$ value.

Table 3.9 LBO simulation fuel mass flow rates ($\dot{m}_f$), experimental blow-off velocities ($U_{BO,exp}$), and the increases in U_b above $U_{BO,exp}$ required to achieve LBO in simulation. The increases are expressed by the ration $U_b/U_{BO,exp}$, and the subscript indicates the elapsed time from $U_b = U_{BO,exp}$ at which the increase occurred.

$\dot{m}_f$ (g/s)	$U_{BO,exp}$ (m/s)	1st incr. $U_b/U_{BO,exp}$	2nd incr.	3rd incr.
0.27	21.6	1.05@ $t=8ms$	-	-
0.30	22.3	1.15@ $t=9ms$	-	-
0.33	23.5	1.05@ $t=6ms$	1.10@ $t=11ms$	1.20@ $t=25ms$

The time $t = 0$ ms in Chapter 6 figures indicates the beginning of the blow-off transient, i.e., the first instances where $U_b = U_{bo,exp}$. The approximate $U_{bo,exp}$ values are shown in Table 3.9. The bulk air velocity in the $\dot{m}_f = 0.27$ g/s simulation was increased by 5% above the $U_{BO,exp}$ value to 22.7 m/s at time $t = 8$ ms after $U_b = U_{bo,exp}$ in order to ensure blow-off would occur, and $U_b = 1.05U_{BO,exp}$ was high enough to bring OH mass fraction and temperature levels low enough to be considered extinguished. The $\dot{m}_f = 0.30$ g/s and 0.33 g/s fuel mass flow rate cases required increased blow-off velocities beyond experimental values due to their rates of change in isosurface area, heat release and evaporation being less sensitive to the increased air than the $\dot{m}_f = 0.27$ g/s case. U_b for the $\dot{m}_f = 0.30$ g/s flame was increased to $1.15U_{BO,exp}$ after $t = 9$ ms from the start of the transient. In the $\dot{m}_f = 0.33$ g/s flame, U_b was increased three times: to $1.05U_{BO,exp}$ after 6 ms, $1.10U_{BO,exp}$ after 11 ms, and $1.20U_{BO,exp}$ after $t = 25$ ms. This is summarised in Table 3.9. A threshold of 80% reduction in volume integrated heat release rate in the LES cells along the $\xi_{st} = 0.0637$ isosurface is used to determine when the flames have blown-off.

3.11.6 Simulation challenges

This section briefly discusses some of the challenges encountered while undertaking the research presented in this thesis. One small challenge occurred early on, relating to utilising the HyChem mechanisms with the 0D-CMC model. The SpeedCHEM package, used for speeding up the solving of the chemical equation reaction rates with the analytical Jacobian method, could not be employed with default settings with the HyChem mechanisms. The HyChem mechanisms defy two major conventions, including: the presence of floating-point numbers as molar stoichiometric coefficients in reaction equations, and some reaction equations containing more than six species total. This is caused by the lumped pyrolysis semi-global reaction sub-mechanism, where non-integer stoichiometric coefficients are everywhere and the equations contain eight to twelve species in total. Adjustment may be needed in chemistry interpreters to account for the large dimensions of the lumped pyrolysis equations. These large equations interfered with SpeedCHEM's sparse analytical Jacobian matrix solver method, requiring a numerical Jacobian solver to be used instead. This slowed down computation significantly. Very small relative and absolute tolerances were required (10^{-14} to 10^{-21}) for the SpeedCHEM method to work with the HyChem mechanisms without runtime numerical errors.

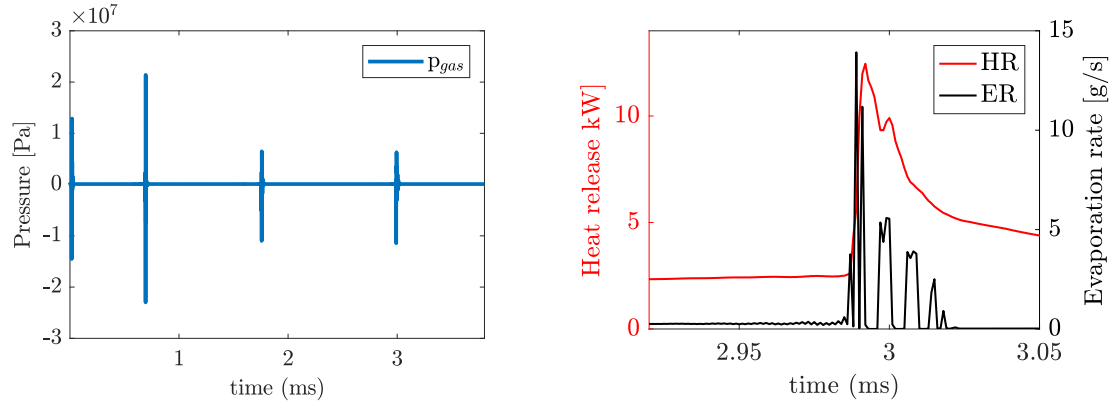
The original scope of this thesis intended to include LES-CMC simulations of the C1 and C5 fuels from the NJFCP for a full comparison of chemistry and fuel effect

3.11 Case Set-up and Solution Strategy

differences between these unusual synthetic jet fuels and the standard Jet-A kerosene. LES-CMC simulations were carried out for all three NJFCP fuels, although with considerable numerical difficulties involving large pressure and velocity fluctuations. Pressure would regularly (every 0.5 to 1 ms) diverge to non-physically high positive and negative values. The pressure fluctuations from one simulation are shown in Fig. 3.14a, with the magnitude reaching 100 to 200 times atmospheric values. Despite these fluctuations, the simulation did not crash and continued iterating through time. Once instantaneous heat release rate and evaporation rate were integrated over the combustion chamber volume, shown in Fig. 3.14b, it was evident the pressure fluctuations were linked to strong oscillations in heat release rate and the evaporation rate. This also affected the flame height in the simulations, causing very short flames and reducing the droplet temperatures to the minimum allowed values.

To fix this numerical instability, the gaseous pressure field p was separated into two variables in the LES solver: p and p_{gas} . p is the default pressure field in the PIMPLE method and is used for thermodynamic calculations as well as for the Lagrangian spray calculations. The p variable was set to a constant value of 101,325 Pa to stop fluctuations in the pressure, heat release and evaporation rates from reinforcing each other to unphysical values. The new p_{gas} variable was used only for solving Eulerian field pressure using the PIMPLE algorithm. With this separation of pressure variables for the Lagrangian/thermodynamics solvers and the Eulerian solver, the pressure divergences were eliminated and p_{gas} varied within an expected range, as shown in Fig. 3.15.

It is unclear why exactly this oscillatory behaviour occurred in the simulations, however due to time limitations further investigation into the cause was not pursued. After the code was modified to prevent the numerical instabilities, the scope of this thesis was reassessed and altered to focus primarily on simulating the lean blow-off behaviour of Jet-A, with LES-CMC simulations of the synthetic C1 and C5 fuels relegated to future works. The primary goal of the thesis was changed to simulating the first blow-off curve of a real fuel spray flame, and to investigate the underlying physics of spray flame local extinction and blow-off phenomena.



(a) A probe tracked instantaneous gaseous pressure over time, pressure periodically diverged to large positive and negative values.

(b) Instantaneous volume integrated heat release rate and evaporation rate influenced by the pressure spike in (a) at $t \approx 3$ ms.

Fig. 3.14 An instability in the code led to large pressure oscillations, which strongly affected heat release rate and the evaporation rate.

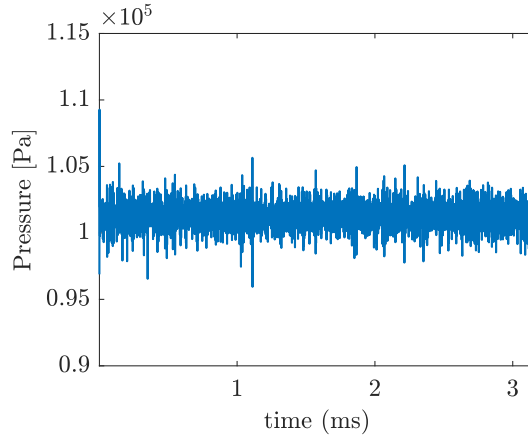


Fig. 3.15 Pressure p_{gas} of the gaseous mixture tracked over time taken using a probe after separating the LES pressure field into two variables: p (held constant at $p = 101,325$ Pa) used for the disperse phase and p_{gas} used for the Eulerian field.

3.12 Summary

The aim of this thesis is to understand the underlying physics of kerosene spray flame local extinction and LBO. This is done by analysing chemical behavioural differences between conventional and alternative fuels as they approach and undergo extinction, and by simulating the blow-off curve of a practical liquid fuel.

The methods and code used to generate the results in the next chapters for the most part already existed prior to this work. The contributions of this work to the body of

research on LBO is the synthesis of several complex models for turbulence-combustion, spray, and fuel chemistry to predict flame LBO in a well-known burner used for fundamental flame studies, as well as in a laminar counterflow diffusion flame context. Detailed analysis through intermediate species trends is offered in a comparatively exhaustive manner to previous numerical studies of sprays and real fuels. This is also the first work to the author’s knowledge to study LBO of a real fuel in numerical simulations through the lens of fuel starvation contributing blow-off.

A few small modifications to the code were necessary to get things running. The Chemkin routine for finding temperature in the CMC code was modified to solve for a lower tolerance around $T = 1000$ K, as divergences would regularly occur as CMC nodes passed through this threshold due to mismatches in the NASA thermodynamics polynomials at that temperature to determine C_p . A modification of the LES OpenFOAM routine was required to prevent non-physical oscillatory behaviour in the gaseous pressure field. This was done by separating the pressure into two quantities: a gaseous field pressure solved for by the PIMPLE routine which is allowed to vary in time and space, and a constant atmospheric pressure field used only by the Lagrangian spray library. By separating the pressure seen by the spray and that of the Eulerian field, numerical stability could be maintained.

Descriptions on the use of CMC in this thesis in both zero-dimensional and 3D contexts is summarised below. 0D-CMC simulations are executed in the context of a counterflow diffusion flame, whereas the LES-CMC simulations are run using the same computational domain as modelled in Tyliczszak et al. [2014] and Giusti & Mastorakos [2017].

0D-CMC

The singly-conditional 0D-CMC code is written in FORTRAN and utilizes Chemkin and SpeedCHEM routines to solve for the chemical reaction rate. The equation is solved using operator splitting, which produces negligible errors as the time step is sufficiently small ($1 \mu\text{s}$). The SpeedCHEM package is used with a numerical Jacobian matrix to work with the lumped pyrolysis HyChem mechanisms in 0D-CMC to account for the stiffness introduced by reaction equations containing more than six species per equation. The scalar dissipation rate is utilised as a parameter analogous to velocity in the 0D framework. As experiments blow off with a critical velocity U_{BO} , 0D-CMC simulations extinguish with a critical scalar dissipation rate $N_{0,ext}$. Stable flamelets with maximum scalar dissipation rate lower than the critical extinction SDR

are simulated, as well as flamelets undergoing extinction transients when the prescribed constant N_0 is increased above the extinction value.

LES-CMC

The turbulence-combustion and spray modelling methodology is largely based on those detailed in Sitte [2019], where LES-CMC was expanded to include premixed combustions regimes (LES-DCMC) with applications toward spray combustion. The LES-CMC model is implemented using the CFD tool OpenFOAM 2.3.1 interfaced with the subgrid scale CMC turbulence-combustion model code, which is written in FORTRAN and utilizes Chemkin and SpeedChem routines. A β -PDF is used to convert the scalars conditioned on the mixture fraction into unconditional scalars in physical space. The Lagrangian-Eulerian polydisperse spray modelling is implemented through the modification of pre-existing OpenFOAM Lagrangian reacting parcel spray routines which are two-way coupled with the gaseous field. The Abramzon & Sirignano [1989] single-droplet evaporation model is employed for the dilute spray. Liquid fuel property relations for Jet-A, dependent on temperature, are taken from Esclapez et al. [2017] and adjusted for the fits used in the OpenFOAM fuel properties routines.

The main difference between methods for the turbulence-combustion modelling in Sitte [2019] and this work are that singly conditional LES-CMC is used here rather than the doubly conditional LES-DCMC, and that the pressure experienced by the spray is separated from the pressure in the gaseous field. The spray pressure is set to a constant value $p = 101,325$ Pa throughout the domain, whereas the pressure of the continuous gaseous field p_{gas} used in the Navier-Stokes transport equations is allowed to vary in space and time. Spray evaporation terms are also included in the mixture fraction variance transport equation as detailed in Giusti & Mastorakos [2017], whereas in Sitte [2019] these terms were unused. The evaporative cooling effect introduced in Sitte [2019], solved using a transport equation for enthalpy including spray terms, is not used in this work.

Chapter 4

0D-CMC Results for Jet-A and Alternative Fuels

When starting projects in combustion and CFD, it is useful to garner information first with simplified models. The simplified version of LES-CMC, known as 0D-CMC, is used here to simulate different chemical mechanisms in a non-dimensional space using the mixture fraction concept to get an initial understanding of the behaviour of the mechanisms and to work out computational kinks. The 0D-CMC results also provide an input solution for the 3D LES-CMC simulation. These simulations allow for evaluation of the recently developed HyChem chemical mechanisms against the more established surrogate/model fuel method in a non-premixed flame context. The HyChem mechanisms are attractive as they are built from real kerosenes, rather than model fuel mixes developed to approximate kerosene behaviour. Their size is not too large as far as detailed mechanisms are concerned. The HyChem mechanisms also include ones developed from synthetic fuels, which need to be evaluated against conventional fuels for their compatibility in current and future jet engines.

This chapter covers the laminar counterflow diffusion flame results using the 0D-CMC combustion model described in Section 3.8.5. Four kerosene fuels are simulated at various scalar dissipation rates and two pressures: 1 atm and 10 atm. The high pressure case is used to gauge species trends closer to more realistic gas turbine engine operating conditions. The differences in chemical species present for the four detailed kinetic mechanisms is discussed for these conditions, and a comparison of the behaviour leading up to the extinction of the fuels is made. The extinction transient (after the critical extinction scalar dissipation rate is applied) and reignition of the HyChem Jet-A flamelet at atmospheric pressure are also explored.

4.1 Stable flamelets at various N_0

The flamelets discussed in this section are solved with the unsteady 0D-CMC equation, which utilises a user-prescribed maximum scalar dissipation rate N_0 in the diffusion term. The flamelets are referred to as stable due to having converged over time to stable, unvarying values of species mass fraction and temperature in mixture fraction space. The maximum scalar dissipation rates N_0 for these stable flamelets are lower than the critical extinction scalar dissipation rates $N_{0,ext}$, beyond which the flamelets are no longer able to sustain a burning condition.

4.1.1 Atmospheric pressure

Figure 4.1 shows 0D-CMC laminar counterflow diffusion flame results for the four different detailed chemical mechanisms (listed in Table 3.7) at atmospheric pressure (1 atm). The HyChem A2 and Dagaut A2 represent Jet-A and the Jet A-1 surrogate respectively, whereas HyChem C5 and C1 are synthetic alternative fuels. Each column of plots is at a different user-prescribed constant scalar dissipation rate N_0 , increasing from left to right. The low N_0 value corresponds to a stable burning slow-diffusion flame, whereas the high N_0 value on the right corresponds to a flame close to extinction due to fast diffusion. The species and temperature are plotted against the CMC mixture fraction η . Stoichiometry for kerosene is at $\eta_{st} = 0.0637$. Temperature is well-matched between the mechanisms with very little discrepancy. Only the C1 fuel in 4.1c shows a visible dip in temperature. OH is included as it is a key radical species in chain branching reactions necessary to sustain the flame, whereas CH_2O is a species marker of incomplete combustion, similar to CO, and is known to build up at near-extinction conditions as well as during extinction transients. The OH behaviour in Fig. 4.1 is very close between all of the mechanisms. CO_2 as well as other major combustion products (not depicted) undergo very similar trends between the Dagaut surrogate and HyChem mechanisms even up to relatively high values of scalar dissipation rate. Overall results from the HyChem mechanism are close to the ones from the surrogate mechanism, albeit with a few exceptions.

One of these exceptions is the level of formaldehyde (CH_2O), with the Dagaut mechanism predicting considerably higher mass fraction values, particularly as the scalar dissipation rate is increased from 30 s^{-1} in Fig. 4.1a to 250 s^{-1} in 4.1c. The CH_2O mass fraction for all the fuels peaks near stoichiometry at low scalar dissipation rates, then as N_0 increases CH_2O peak mass fraction moves into fuel-rich zones of mixture fraction ($\eta > \eta_{st}$). The HyChem A2 CH_2O trend in Fig. 4.1c mirrors the

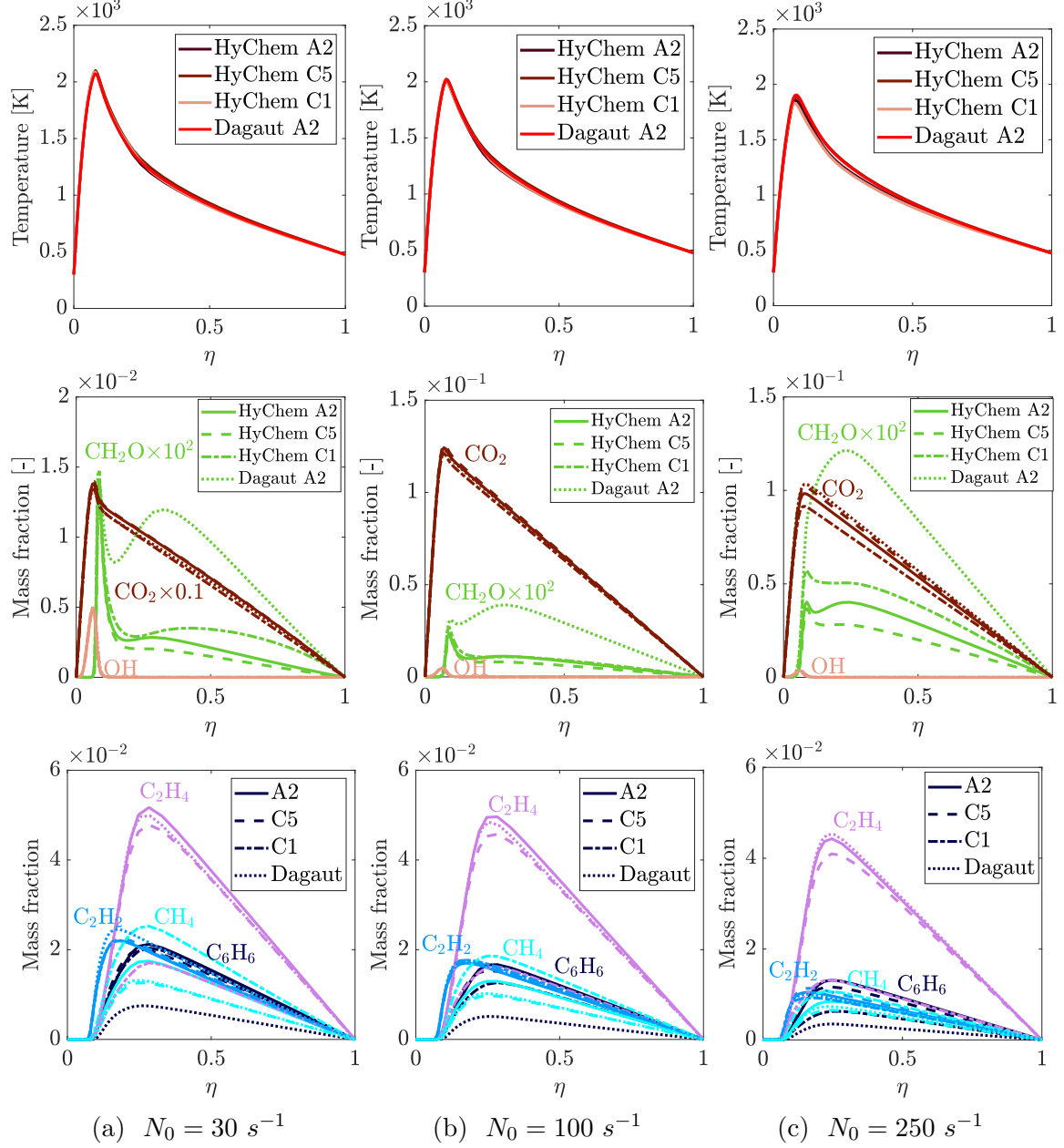


Fig. 4.1 Species mass fractions and temperature (K) in mixture fraction space from laminar counterflow diffusion flames of the different fuels at $P = 1$ atm, $T_{fuel} = 475$ K and $T_{air} = 300$ K, using the HyChem and Dagaut mechanisms. The three columns show results at scalar dissipation rates $N_0 = 30$ s $^{-1}$, $N_0 = 100$ s $^{-1}$, and $N_0 = 250$ s $^{-1}$.

shape of the Dagaut surrogate CH_2O trend in Fig. 4.1a, indicating that the A2 formation of CH_2O follows same trend as the surrogate Jet A-1 but at higher values of N_0 . Amongst the three HyChem fuels, formaldehyde levels are higher for fuel C1 than C5 and A2, with a significant increase in formaldehyde at high scalar dissipation rate. All of the mechanisms exhibit overall increase in formaldehyde mass fraction as scalar dissipation rate is increased— this is due to the mechanisms containing enough intermediate chemistry to model incomplete combustion from the intensity of the high mixing rates and lowering of the overall temperature. This behaviour indicates that the flame may be approaching blow off if the amount of CH_2O becomes especially high. The main reason for the differences in CH_2O between the Dagaut surrogate and the HyChem A2 mechanism is likely due to the HyChem mechanism being developed for high-temperature applications, whereas the Dagaut mechanism contains more reactions relevant for mid- to low-temperature chemistry.

The bottom images in Fig. 4.1 display another discrepancy between the Dagaut and HyChem chemical mechanisms concerning the aromatic soot precursor benzene (C_6H_6). The HyChem mechanisms in Fig. 4.1a predict more than twice the amount of benzene than the surrogate mechanism. The Dagaut surrogate kerosene mechanism uses n-propylbenzene and n-propylcyclohexane to model the aromatic content of conventional kerosene, representing about 23% of the model fuel (the rest modelled using n-decane). This is a slightly larger proportion of aromatics than the composition of the HyChem A2 fuel (19%) but considerably lower than the C5 aromatic content (30%). The C1 fuel is less than 1% aromatics and yet has comparable benzene production to the other HyChem fuels. Thus it is not the proportion of aromatics in the fuel composition causing this difference. It is most likely due to differences with the oxidation part of the HyChem mechanism based on USC Mech II, a high-temperature $\text{H}_2/\text{CO}/\text{C1-C4}$ kinetic model [Wang et al., 2007] which is utilized by all the HyChem fuels. The Dagaut mechanism captures more intermediate temperature chemistry, which results in lower observed mass fractions of benzene. At the highest scalar dissipation rate in Fig. 4.1c, the peak values of benzene from all of the mechanisms have decreased due the very high rates of mixing which cause lower temperatures and incomplete combustion. However, the C1 fuel displays a larger decrease in benzene compared to the other HyChem fuels. This trend coupled with the larger quantities of formaldehyde indicates that the C1 flame is approaching extinction earlier than the other fuels.

The ethylene (C_2H_4) mass fraction in Fig. 4.1 is drastically different for the C1 flame compared to the other fuels, reaching values nearly three times lower— closer to benzene at all scalar dissipation rates. The C1 mechanism differs from the A2 and

C5 mechanisms as its primary products are propene (C_3H_6) and iso-butene ($i-C_4H_8$), rather than ethylene and methane (CH_4) [Colket et al., 2017], which accounts for why there is considerably less ethylene present in the C1 flame. This difference should have a large effect on sooting propensity due to the sooty tendency of ethylene flames. A low presence of ethylene combined with having very few aromatics portends that the C1 flame ought to have much lower sooting tendencies than the conventional Jet-A, making it potentially a more preferable alternative jet fuel.

Methane is another species exhibiting differences in trends between the fuels at lower scalar dissipation rates. The Dagaut and C5 mechanisms match consistently, whereas the C1 fuel surprisingly displays the highest peaks of CH_4 , despite the lack of methane in the fuel-cracking pyrolysis step in the C1 mechanism.

The benzene and acetylene presences in Fig. 4.1 are quite similar between all of the HyChem kerosenes— if soot modelling were based on either of these soot precursors then it is likely that C1 would have a similar sooting tendency to petroleum-derived kerosene. In the context of these kerosene mechanisms, ethylene would be the most informative choice as a soot precursor. The HyChem A2 mechanism compares well overall against the Dagaut surrogate. Although it was formulated for high-temperature conditions, it still captures most species trends relatively well and at a reduced computational cost especially in terms of computer memory.

Going more in-depth with the HyChem results, species profiles varying with scalar dissipation rate in mixture fraction space for the A2, C5, and C1 fuelled flames are displayed in Figures 4.2, 4.3, and 4.4 respectively. The scalar dissipation rates range from stable burning up to the highest possible N_0 values prior to extinction of the flame. The benefit of using detailed chemical schemes is visible for the sheer number of species available for analysis. The species in the figures can be grouped as follows:

Row 1: Combustion equation reactants and products

Row 2: Intermediate indicators of heat release and extinction, plus
CO

Row 3: Pyrolysis species plus common soot precursor C_2H_2

Row 4: Pyrolysis species plus extinction marker HCO

Most peak species mass fractions decrease with increasing scalar dissipation rate, whereas O_2 , CH_2O , CO , CH_3 , HCO , and the fuel mass fraction Y_{fuel} experience the inverse of this trend. At very high scalar dissipation rates, many reactant species are flung away from each other before they have time to react, resulting in a build

up of unburnt quantities like fuel and oxygen mass fractions, as well as incomplete combustion products such as CH_2O and CO . CH_3 is a chain reaction accelerating radical and a producer of CH_2O through reactions with O [Najm et al., 1998]. HCO is a key species involved in the oxidation of hydrocarbons formed by reactions with CH_2O , and it reacts with many other species to produce CO radicals [Najm et al., 1998].

The selected species profiles are very similar between the A2 and C5 fuels in Figs. 4.2 and 4.3 aside from one or two exceptions. The fuel chemistry between the two mechanisms differs only in the molar quantities of products and some mild variations in the reaction rate terms in the first seven semi-global reaction steps. Other than these, the mechanisms are identical. The main reason for interest in the C5 fuel was due to its unusual physical properties, rendering its comparison to conventional Jet-A in 0D-CMC somewhat less illuminating. Nonetheless, for reference purposes it is noted from the selected species in Fig. 4.3 that there are some differences in the CH_2O and CH_3 mass fractions. Compared to the A2 results, the C5 flame at higher scalar dissipation rates experiences a lower peak in CH_2O at richer mixture fractions, whereas the CH_3 changes from a double-peak bimodal shape to a unimodal one. Toluene follows the same trend as in A2, however at considerably higher peak mass fraction values (nearly double). Other than these discrepancies the HyChem A2 and C5 mechanisms produce very similar results.

As for the C1 flame in Fig. 4.4, there are more differences. Peak values of formaldehyde are considerably higher, though still without the higher peak at richer mixture fractions observed in the A2 flame. The CO profile hardly changes at all with increasing N_0 , although the trend is inverted compared to the A2 and C5 flames, with CO actually decreasing with increasing scalar dissipation rate. The methyl radical CH_3 displays different behaviour from both A2 and C5, instead peaking strongly at a leaner mixture fraction and with the largest disparity between the bimodal peaks. This is likely partly due to the reduced presence of aromatic hydrocarbons in the C1 flame, which peak in mass fraction at rich mixture fractions around $\eta = 0.25$. CH_3 is a chain accelerator radical, so its increase in presence as N_0 is increased indicates that fewer reactions are consuming the radical, and thus some of the chain reactions needed to sustain a strong flame are no longer occurring as frequently. Increases in CH_3 mass fraction can then contribute to increased quantities of CH_2O and HCO as the flames approach extinction or lean blow-off.

The ethylene mass fraction, as was observed in Fig. 4.1, is much lower than in the A2 and C5 flames, whereas the $i\text{-C}_4\text{H}_8$ peak mass fraction in the C1 flame is 30 times larger, due to it being the primary decomposition species for the alcohol-to-jet

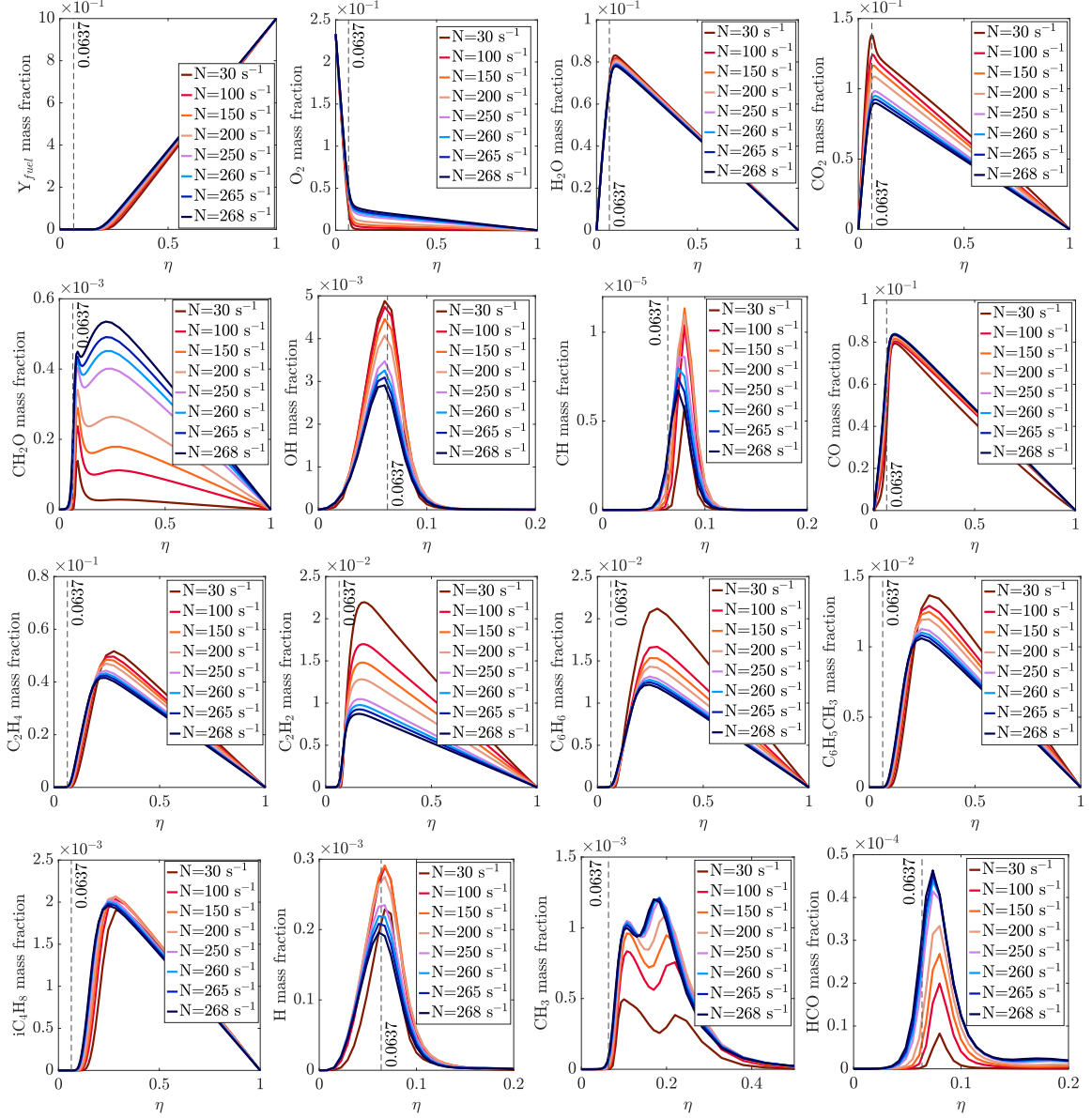
A2: P = 1 atm

Fig. 4.2 Species from 0D-CMC in mixture fraction space for the HyChem A2 flame at $P = 1$ atm, $T_{fuel} = 475$ K and $T_{air} = 300$ K varying with scalar dissipation rate N_0 (s^{-1}). N_0 values range from stable burning to near-extinction. The stoichiometric mixture fraction η_{st} is indicated with the dashed line.

C5: P = 1 atm

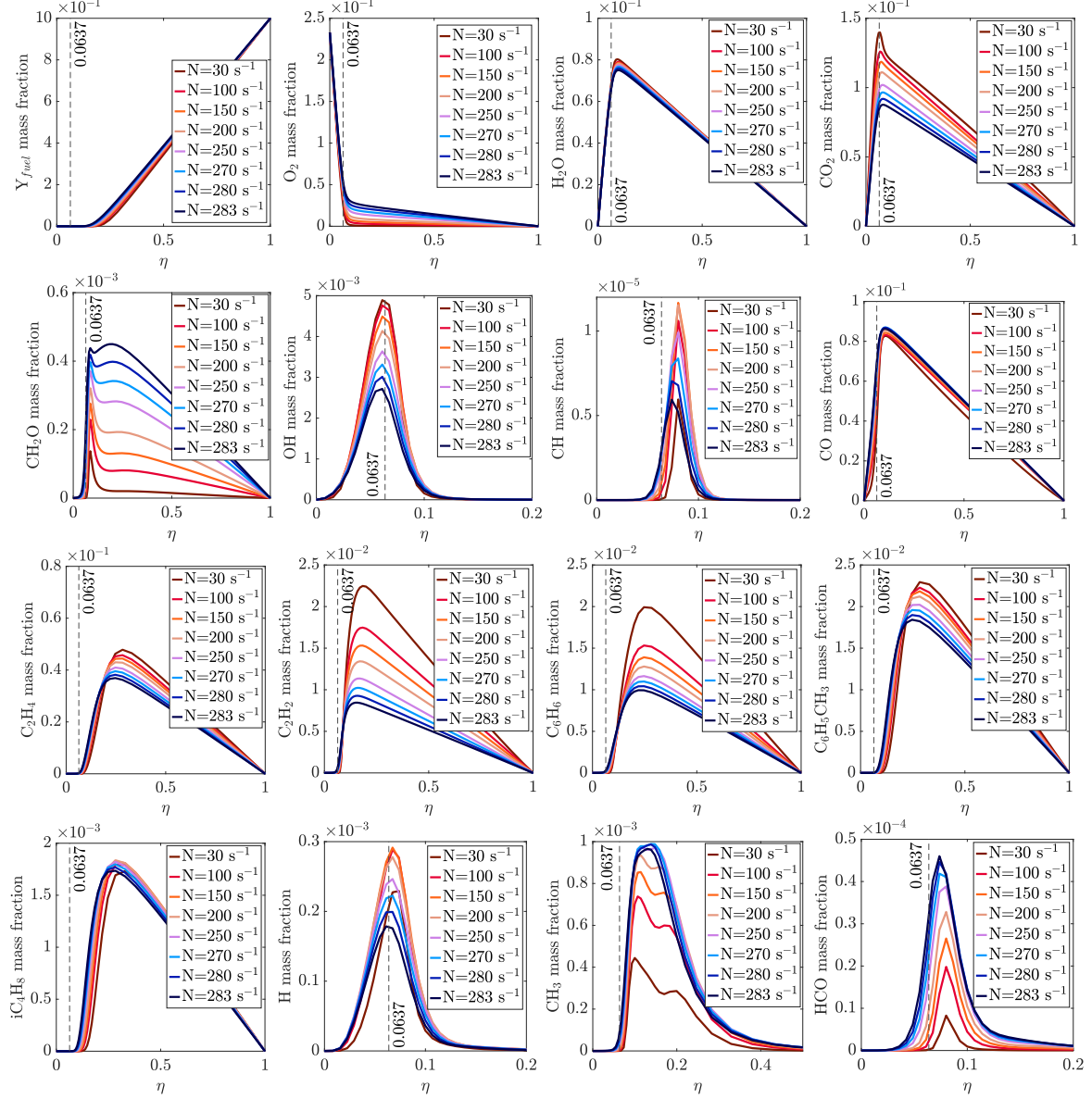


Fig. 4.3 Species from 0D-CMC in mixture fraction space for the HyChem C5 flame at $P = 1$ atm, $T_{fuel} = 475$ K and $T_{air} = 300$ K varying with scalar dissipation rate N_0 (s^{-1}). N_0 values range from stable burning to near-extinction. The stoichiometric mixture fraction η_{st} is indicated with the dashed line.

C1: P = 1 atm

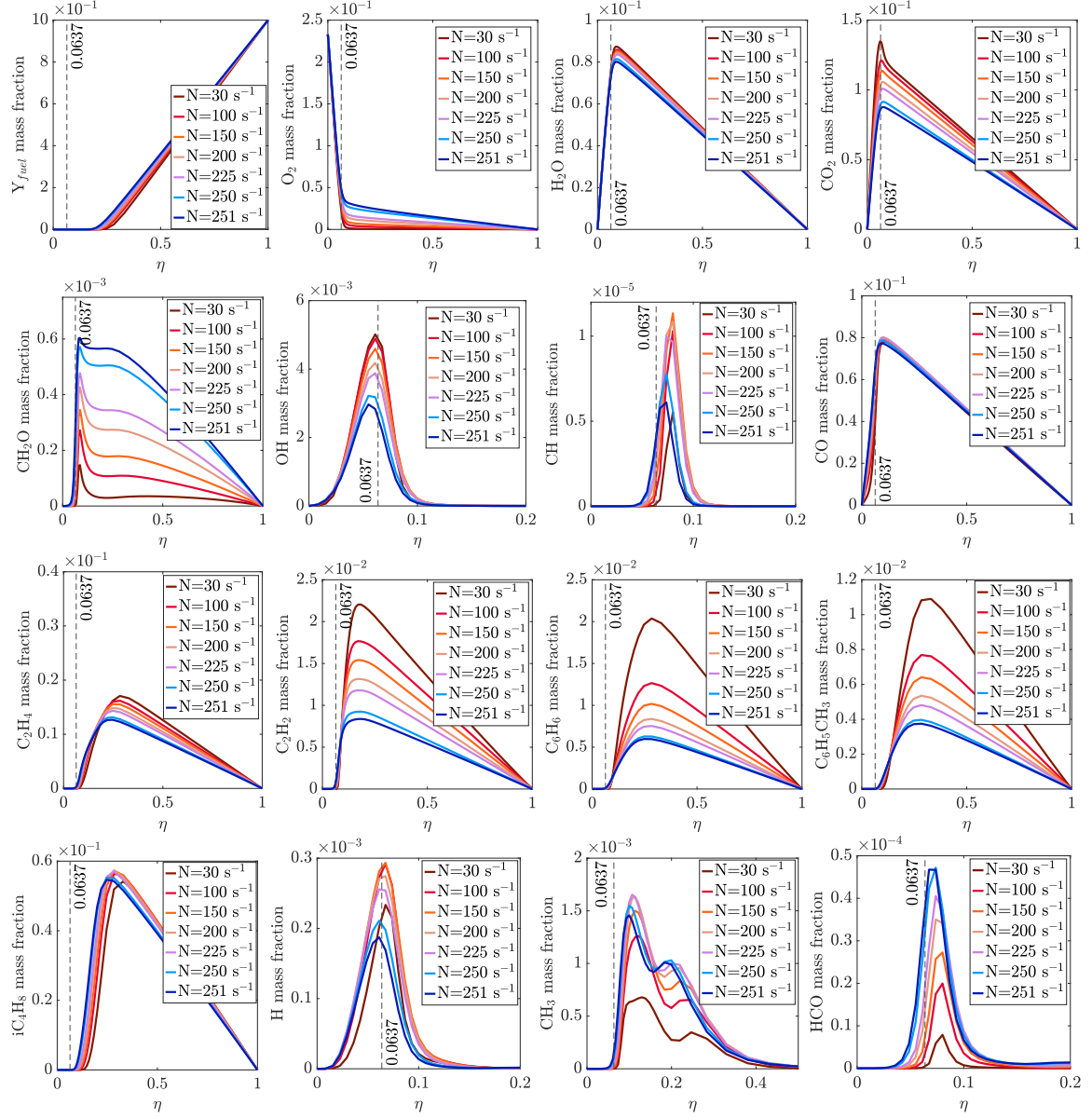


Fig. 4.4 Species from 0D-CMC in mixture fraction space for the HyChem C1 flame at P = 1 atm, $T_{fuel} = 475$ K and $T_{air} = 300$ K varying with scalar dissipation rate N_0 (s^{-1}). N_0 values range from stable burning to near-extinction. The stoichiometric mixture fraction η_{st} is indicated with the dashed line.

fuel. Common soot precursor C_2H_2 is about the same as for the other flames, but the aromatics benzene and toluene on the other hand display a much larger range in mass fraction across increasing N_0 in the C1 flame. C_6H_6 levels are about the same between the C1 and A2 flames at low N_0 , however at high N_0 benzene mass fraction in the C1 flame is about half that of the A2 flame. $C_6H_5CH_3$ behaves similarly. This strong reduction in aromatic hydrocarbons at high N_0 could be a desirable characteristic for new fuels as jet engines continually designed to operate at leaner conditions, as it would contribute to the reduction in soot.

4.1.2 High pressure (10 atm)

The simulation mass fractions in mixture fraction space shown in Fig. 4.5 are run at high pressure (10 atm) and $T_{fuel} = 570K$. Figure 4.5a is at the same scalar dissipation rate $N_0 = 30 s^{-1}$ as in Fig. 4.1a, however the subsequent increases in N_0 for the 10 atm simulations are much greater, reaching up to $900 s^{-1}$.

Once again, the Dagaut surrogate and the HyChem mechanisms compare very well in the temperature profiles, which peak at a higher temperature due to the increased pressure. The $N_0 = 500 s^{-1}$ results in Fig. 4.5b are nearly identical to the $100 s^{-1}$ results at 1 atm in 4.1b. However at low and high scalar dissipation rates the pressure increase alters the CH_2O behaviour. At $N_0 = 30 s^{-1}$ in 4.5a, the formaldehyde peaks of all the mechanisms are about one-third of the peak mass fractions observed at 1 atm in Fig. 4.5a, and the profiles have only one peak close to stoichiometry. The formaldehyde mass fraction peaks and profile shapes at the mid- and high-scalar dissipation rates for the two pressures are practically the same (although at high N_0 the peak has shifted to the right), whereas at $N_0 = 30 s^{-1}$ the CH_2O peaks are significantly lower in the 10 atm case. The Dagaut mechanism interestingly matches the HyChem A2 mechanism even better at high pressure, especially in the low- and high-scalar dissipation rate simulations.

Soot precursors as well as CH_4 are in the bottom row of Fig. 4.5. The ethylene mass fraction is virtually unchanged from the 1 atm results for all mechanisms and still hardly responds to increase in the scalar dissipation rate. Benzene, methane and acetylene mass fractions are all significantly increased from 1 atm levels at the low N_0 in Fig. 4.5a. These three soot precursors' presence decreases as scalar dissipation rate is increased, matching the 1 atm behaviour as the weak limit of the flame is approached. The C5 precursor mass fractions match the A2 results well, with methane being the one exception at low N_0 . At high pressure and low N_0 , C1 has the highest peaks in

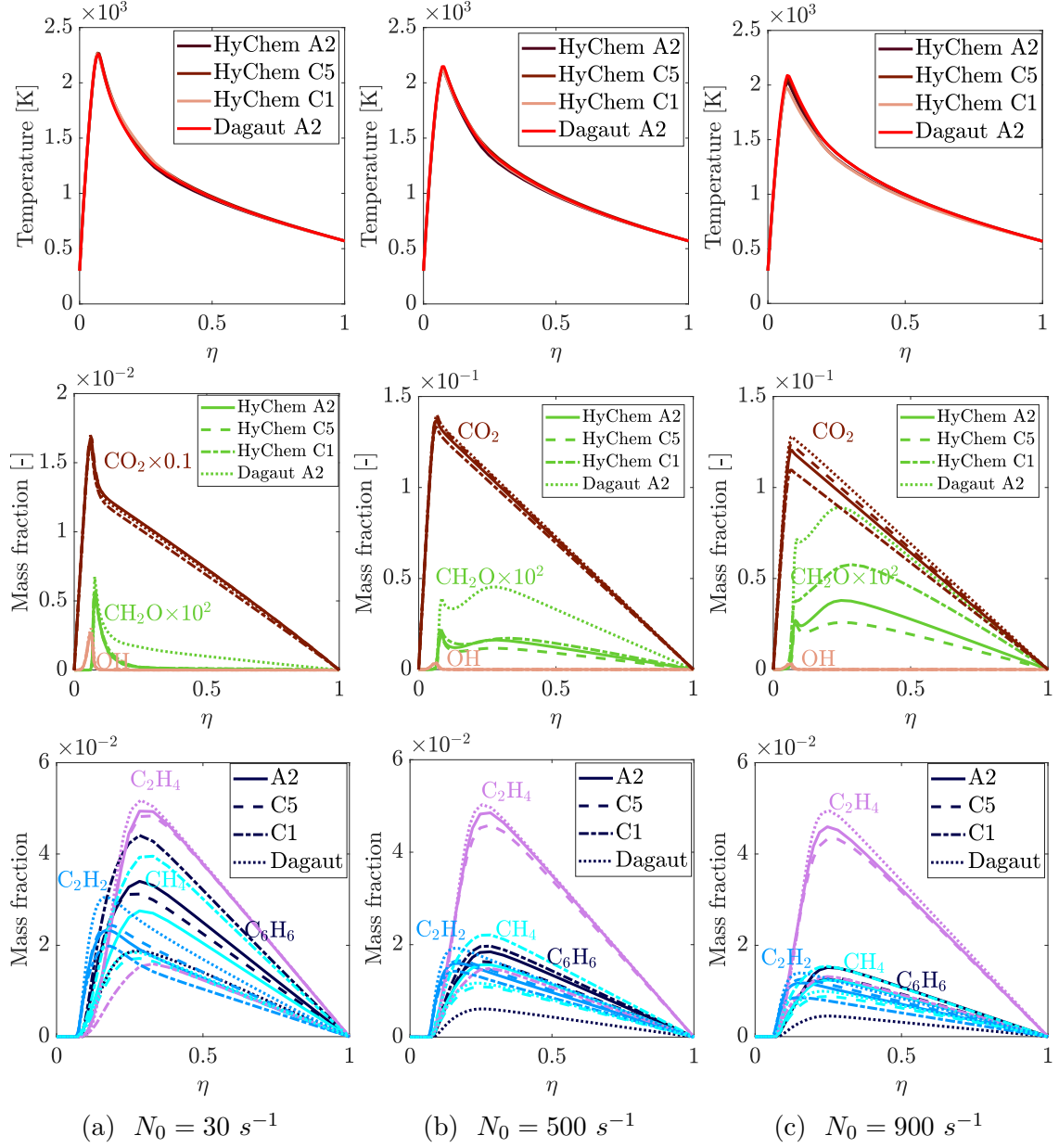


Fig. 4.5 Species mass fractions and temperature (K) in mixture fraction space from laminar counterflow diffusion flames of the different fuels at $P = 10$ atm, $T_{fuel} = 570$ K and $T_{air} = 300$ K, using the HyChem and Dagaut mechanisms. The three columns show results at scalar dissipation rates of $N_0 = 30$ s $^{-1}$, $N_0 = 500$ s $^{-1}$, and $N_0 = 900$ s $^{-1}$.

benzene and methane, although their presence decreases considerably with increasing N_0 .

These laminar flame results show that ethylene is not sensitive to pressure change or molecular mixing, even when nearing extinction. Benzene and methane on the contrary are very sensitive to both pressure and N_0 , exhibiting the most variability between the fuels. The mechanisms follow very similar trends overall at atmospheric and high pressure, especially as the scalar dissipation rate is increased toward extinction. Differences between the Dagaut surrogate and the HyChem mechanisms are generally reduced with increases in scalar dissipation rate and pressure.

In-depth comparison of selected species mass fractions in mixture fraction space for the three HyChem fuels at a pressure of 10 atm are shown in Figs. 4.6, 4.7, and 4.8.

The species trends overall appear very similar to their $P = 1$ atm counterparts. This is indeed the case for most of the pyrolysis products and the major reactants and combustion products, whose profiles and peak mass fraction values remain close to those at atmospheric pressure. In all the HyChem fuels, however, pressure has affected the behaviour of the lighter radical species involved in the chain reactions for sustaining combustion. Peak mass fractions of species H, OH, and CH at high pressure no longer continually decrease with increasing scalar dissipation rate. Peak mass fractions start low, and then increase as N_0 is increased up to about $N_0 = 500 \text{ s}^{-1}$. As N_0 is increased further, species mass fraction peaks begin to decrease, having reached their peaks in the middle of the flame stability range, far from mixing extremes. Nonlinear behaviour in reaction rates and species production are enhanced as pressure is increased.

Most species exhibit unimodal dependence on the mixture fraction, although CH_3 and CH_2O still demonstrate bimodal trends which are more pronounced as scalar dissipation rate is increased. Increased pressure has also enhanced the bimodal behaviour of these two species, with more dramatic dips between the peaks especially for CH_3 . Species such as HCO and CH_3 still follow the same trends with scalar dissipation rate as in the 1 atm simulations, but at high pressure the peak species mass fractions are about three times lower. The peak mass fractions of H and CH are similarly reduced. These reductions indicate that the combustion reactions and chain reactions occur at a higher frequency than at atmospheric pressure, resulting in fewer leftover radical species present. Increased pressure enhances complete combustion, evidenced here by the reduction in peak CO mass fraction by more than 10%.

A pressure of 10 atm is still only in the mid-range of operating pressures for existing jet engines, so more studies should be made at even greater pressures (20-40 atm) to understand how species respond. At 10 atm, soot precursors such as ethylene

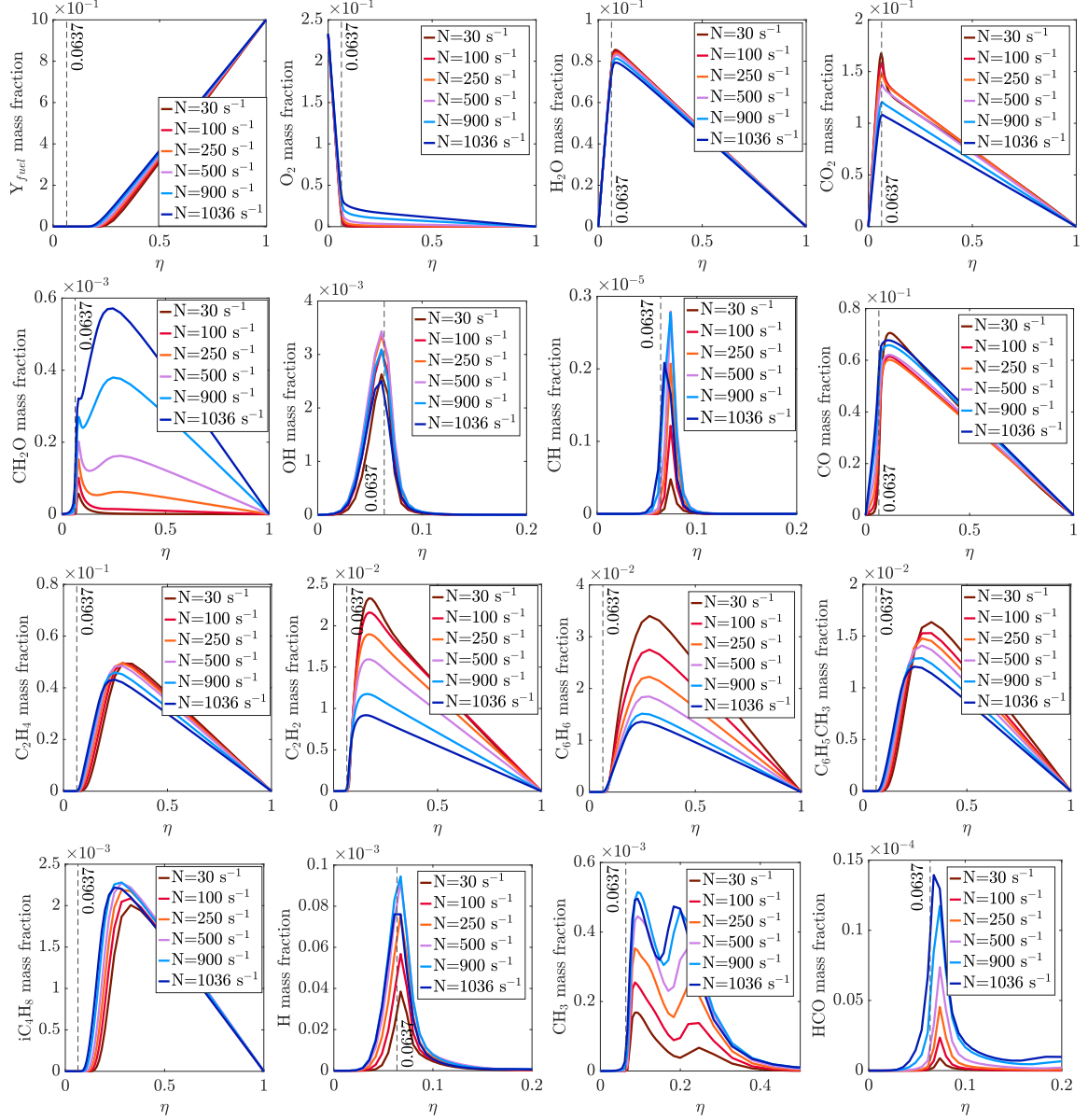
A2: P = 10 atm

Fig. 4.6 Species from 0D-CMC in mixture fraction space for the A2 flame at P = 10 atm, $T_{fuel} = 570\text{ K}$ and $T_{air} = 300\text{ K}$ varying with scalar dissipation rate N_0 (s^{-1}). N_0 values range from stable burning to near-extinction. The stoichiometric mixture fraction η_{st} is indicated with the dashed line.

C5: P = 10 atm

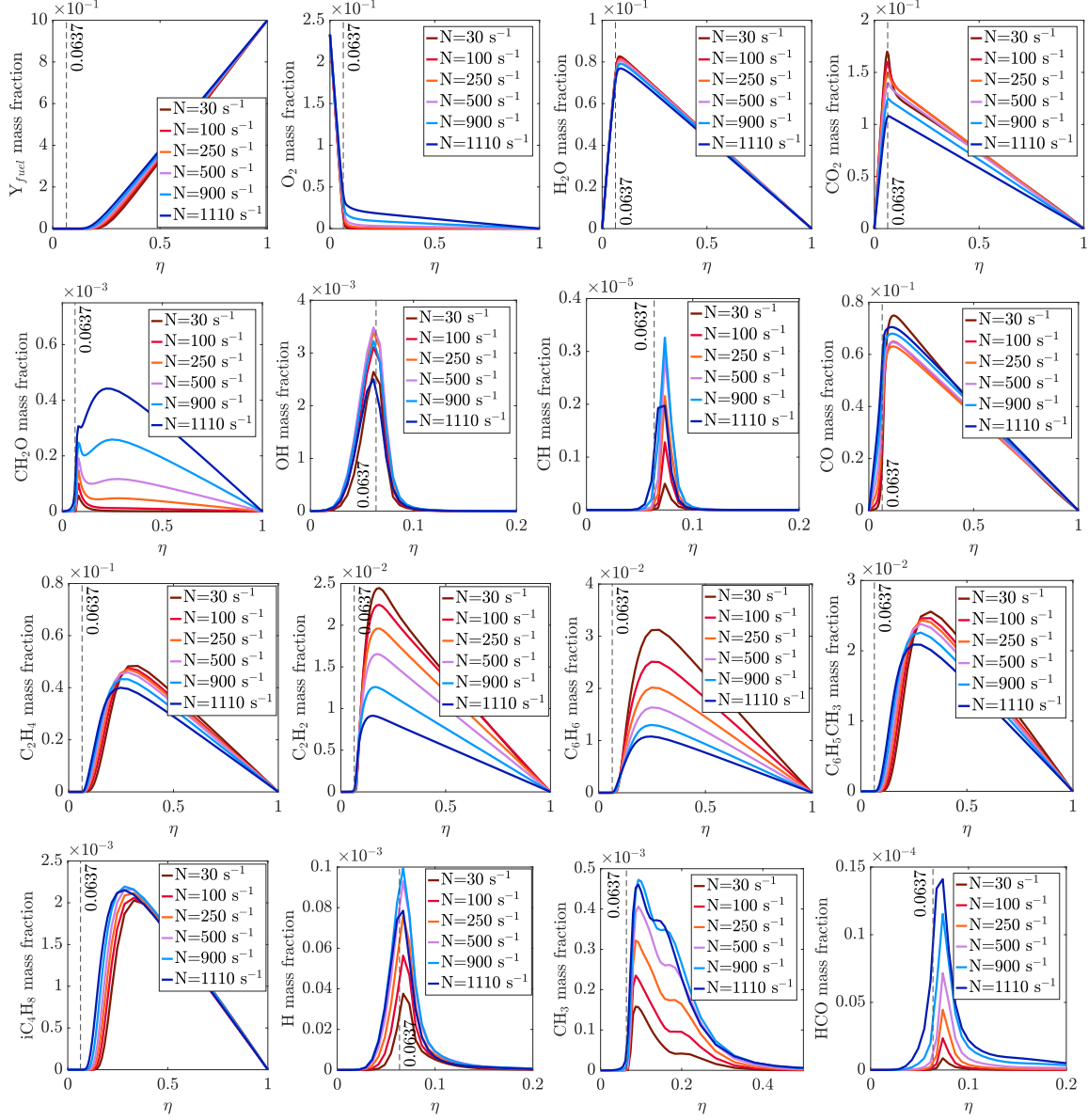


Fig. 4.7 Species from 0D-CMC in mixture fraction space for the C5 flame at P = 10 atm, $T_{fuel} = 570\text{ K}$ and $T_{air} = 300\text{ K}$ varying with scalar dissipation rate N_0 (s^{-1}). N_0 values range from stable burning to near-extinction. The stoichiometric mixture fraction η_{st} is indicated with the dashed line.

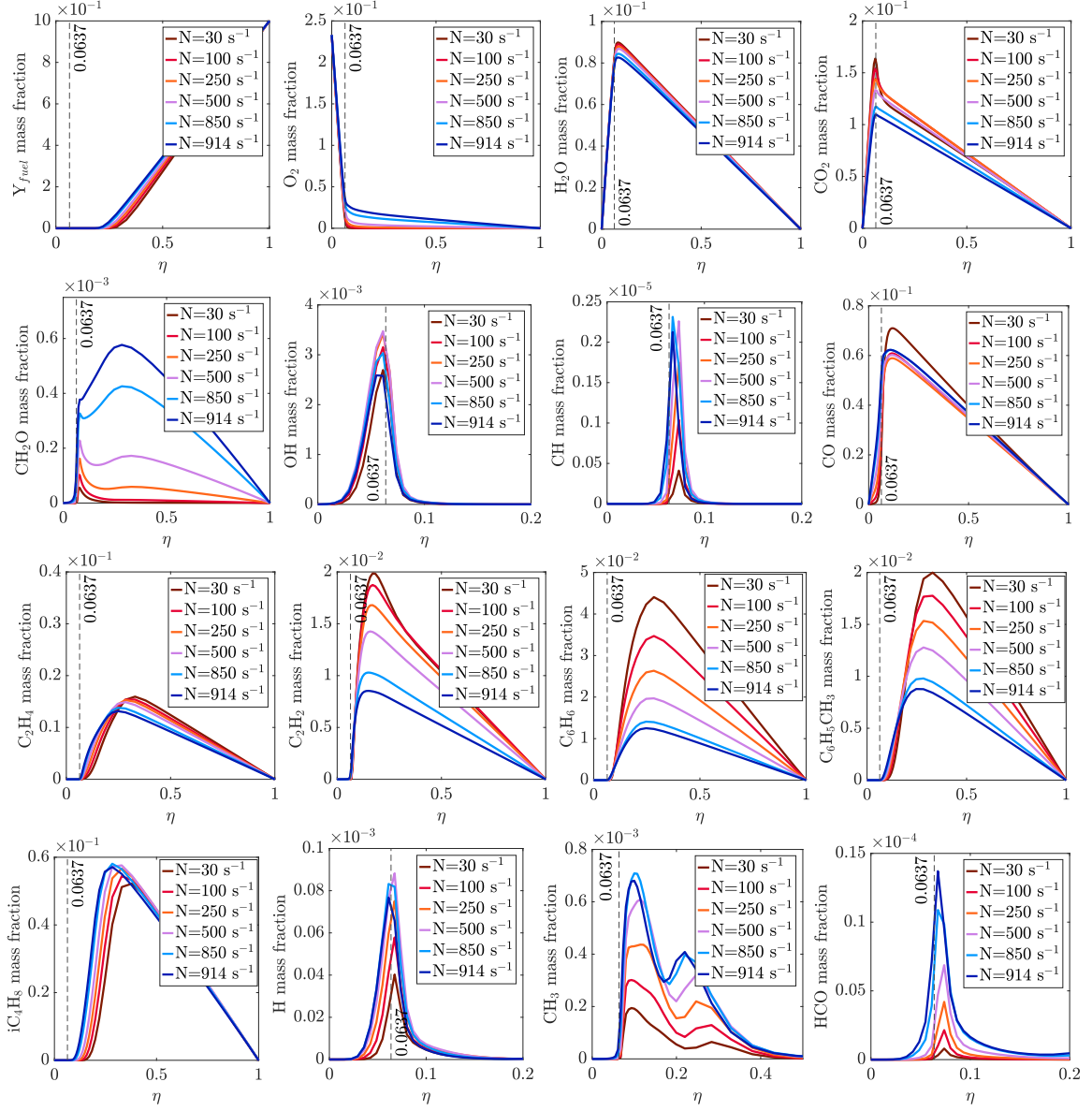
C1: P = 10 atm

Fig. 4.8 Species from 0D-CMC in mixture fraction space for the C1 flame at P = 10 atm, $T_{fuel} = 570\text{ K}$ and $T_{air} = 300\text{ K}$ varying with scalar dissipation rate $N_0\text{ (s}^{-1}\text{)}$. N_0 values range from stable burning to near-extinction. The stoichiometric mixture fraction η_{st} is indicated with the dashed line.

and acetylene and aromatics like benzene and toluene do not increase significantly, suggesting that these fuels at high pressure conditions may not produce much sootier flames compared to the atmospheric cases.

4.2 Extinction

4.2.1 The approach to extinction

The results from the simulations in the previous section are plotted in Fig. 4.9 to show the approach toward extinction for both atmospheric pressure and at 10 atm. Prescribed scalar dissipation rates N_0 are increased until the simulations are unable to sustain a burning flame, causing flame extinction. The maximum temperature in mixture fraction space for each simulation is recorded along with the maximum scalar dissipation rate N_0 supplied as input for that simulation. At $P = 1$ atm, the C1 fuel extinguishes at the lowest N_0 at about 251 s^{-1} with a maximum temperature of 1800 K. HyChem A2 then extinguishes at the next highest scalar dissipation rate, followed by the Dagaut kerosene, and C5 extinguishes at the highest scalar dissipation rate.

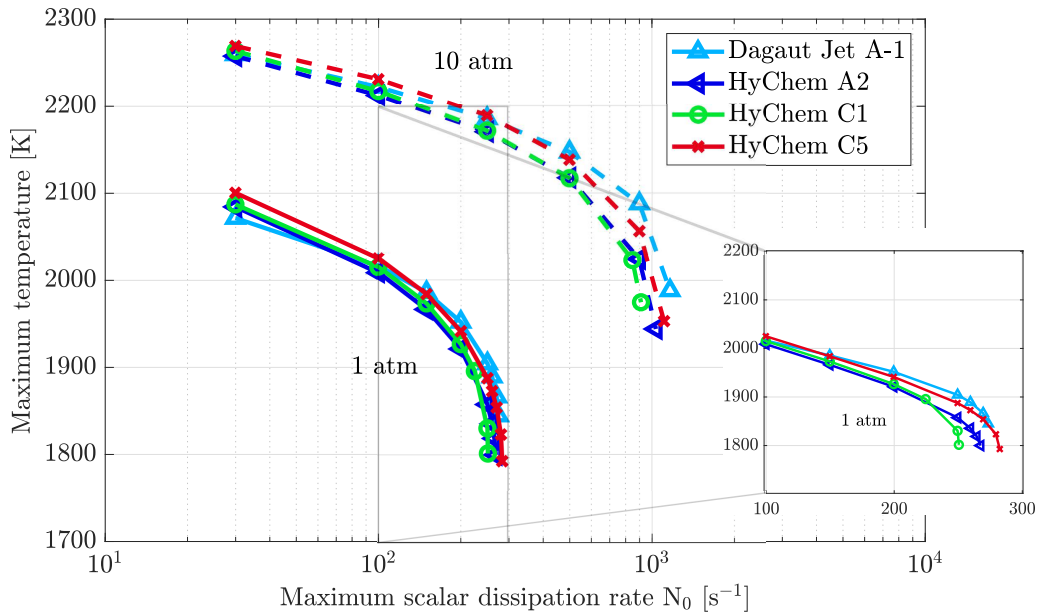


Fig. 4.9 Comparison of the approach to extinction for the four kerosene mechanisms at $P = 1$ atm (solid lines) and 10 atm (dashed lines) on a logarithmic x-axis for N_0 against maximum temperature (K). Small inset plot is an enhancement of the 1 atm curve on a linear x-axis.

Table 4.1 Extinction scalar dissipation rates from 0D-CMC simulations at 1 atm and 10 atm for the four kerosene flames.

Chemical mechanism	$N_{0,ext}$ (s^{-1}) @ 1 atm	$N_{0,ext}$ (s^{-1}) @ 10 atm
Dagaut Jet A-1	275	1168
HyChem A2	269	1040
HyChem C1	252	915
HyChem C5	284	1112

At 10 atm, the HyChem fuels follow the same trends with C1 extinguishing at lowest N_0 and C5 at the highest N_0 , but the Dagaut surrogate mechanism extinguishes at the highest N_0 overall. The critical values of scalar dissipation rate causing extinction of the flames $N_{0,ext}$ are listed in Table 4.1. These fuel extinction trends are in agreement with the non-premixed counterflow simulation results of Gao & Lu [2017].

C1 extinguished at the lowest rate of mixing of all the fuels, which follows experimental trends where C1 extinguished at richer equivalence ratio than A2 and C5 in both the bluff body swirl burner configuration in Allison et al. [2018] as well as the realistic gas turbine experiments discussed in Esclapez et al. [2017]. In these experiments it was observed that A2 should have been the most robust against higher scalar dissipation and blow-off, but these preliminary computational 0D results indicate that C5 exhibits the most resilient behaviour toward extinction. This result indicates that it is the liquid fuel physical properties of C5 which caused it to blow-off at richer equivalence ratio than A2 in experiments, rather than chemical differences.

When it comes to different chemical mechanisms capturing extinction and LBO phenomena, Gao & Lu [2017] suggest based on bifurcation analysis that it is the same set of reactions involving small molecules (such as H, OH, O₂, HCO, CO and CO₂) controlling how the flame will extinguish. This is a key reasoning for the feasibility of the lumped pyrolysis model used in the HyChem mechanisms and the utilization of detailed mechanisms for smaller species [Gao et al., 2016], hence the use of USC Mech II. Since both the surrogate and HyChem methods have detailed oxidation mechanisms of small species, they should both be able to capture LBO and extinction to a fairly similar degree. This is certainly true at atmospheric pressure, where there largest difference in $N_{0,ext}$ is 12.7%, between C1 and C5. At 10 atm, the largest difference is between the Dagaut surrogate and C1, reaching 27.7%. To make a more fair comparison, the HyChem A2 and Dagaut mechanisms however differ in $N_{0,ext}$ by only 2.2% and 12.3% at 1 atm and 10 atm respectively. This is favourable to the HyChem A2 mechanism,

which overall fares well in comparison to the significantly larger Dagaut surrogate scheme. However there is still the surprising result of the HyChem C5 fuel being the most resistant to extinction, despite having a nearly identical mechanism to the A2 fuel. The reason for the discrepancy may lie in the minor differences in CH_2O and CH_3 mass fractions, and CH_2O has been noted to react most with OH during extinction [Paxton et al., 2019]. C5 has lower peaks of both CH_2O and CH_3 , which may allow more OH to persist for longer, extending the flame stability of C5. Deeper analysis must be made however to come to more definite conclusions, perhaps through reaction pathway analysis or bifurcation analysis.

4.2.2 Transient response: extinction

Up to this point the 0D-CMC simulation results have all been stable solutions. In this section the 0D-CMC transient response during extinction will be explored for the HyChem A2 fuel. This will provide some context for the LES-CMC local extinction and global blow-off analysis in the next chapters.

The simulations in this section follow similar methodology and analysis to the work in Paxton et al. [2019], which observed extinction transients of non-premixed methane and n- $\text{C}_{12}\text{H}_{26}$ using 0D-CMC. A steady-state solution at the scalar dissipation rate $N_0 = 0.93N_{0,ext}$ is used to start, then a step change in N_0 is imposed at $t = 0$ s. Three step changes are examined: $N_0 = 1.0N_{0,ext}$, $N_0 = 1.1N_{0,ext}$, and $N_0 = 1.2N_{0,ext}$ at both 1 atm and 10 atm (using the relevant $N_{0,ext}$ values for the different pressures) and are shown in Figs. 4.10 and 4.11 respectively. The selected species mass fractions of interest during the extinction transient are normalized by their initial value, and their changes in behaviour are observed over non-dimensionalised time, using the relevant $N_{0,ext}$ for each pressure. In all cases the peak species mass fraction values are plotted.

The selected species for observation during the transient are ethylene (C_2H_4), acetylene (C_2H_2), formaldehyde (CH_2O), OH, HCO, CH, OH* and the product of $\text{CH}_2\text{O} \times \text{OH}$. OH*, the excited OH molecule, is commonly used in experiments as a qualitative marker for heat release rate and flame structure. CH is created in the thin reaction zone of the flame and decays rapidly, resulting in thin profiles [Grish & Orain, 2009]. It is used as a marker for the flame front similarly to OH, and is potentially a more accurate marker especially in highly wrinkled flame topologies [McManus et al., 2020]. HCO is regarded a good experimental observable species for marking flame burning and heat release rate [Najm et al., 1998], although it is noted in Paul & Najm [1998] that it has been difficult to obtain sufficiently high signal intensities for HCO in experiments. This has led to interest in the combined signal of $\text{CH}_2\text{O} \times \text{OH}$ (as both

species contribute to the production of HCO) as a marker of heat release rate [Paul & Najm, 1998], and has been explored experimentally in both gaseous and spray flame contexts [Kariuki et al., 2015; Yuan et al., 2015].

The extinction of the flame is complete in Fig. 4.10 once the markers of heat release reach zero. In Fig. 4.10a the extinction transient for the $N_0 = N_{0,ext}$ case lasts for a much longer duration (the duration is about 5.6 ms in total) than the other two cases with larger step changes in the scalar dissipation rate. It is about 15 times longer than the $N_0 = 1.1N_{0,ext}$ transient and 30 times longer than the $N_0 = 1.2N_{0,ext}$ transient. This is reasonable, as sharper step increases should result in increasingly faster extinction. Most of the species in Fig. 4.10a change very slowly during the transient, with CH_2O being the major exception, as well as OH, CH, and interestingly C_2H_2 to a lesser extent. CH_2O continually increases during the transient while OH, CH, and C_2H_2 mass fractions decrease. CH is the herald of the oncoming extinction, reducing more sharply earlier than any of the other species. This is more evident in 4.10b and 4.10c where CH decreases to zero before any other species, with OH^* being a close second. This result replicates the findings for non-premixed methane and n- $\text{C}_{12}\text{H}_{26}$ in Paxton et al. [2019], where CH^* was determined to be a key indicator of when an extinction will occur.

The sharp increase in the CH_2O profile appears most linked to the steeper decrease in OH mass fraction, as the primary consumption pathway for CH_2O is through reaction with OH [Paxton et al., 2019]. As OH decreases at a faster rate, the CH_2O presence experiences a runaway increase, peaking at over twice its initial value from the steady-state solution. These peaks are slightly reduced with greater N_0 step increases. The CH_2O peaks occur after the loss in OH with a small offset. This offset appears to line up more or less with the loss in HCO. Once HCO and similar radicals are all gone, CH_2O is no longer produced in greater quantities than it is consumed, and its levels proceed to decrease at a fairly steep rate. In 4.10a, the HCO and $\text{CH}_2\text{O} \times \text{OH}$ profiles follow nearly identical trends, but as the step change in N_0 is increased the $\text{CH}_2\text{O} \times \text{OH}$ profile is more similar to the OH^* trend.

The 10 atm HyChem A2 extinction transients in Fig. 4.11 have a few differences from their atmospheric counterparts. While the $N_0 = N_{0,ext}$ case extinguishes at proportionally the same duration as at 1 atm, the $N_0 = 1.1N_{0,ext}$ and $N_0 = 1.2N_{0,ext}$ transients in 4.11b and 4.11c extinguish even more quickly. At higher pressure, the OH and CH profiles are closer together, though CH still decreases to zero before OH. HCO and OH^* peak at higher proportions than at atmospheric pressure before sharply decreasing after the loss of OH mass fraction. Peaks of CH_2O are also higher, and the

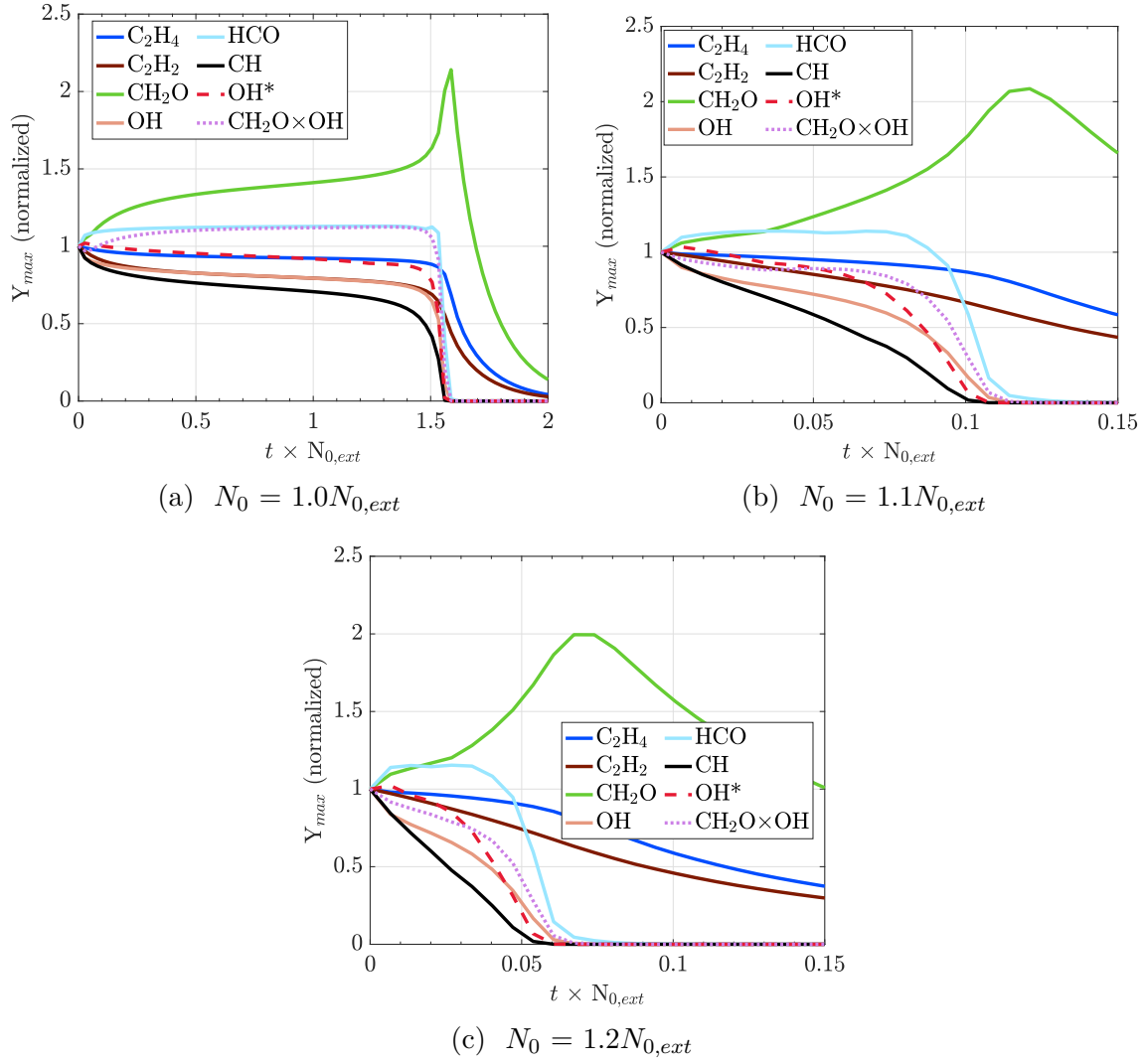


Fig. 4.10 Species mass fraction changes during the HyChem A2 flame extinction transient, $T_{air} = 300$ K, $T_{fuel} = 475$ K, $P = 1$ atm.

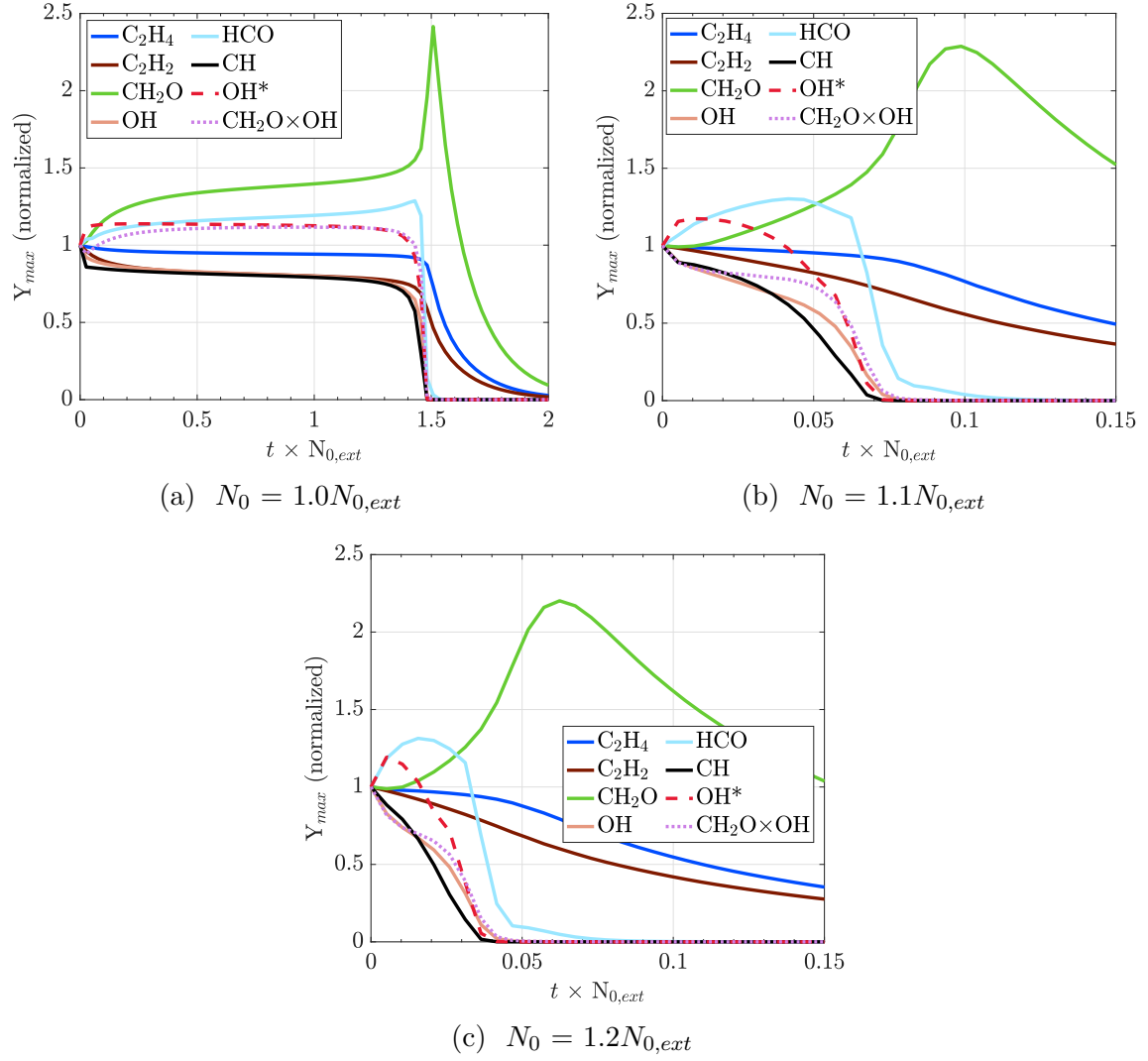


Fig. 4.11 Species mass fraction changes during the HyChem A2 flame extinction transient, $T_{air} = 300$ K, $T_{fuel} = 570$ K, $P = 10$ atm.

offset from the loss of OH is longer. In 4.11a all three major indicators of heat release rate (OH^* , HCO and $\text{CH}_2\text{O} \times \text{OH}$) line up very closely, however at larger N_0 values these trends once again separate, with $\text{CH}_2\text{O} \times \text{OH}$ lining up most closely with the OH profile at higher pressure. Both OH^* and $\text{CH}_2\text{O} \times \text{OH}$ are quite good metrics for extinction, lining up closely with the loss of CH, whereas HCO presence is considerably more prolonged, especially at higher pressure.

CH_2O is dependent on temperature in a different manner compared to the radical species. Normalized quantities plotted against corresponding maximum temperature during the extinction transient are shown in Fig. 4.12 for the HyChem A2 1 atm and 10 atm cases at $N_0 = 1.1N_{0,ext}$. In 4.12a CH is lost by the time temperature dips below 1500 K, while HCO is still around until temperatures reach as low as 1200 K. On the other hand CH_2O as well as pyrolysis product C_2H_4 and its decomposition product C_2H_2 are seen to be much less directly affected by the temperature. A shift

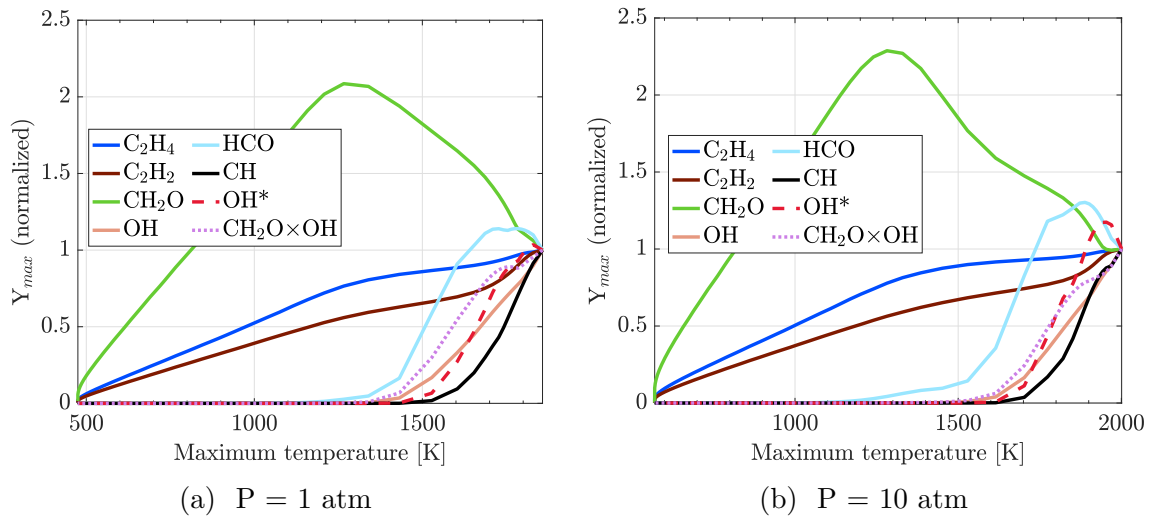


Fig. 4.12 Normalized maximum species mass fractions and heat release rate markers dependence on maximum temperature in the HyChem A2 extinction transient at both 1 atm and 10 atm, $N_0 = 1.1N_{0,ext}$.

in rates of decrease for C_2H_4 and C_2H_2 is discernible once the maximum temperature reaches about 1250–1300 K, after which the species mass fractions decrease at a faster rate. This temperature threshold corresponds to the lowest temperature at which full pyrolysis of the parent fuel can take place [Han et al., 2019]. Below this temperature, the fuel is no longer fully broken down into the smaller hydrocarbon molecules. This shift also roughly lines up with the peak in CH_2O , which decreases at a nearly linear rate as temperature decreases. An increase in pressure in Fig. 4.12b appears to shift

the small radical species extinctions to the right, where OH, CH and heat release rate markers OH* and CH₂O×OH all fall to zero above 1500 K. HCO initially follows the extinction transient profiles of OH and CH, but after a certain point around 1600 K its gradient becomes less steep and HCO then decreases at a much more gradual rate, disappearing below 1200 K. CH₂O, C₂H₄, and C₂H₂, however, respond nearly identically to temperature as in the atmospheric pressure case, suggesting that pressure does not change the extinction transient behaviour of species that are less temperature sensitive.

4.2.3 Transient response: reignition

Once the extinction transient begins, is it possible to reignite the flamelet? This is tested using the transient of the $N_0 = 1.1N_{0,ext}$, $P = 1$ atm case from Fig. 4.10b through plots of maximum species mass fractions and maximum temperature over time. The extinction-reignition transient attempts are displayed in Fig. 4.13. A step change of $1.1N_{0,ext}$ is applied to the steady-state solution $N_0 = 0.93N_{0,ext}$ at $t = 0$ s and is allowed to begin progressing toward extinction. At three different times during the extinction transient, the scalar dissipation rate is reduced to $0.93N_{0,ext}$ to see if the flame could reignite. The three times at which this step decrease in N_0 is applied are indicated by the vertical lines at $t = 2\delta$, 3δ , and 3.25δ after the initial $1.1N_{0,ext}$ step increase, where δ is equal to 1×10^{-4} s.

The normalized CH₂O and OH responses to the reduction in scalar dissipation rate are shown in Fig. 4.13a. As the extinction response begins, CH₂O increases as OH decreases as observed previously. Then at $t = 2\delta$ the N_0 is decreased and the species mass fractions quickly return to initial steady-state values, indicating a successful reignition of the flamelet. The corresponding temperature and heat release rate in 4.13b for this first attempt also show a return to nominal values, although not without a considerable jump in heat release rate just after N_0 is reduced. Then at $t = 3\delta$ the second attempt is made. At this point OH has decreased by nearly 50% and CH₂O is nearly 50% larger than steady-state values. After N_0 is reduced, OH and CH₂O begin to return to steady-state levels, however at a much slower rate. OH and temperature recover considerably more quickly than CH₂O, reaching initial values when CH₂O mass fraction is still about 25% greater. CH₂O×OH this time increased even more, going from 80% to nearly 140% nominal values. This is a second successful reignition attempt. At $t = 3.25\delta$, a third attempt is made to reignite the extinguishing flamelet. By this point in the $N_0 = 1.1N_{0,ext}$ transient OH levels are less than half their original values and CH₂O has surged up by greater than 50%. Temperature is still at

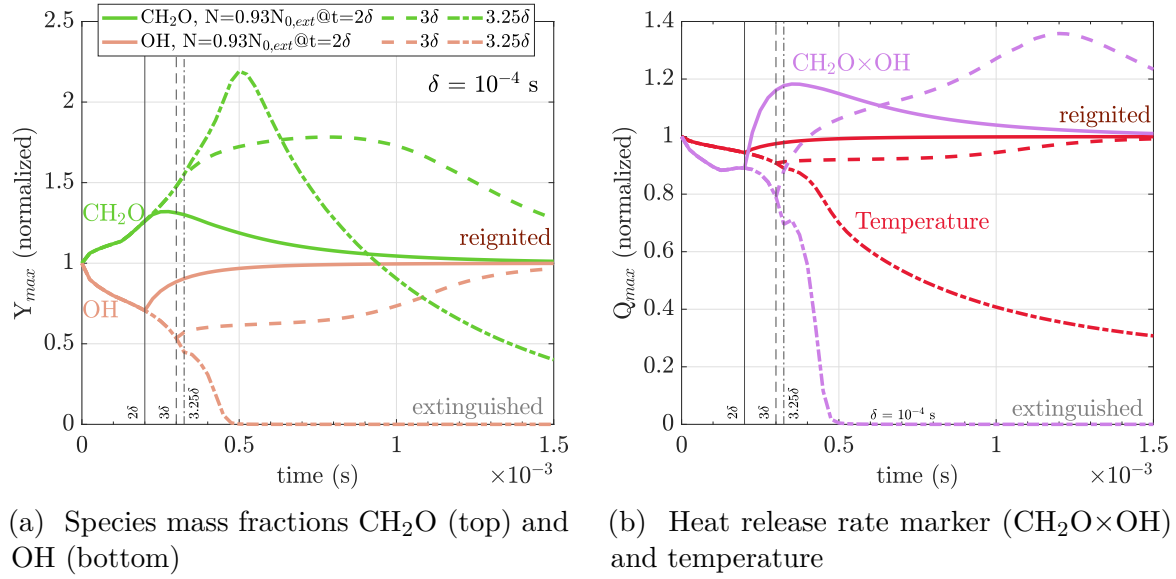


Fig. 4.13 The extinction transient from the $N_0 = 1.1N_{0,ext}$, $P = 1$ atm case is used to test possibility of flamelet reignition during extinction. Time $t = 0$ s indicates the start of the extinction transient when N_0 was increased from $0.93N_{0,ext}$ to $1.1N_{0,ext}$. Solid, dashed, and dash-dot lines indicate times 2δ , 3δ , and 3.25δ respectively (where δ is equal to 1×10^{-4} s) when N_0 was reduced to $0.93N_{0,ext}$. Reignition of the flamelet is observed when $N_0 = 0.93N_{0,ext}$ is applied at times $t = 2\delta$ and 3δ . Flamelets continue to extinguish despite the reduction in N_0 at times $t = 3.25\delta$ and greater.

about 90% of steady-state, however the loss of critical species to this extent makes the flame irrecoverable. OH and $\text{CH}_2\text{O} \times \text{OH}$ plummet to zero while CH_2O peaks to more than double its initial mass fraction. Reignition at this point in the transient and later is no longer possible. Temperature gradually decreases, its rate slowing after OH is lost. The maximum temperature is equal to 70% of steady-state when the flame is extinguished, the same as the threshold used to quantify extinction in LES-CMC simulations mentioned in Section 4.2.1.

Loss of small chain-branching reaction radical species is the biggest reason for the extinction of a flamelet. Once these radical species reach a certain low threshold, there is no turning back and the extinguishing flame can no longer be reignited. These results emphasize the importance of predicting these radical species as accurately as possible in order to appropriately model flame extinction and lean blow-off. Small changes in mass fraction can mean the difference between a burning and an extinguished flame.

4.2.4 Extinction thresholds for LES-CMC

Laminar counterflow simulation results provide valuable information which can be used to quantify extinction in mixture fraction space in LES-CMC simulations (the subject of the next two chapters). In Zhang et al. [2015], the final stable 0D-CMC solution prior to extinction is used to generate thresholds to demarcate extinction in the mixture fraction space context for a non-premixed methane flame. Applying that method here, the HyChem A2 solution at atmospheric conditions and $N_0 = 268 \text{ s}^{-1}$ discussed in the previous section is used to determine extinction thresholds, shown in Fig. 4.14.

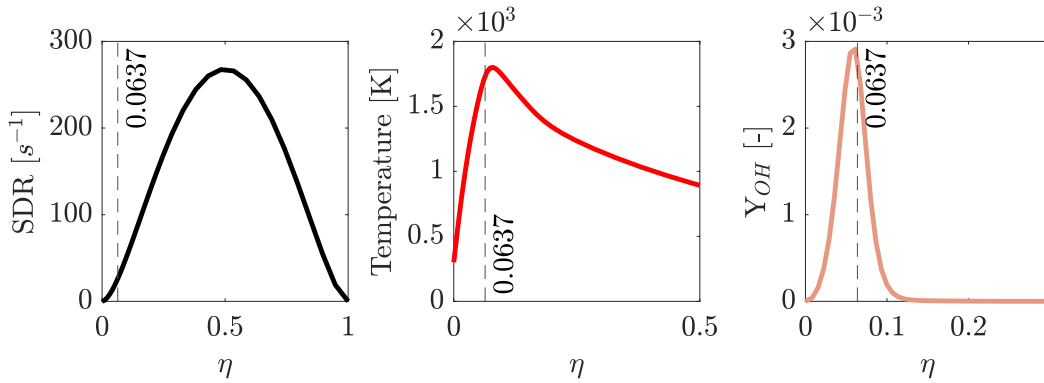


Fig. 4.14 Plots showing scalar dissipation rate, temperature, and OH mass fraction in η -space are shown from left to right. Extinction threshold values for LES-CMC are taken from the final stable solution of the 0D-CMC HyChem A2 flame at $P = 1$ atm, $N_0 = 268 \text{ s}^{-1}$, using the values at stoichiometry ($\eta_{st} = 0.0637$) for critical scalar dissipation rate, $N|\eta_{st}$. 70% and 15% of the $T|\eta_{st}$ and $Y_{OH}|\eta_{st}$ values respectively are used to determine critical temperature and critical OH mass fraction.

The critical values of scalar dissipation rate, taken at stoichiometry (the intersection of the dashed and solid lines in Fig. 4.14) is $N|\eta_{st} = N_{st,cr} = 24.5 \text{ s}^{-1}$. Thresholds of 70% and 15% are used to determine the critical values of temperature and OH mass fraction, resulting in: $T|\eta_{st} \times 70\% = T_{st,cr} = 1194 \text{ K}$ and $Y_{OH}|\eta_{st} \times 15\% = Y_{OH,st,cr} = 0.00045$. These criteria are utilized in the subsequent chapters to quantify local extinctions in the LES-CMC flames.

4.3 Conclusions

Laminar counterflow flames are run at various pressures and scalar dissipation rates using 0D-CMC. Four detailed chemical mechanisms are used: the Dagaut surrogate

0D-CMC Results for Jet-A and Alternative Fuels

mechanism for Jet A-1, and the HyChem lumped-pyrolysis mechanisms A2, C1 and C5, which represent standard Jet-A and two synthetic fuels.

Increasing the scalar dissipation rate typically decreases temperature and peak species mass fractions, with some notable exceptions such as CH_2O , CH_3 and HCO . The Dagaut surrogate and HyChem Jet-A results compare favourably with each other overall. Differences between the Dagaut surrogate and the HyChem mechanisms are generally reduced with increases in scalar dissipation rate and pressure. The HyChem C1 fuel has some distinctly different trends concerning ethylene and iso-butene, due to its very different chemical composition.

The mechanisms follow very similar trends overall at atmospheric and high pressure, especially as the scalar dissipation rate is increased toward extinction. Increasing pressure from atmospheric to 10 atm does not strongly affect large species behaviour, however small radical species are more significantly affected in peak levels of mass fraction. Ethylene is not sensitive to pressure change or molecular mixing, even when nearing extinction. Benzene and methane on the contrary are very sensitive to both pressure and N_0 , exhibiting the most variability between the fuels.

Scalar dissipation rates are increased to the point of flame extinction and the different extinction rates for the four fuels are compared at 1 atm and 10 atm. At 1 atm the C1 flame extinguishes at the lowest N_0 , making it most susceptible to blow-off, which follows experimental observations. The most resistant fuel to blow-off however is C5, rather than the HyChem A2 fuel as observed in experiments. Small differences in the chain-branch reaction species like CH_3 which affect CH_2O and subsequently OH production may be the reason for robustness of the C5 fuel. Its extinction scalar dissipation rate is 5.6% greater than the HyChem A2 value and 3.3% greater than the Dagaut surrogate extinction rate. At 10 atm the C1 fuel is still most prone to extinction, and amongst the HyChem fuels C5 is again the most robust against extinction. This result indicates that it is the liquid fuel physical properties of C5 which caused it to blow-off at richer equivalence ratio than A2 in experiments, rather than chemical differences. The Dagaut Jet-A1 surrogate extinguished at the highest value of scalar dissipation rate.

The extinction transients for the HyChem A2 fuel at 1 atm and 10 atm are explored through observation of several radical species, heat release rate markers as well as ethylene and acetylene mass fractions. OH^* and $\text{CH}_2\text{O} \times \text{OH}$ appear to correlate well as indicators of heat release rate. At 1 atm HCO matches relatively well against these heat release rate markers, however at 10 atm there are larger discrepancies between HCO and the other heat release rate markers. Increasing the extinction scalar dissipation rate

correspondingly reduces the duration of the extinction transient. CH is the first species to fall to zero, reaffirming it as a marker for the potential occurrence of an extinction event. CH₂O steadily increases during the extinction transient, reaching a distinct peak just after the flame is extinguished. This is linked to its primary consumption pathway involving OH; as OH is reduced, there is more and more CH₂O building up. Then once OH and other radical species are lost, CH₂O decreases monotonically as its rate of production becomes smaller than its rate of consumption by other species. Reignition of the extinction transient is successfully attempted up to a point in the transient, after which radical species mass fractions are too small to allow for recovery of the flame.

Chapter 5

Stable LES-CMC flame

Based on the 0D-CMC analysis of the various kerosene mechanisms in Chapter 4, the HyChem A2 mechanism is deemed suitable for use in LES-CMC simulations to replicate experiments using Jet-A in a bluff body swirl spray flame configuration. The focus of these experiments was to compare lean blow-off behaviour of the three kerosene fuels using a blow-off curve, with Jet-A as a reference fuel, and to determine how fuel chemistry contributes to LBO. As simulating LBO using LES-CMC for all three HyChem fuels is out of the scope of this work, focus is directed onto LES-CMC simulations of HyChem A2 (Jet-A) to create a reference for comparison against future simulations with the synthetic HyChem fuels.

This chapter covers the analysis of the initial stable HyChem A2 spray flame modelled using LES-CMC. The LES-CMC approach, which has had demonstrated success capturing local and global extinction for gaseous [Zhang, 2015; Zhang & Mastorakos, 2016] and spray flames [Giusti & Mastorakos, 2016, 2017], is used here with Lagrangian spray modelling and a detailed Hybrid Chemistry mechanism for Jet-A [Wang et al., 2018a; Xu et al., 2018]. The flame is simulated at the following conditions: fuel mass flow rate $\dot{m}_f = 0.27$ g/s, bulk air velocity $U_{b,air} = 15.9$ m/s $= 0.74U_{BO,exp}$, and equivalence ratio $\phi_{overall} = 0.37$. Unconditional quantities are presented in spatial visualizations. Comparisons of the flame size and shape, as well as the fuel sprays and heat release between the simulation and experiments are made. Time-averaged and instantaneous images of the stable LES-CMC solutions are presented, as well as evidence of the occurrence of local extinctions.

This solution is then used to start LBO simulations of the Jet-A flame, discussed in the next chapter.

5.1 Comparison with experiment

The comparison between the experiments and simulations in this work are limited to those of a qualitative nature, primarily related to flame shape and structure through time-averaged OH^* chemiluminescence and instantaneous OH-PLIF images. These are the only experimental data currently available for this flame. The flow velocity field in the same burner has already been computed using LES-CMC for methane [Zhang et al., 2015], n-heptane [Tyliszczak et al., 2014], and ethanol [Giusti & Mastorakos, 2017] with good agreement. The droplet size and velocity data from spray experiments in Yuan et al. [2018] were also numerically validated in Giusti & Mastorakos [2017] with very good agreement. The computational set-up in this work was deemed similar enough to those previously studied to allow for primary focus on qualitative flame behaviour.

Chemiluminescence is a useful qualitative method for characterizing flame shape and intensity in experiments. Optical radiation can be directly linked to the chemical reactions in combustion, i.e., the light intensity is proportional to the chemical production rate [Muruganandam et al., 2004]. Light intensity is generated by excited oxidized molecules which then relax to lower energy states by emitting photons. This light intensity is commonly captured using species such as OH^* , CH^* , C_2^* , and CO_2^* . The chemiluminescence of these excited species has been observed to scale linearly with fuel consumption rate, which allows it to be used as a rough indication of global heat release rate (HRR) [Balachandran et al., 2005].

Figure 5.1 shows a comparison between the time-averaged inverse Abel-transformed OH^* chemiluminescence from experiments in Sidey et al. [2017] (left) and time-averaged OH^* mass fraction from the numerical simulation of the flame (right). The images are denoted with EXP for experiment and LES for simulation. The LES results experience strong gradients along the spray and the shear layer, which affects quantities related to heat release. This causes a blocky appearance in the results due to the coarse size of the CMC mesh. The simulation captures the overall size and shape of the flame relatively well. These time-averaged LES-CMC OH^* results are similar to the heat release rates observed for the stable ethanol flame in the same geometry modelled in Giusti & Mastorakos [2016], where spray terms in the subgrid mixture fraction variance equation were introduced to model the additional subgrid mixing related to evaporation source terms. Increased subgrid mixing leads to an increase of the mixture fraction variance and scalar dissipation rate, which results in an increase of heat release rate observed along the spray cone.

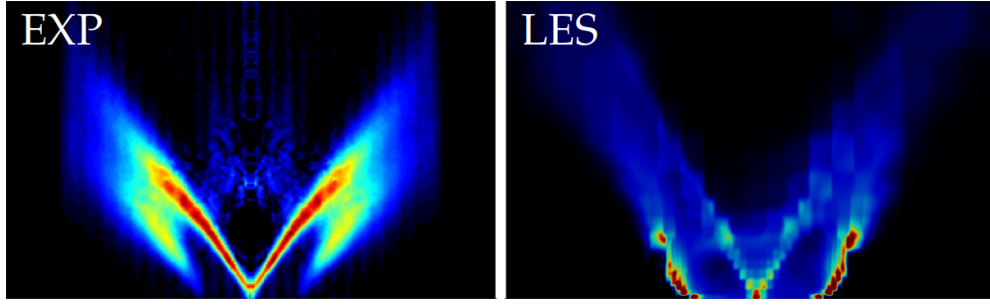


Fig. 5.1 Experimental inverse Abel-transformed time-averaged OH^* from Sidey et al. [2017] (left) for the Jet-A flame compared against time-averaged OH^* from LES-CMC (right), where maximum OH^* mass fraction is $2e^{-11}$. Conditions: $U_b = 0.74U_{BO,exp} = 15.9 \text{ m/s}$, $\dot{m}_f = 0.27 \text{ g/s}$. Images shown are $0.08 \times 0.05 \text{ m}$.

In the LES results in Fig. 5.1 the air-flame shear layer along the bluff body edge experiences the highest peaks of OH^* , whereas in experiments the highest peaks are encountered along the spray cone. The high OH^* signal along the spray in the experiments may be caused by higher rates of mixing due to evaporation compared to the rates modelled in the simulation. The low-volatility of Jet-A may contribute to increased levels of heat release and OH presence near the bluff-body and along the air shear layer, which was observed in experiments with n-decane and n-dodecane flames in the same burner in Yuan et al. [2018]. Similar differences between experiment and simulation for a stable n-heptane flame in the same burner using LES and Discrete Particle Simulation are observed in Paulhiac et al. [2020]. It is common for simulations to predict higher heat release along the shear layer with connection to the bluff body edge. This is possibly due to inadequate wall-induced heat loss caused by the bluff body surface in numerical models.

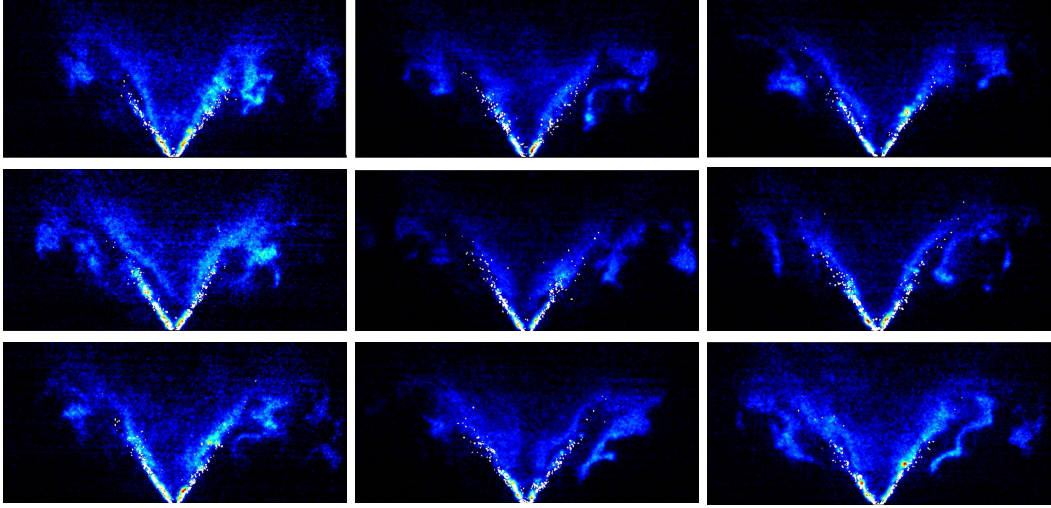
Planar laser induced fluorescence (PLIF) is a 2D experimental imaging technique which can provide instantaneous information across the entire plane of the flow field, revealing important information on species composition, temperature and the structure of the flow [Grisch & Orain, 2009]. Mie scattering is used to measure the size distribution of droplets in sprays by elastic scattering of laser light [Masri et al., 1996]. Simultaneous OH-PLIF and Mie scattering experimental techniques were applied to the Jet-A flames; instantaneous images at two different air flow rates are shown in Fig. 5.2. The details of the experimental imaging methodology can be found in Sidey et al. [2017]. In Fig. 5.2a the droplets are nearly all vaporised before leaving the flame zone, whereas in Fig. 5.2b droplets are visible higher up outside of the flame, continuing out of the frame. In Fig. 5.2b the OH-PLIF signal is notably greater around the outer flame branches at

the higher air velocity $U_b = 0.93U_{BO,exp} = 20.2$, and the outer flame more frequently attaches to the edge of the bluff body.

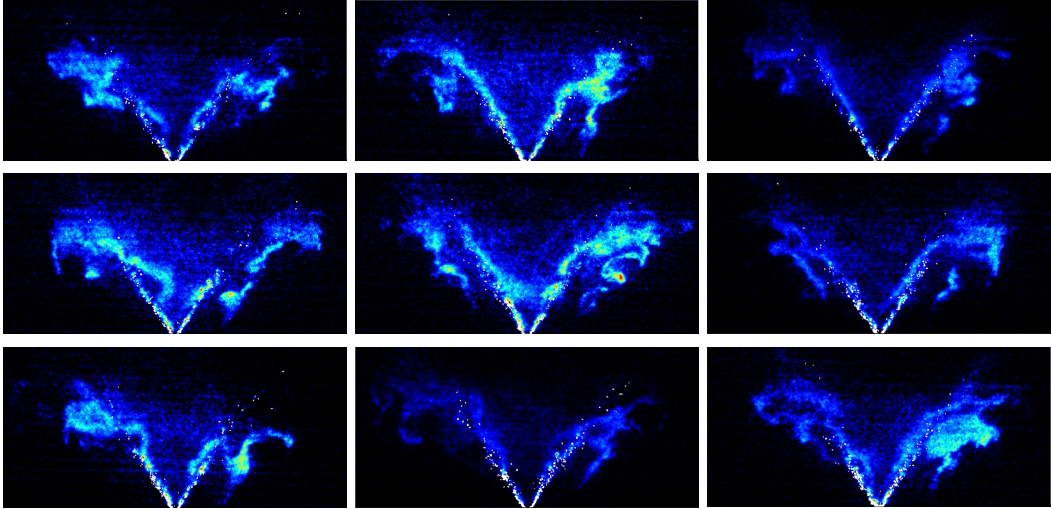
LES-CMC instantaneous heat release rate and the Lagrangian spray parcels at the same air and mass flow rates as the flame in Fig. 5.2a are shown in Fig. 5.3. The experimental results show a large amount of flame lift-off at both conditions, although with increased attachment as air velocity is increased. The LES-CMC HRR results have a much more attached flame, with highest signal observed not along the spray, but rather along the air shear layer, corresponding to the time-averaged OH* results in Fig. 5.1. In experiments by Cavaliere et al. [2013], n-heptane spray flame OH* signal reduces along the spray and increases along the air shear layer as bulk air was increased. Similar trends were also observed with OH-PLIF of decane and dodecane spray flames in Yuan et al. [2018].

The presence of this behaviour in the LES-CMC results indicates that the simulation is possibly exhibiting signs of a flame closer to blow-off conditions than expected. Some droplets are also still visible at heights well above the flame despite it being a stable condition with lower bulk air flow rate. Another reason for the difference in peak heat release location between experiments and simulations may be due to the use of the detailed chemical mechanism. In Giusti & Mastorakos [2016, 2017], time-averaged heat release rate from LES-CMC of both a one-step and a detailed ethanol mechanism were used and compared with experimental inverse Abel-transform time-averaged OH*. Interestingly the one-step ethanol chemistry captured the locations of higher heat release along the spray significantly better against the experiments than the detailed chemical mechanism. The detailed ethanol mechanism produced higher rates of heat release along the air shear layer than along the spray, similar to the detailed HyChem mechanism results here.

Instantaneous cut-planes of OH mass fraction and the Lagrangian spray parcels from LES-CMC at the same conditions as Fig. 5.3 are shown in Fig. 5.4. Compared to the OH-PLIF results in Fig. 5.2, OH presence in the simulation is much more spatially distributed with peak mass fraction located both near the spray and along the air shear layer. But the simulations are similar to experiments in that there is peak OH in the recirculation zone, along the spray and the edge of the central recirculation zone, and along the shear layer at axial heights greater than 10 mm. See Fig. 3.6 for location of the recirculation zones. Correspondingly to the HRR results, the OH in the simulation is attached to the bluff body, but there is also notable OH mass fraction present downstream of the flame region along the spray and the shear layer. The downstream presence of the OH is due to the lumped pyrolysis method of the



(a) $U_b = 0.74U_{BO,exp} = 15.9 \text{ m/s}$



(b) $U_b = 0.93U_{BO,exp} = 20.2 \text{ m/s}$

Fig. 5.2 Instantaneous simultaneous OH-PLIF and Mie scattering images of Jet-A experiments at two different air mass flow rates from the work of Sidey et al. [2017]. Fuel mass flow rate $\dot{m}_f = 0.27 \text{ g/s}$ is the same for both (a) and (b). Domain window is $0.08 \text{ m} \times 0.04 \text{ m}$.

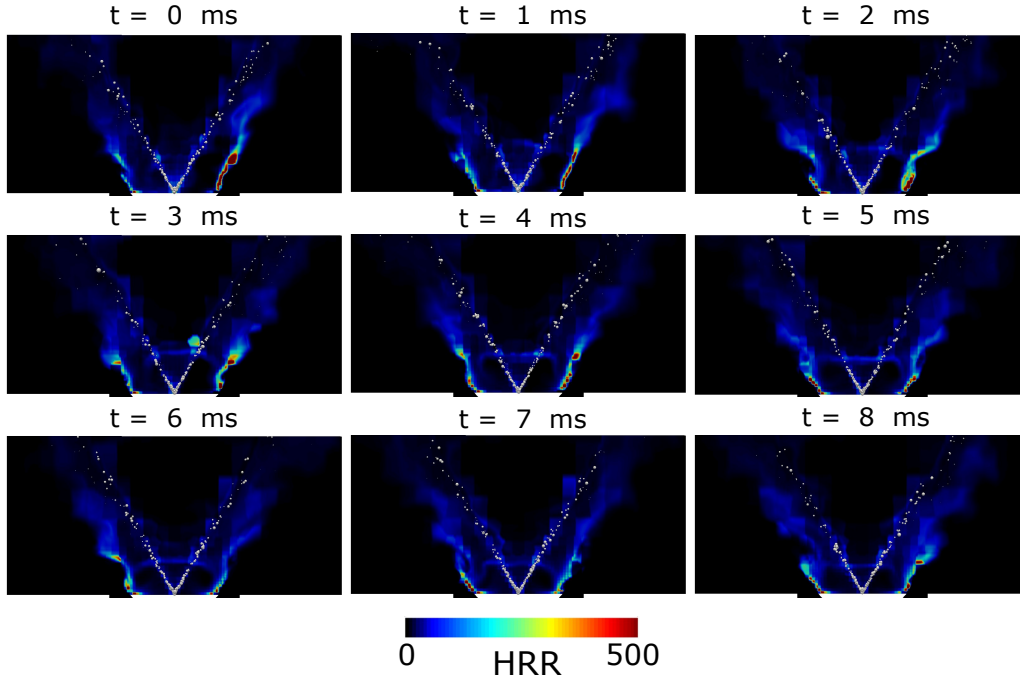


Fig. 5.3 Instantaneous 2D cut-planes of heat release rate (MW/m^3) from LES-CMC simulations overlaid with the Lagrangian spray parcels located in the same plane, scaled by droplet diameter. Conditions: $U_b = 0.74U_{BO,exp} = 15.9 \text{ m/s}$, $\dot{m}_f = 0.27 \text{ g/s}$. Domain window is $0.095 \text{ m} \times 0.045 \text{ m}$.

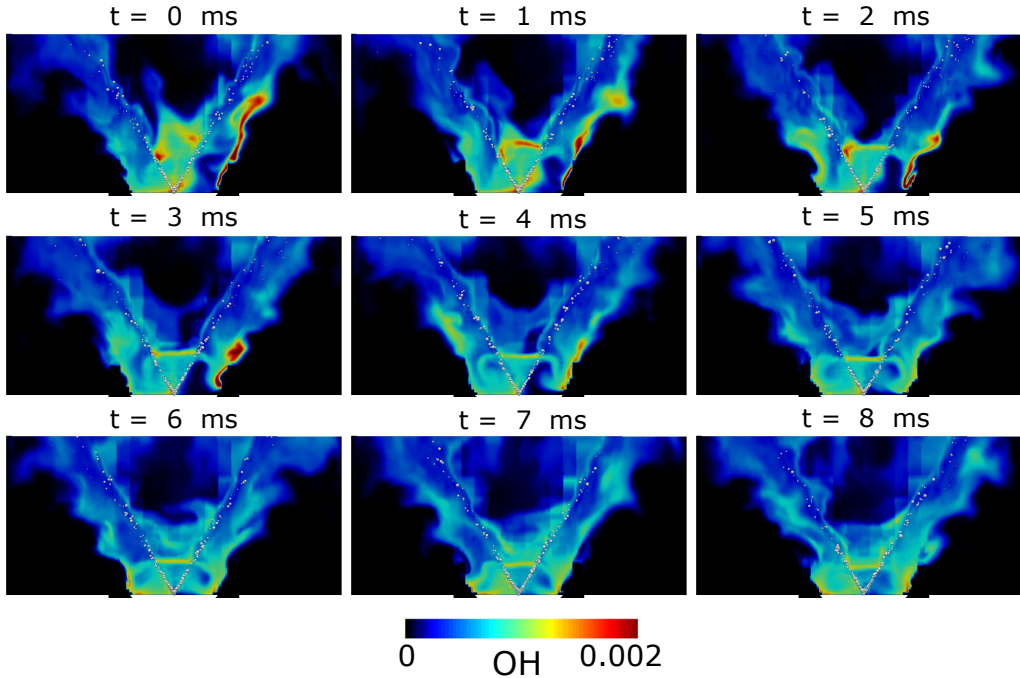


Fig. 5.4 Instantaneous 2D cut-planes of OH mass fraction from LES-CMC simulations overlaid with the Lagrangian spray parcels located in the same plane, scaled by droplet diameter. Conditions: $U_b = 0.74U_{BO,exp} = 15.9 \text{ m/s}$, $\dot{m}_f = 0.27 \text{ g/s}$. Domain window is $0.095 \text{ m} \times 0.045 \text{ m}$.

detailed HyChem kerosene mechanism. OH is produced by the seventh global reaction equation wherever there is vaporised fuel and single oxygen atoms (O) [Wang, 2018].

Figure 5.5 shows 2D cut-planes of vaporised fuel mass fraction overlaid with Lagrangian spray parcels scaled by droplet diameter. White isolines indicate stoichiometric mixture fraction. In the enlarged window it is even more evident that some droplets are travelling quite far downstream away from the flame. The vaporised fuel in the 2D gaseous field trails after the droplets in small quantities downstream, whereas significant levels of fuel mass fraction are located primarily along the spray cone near the stoichiometric isolines. Wherever there are high levels of fuel mass fraction, there is a lack in OH mass fraction in Fig. 5.4. Too much fuel vapour quenches the branches of stoichiometric regions along the fuel spray cone.

Not only fuel vapour may be causing the quenching of these stoichiometric regions between the shear layer and the spray in Fig. 5.5. In Paulhiac et al. [2020], they noted that vortical structures generated by the coupling between the injected spray and the gas phase could locally extinguish the flame, expelling hot products, fuel vapour and droplets outside the stoichiometric envelope. Small quantities of fuel mass fraction can even be observed at radii greater than that of the air inlet annulus, where tiny droplets have been convected axially downward to the upstream region by the side recirculation zones and vaporised upon encountering the fresh oxidants entering the chamber from the annulus. There is however no fuel at all observed in the central recirculation zone, indicating this region is well-mixed.

Overall the simulation results look closer to the experimental OH-PLIF Mie results at the higher air mass flow rate in Fig. 5.2b, exhibiting some behaviour of a flame closer to blow-off. One reason for this may be due to the spray modelling used in simulation. When the simulations were set up, the injected spray velocity $U_{droplets} = 25$ m/s was the same as in Sitte [2019] for the Rouen lifted heptane spray flame [Verdier et al., 2018]. Information on the droplets speeds used in the kerosene experiments were lacking at the time. However in Yuan et al. [2018] the experimental liquid spray velocities U_l used were listed for decane and dodecane to be between 11–12 m/s. This significant difference in droplet speed may account for some of the differences between the experiments and simulation. The droplets move so quickly through the flame zone that the larger ones are not fully vaporised before they exit the flame to the downstream region of the combustor, reducing the availability of fuel vapour in the hot burning region.

Under ideal circumstances this stable LES-CMC simulation would have been compared and validated against experiments well before blow-off simulations were

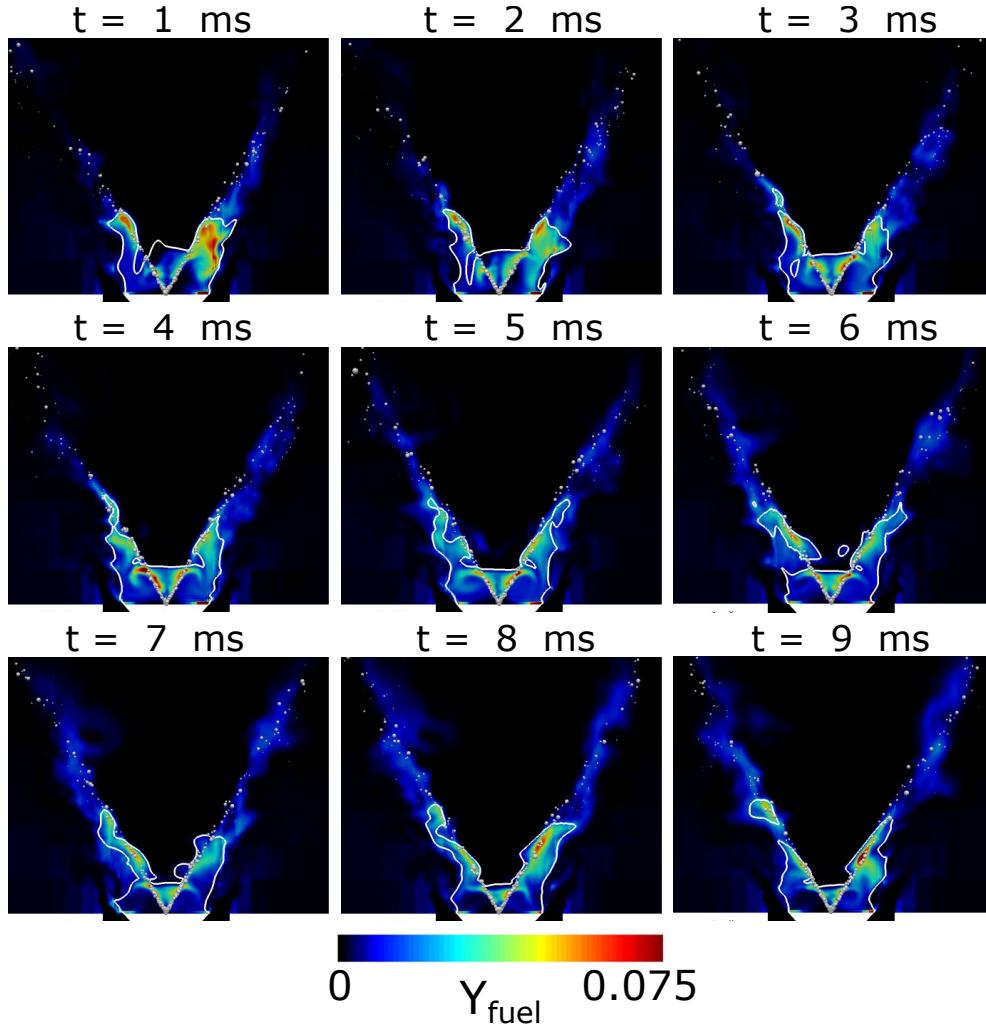


Fig. 5.5 Instantaneous 2D cut-plane of gaseous parent fuel mass fraction, overlaid with white isolines indicating the stoichiometric mixture fraction $\xi_{st} = 0.0637$, as well as the Lagrangian spray parcels located in the same plane, scaled by droplet diameter. Conditions: $U_b = 0.74U_{BO,exp} = 15.9 \text{ m/s}$, $\dot{m}_f = 0.27 \text{ g/s}$. Domain window is $0.095 \text{ m} \times 0.075 \text{ m}$.

initiated. Discrepancies between modelling and experiments would be identified and fixed given the time and appropriate metrics for comparison. The spray behaviour in particular required more time and data for validation. The CMC mesh also likely required a sensitivity study to determine the refinement needed to get a good comparison with experimental results. In the case of this work however, the stable flame was run to gain time-averages simultaneously as LBO simulations were initiated to make up for lost simulation time due to large setbacks with the stability of the code for the spray modelling. Thus the behaviour of the stable flame of the chapter was only fully characterised as the blow-off simulations were being completed.

The simulations in this work provide a first look at the structure of simulated kerosene spray flames before and during lean blow-off, and provide insights into the physics of local extinction and blow-off for spray flames using practical fuels. However these simulations will require more extensive validation against experiments before stronger conclusions can be drawn about the capabilities of the LES-CMC model in capturing LBO phenomena in heavy hydrocarbon spray flames. The stable flame explored in this chapter provides a baseline reference for comparison for the blow-off simulations discussed in Chapter 6.

5.2 Time-averaged LES-CMC results

Time-averaged quantities from the stable $\dot{m}_f = 0.27$ g/s simulation are shown in Fig. 5.6. OH^* and iC_4H_8 were averaged over 10 ms, while all other quantities were averaged over 17 ms. The stable flame structure is asymmetric, indicated by the white stoichiometric isoline. This tendency toward single flame branch behaviour has been observed in previous experiments with other low-volatility fuels like decane and dodecane in Yuan et al. [2018], both at stable and blow-off conditions. The recirculation zone is conical and flows downward within the spray cone toward the bluff body. High temperatures occur near to the bluff body. Spray flames and particularly low-volatility fuels have been observed to have low lift-off heights [Cavaliere et al., 2013] compared to gaseous flames, with strong attachment to the bluff body. OH presence is spatially distributed along the stoichiometric isolines as well as at richer mixture fractions close to the bluff body. Low levels of OH mass fraction are also observed along the entire spray region. As many droplets are not fully vaporised in the flame zone, they head downstream where temperatures are still warm enough for slower evaporation and oxidation, resulting in the extended low-mass fraction OH presence downstream. This has not been observed in experiments with OH-PLIF imaging; it is possibly a

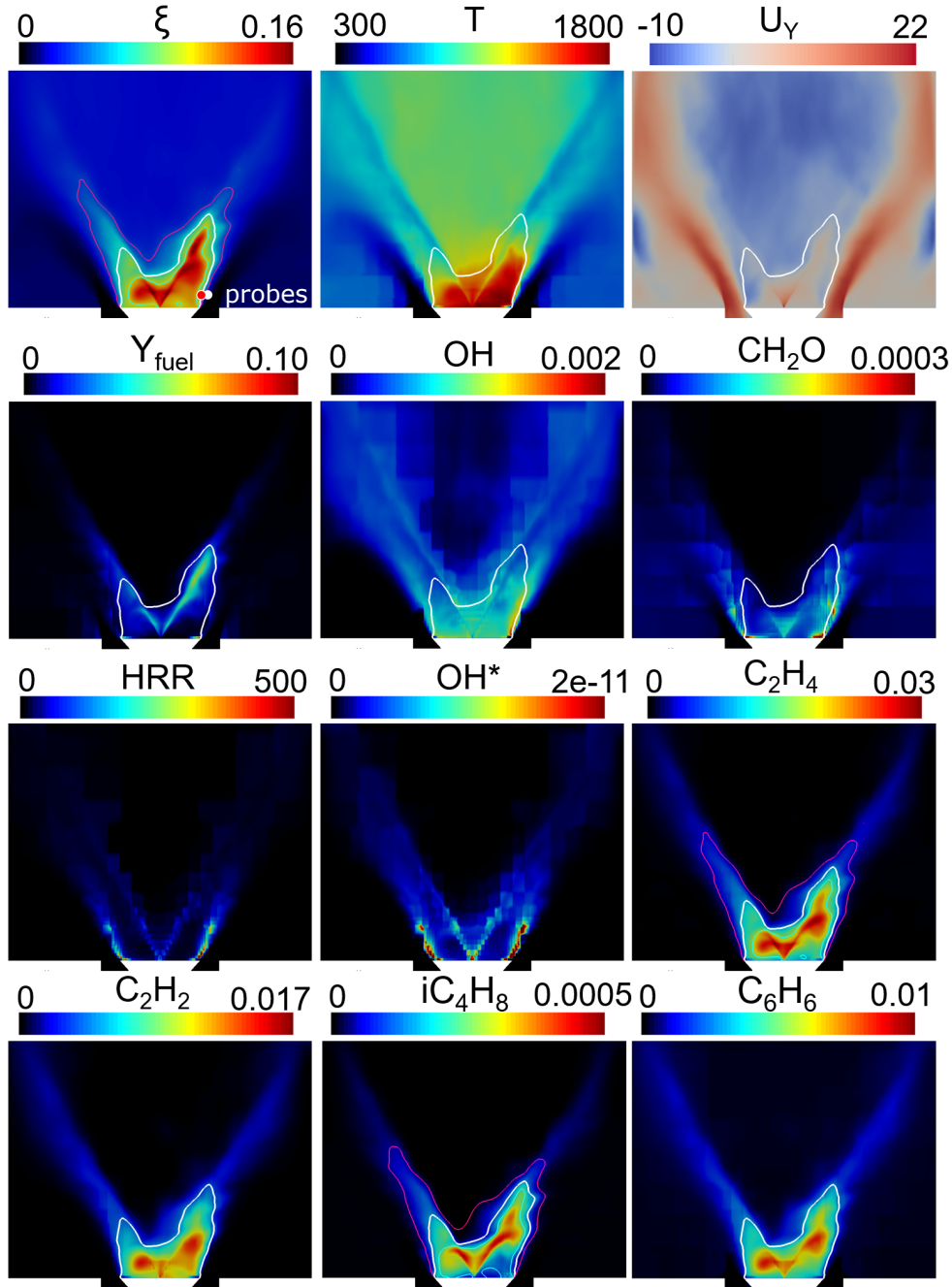


Fig. 5.6 Time-averaged filtered quantities from the stable $\dot{m}_f = 0.27$ g/s flame, including mixture fraction ξ , temperature (K), axial velocity (m/s), heat release rate (MW/m³), and various species mass fractions including OH*. White isolines indicate stoichiometric mixture fraction $\xi_{st} = 0.0637$, light green isolines correspond to rich mixture fraction $\xi = 0.1$ and pink isolines correspond to lean mixture fraction $\xi = 0.03$. Q probe locations are indicated along the air-shear layer with dots in the ξ field. Domain window is 0.095 m x 0.075 m.

computational artefact from the HyChem lumped pyrolysis technique. There is no OH presence in the lower corners of the chamber.

CH₂O does not exist in the recirculation zone, rather it peaks near to the stoichiometric isolines and the air-shear layer, where it is produced by incomplete combustion reactions. Some amount of CH₂O collects in the corners of the chamber, where temperatures are low (400-800 K) and there is no OH mass fraction present. Once convected to these corners the CH₂O remains there, trapped by the fluid motion of the side recirculation zones.

Regions of high parent fuel mass fraction correlate to regions of high mixture fraction along the spray. The gaseous fuel mass fraction acts as a heat sink and quenches parts of the flame, visible in the temperature and OH fields. Pyrolysis products such as C₂H₄, C₆H₆ and iC₄H₈ are all primarily located in fuel-rich regions within the stoichiometric isolines, although iC₄H₈ has less presence close to the bluff body. There is some residual presence of these pyrolysis products downstream of the flame following the evaporating droplets, similar to OH mass fraction. Shock tube experiments using Jet-A in Han et al. [2019] showed that at temperatures below 1400 K, C₂H₄ is the dominant pyrolysis product powering the flame. At temperatures above 1400 K, C₂H₄ breaks down to C₂H₂, which then dominates as the main fuel sustaining combustion. This can be seen in Fig. 5.6, where peak C₂H₂ occurs closer to the bluff body in the very high temperature regions, whereas C₂H₂ peaks higher up, closer to the spray.

The HyChem mechanism includes reactions for OH*, which can provide another reference for comparison between heat release rate from simulation and OH* signals from experiments. The heat release rate and OH* results show that reactions occur with highest intensity along the air shear layer off the edges of the bluff body. The HRR along the spray is considerably lower in proportion to the OH* signal, and significantly lower than that observed in the experimental results in Fig. 5.1. It may be that OH* signal perhaps overestimates the HRR along the spray cone.

5.3 Instantaneous LES-CMC results

5.3.1 3D stoichiometric isosurfaces

The flame is visualised above the bluff body and annulus in three-dimensional space in Fig. 5.7 using the stoichiometric mixture fraction ($\xi_{st} = 0.0637$) isosurface coloured with various quantities. The isosurface corresponds to $t = 0$ ms in Figs. 5.3 and 5.4. Compared to the LES-CMC spray flame simulation of ethanol [Giusti & Mastorakos,

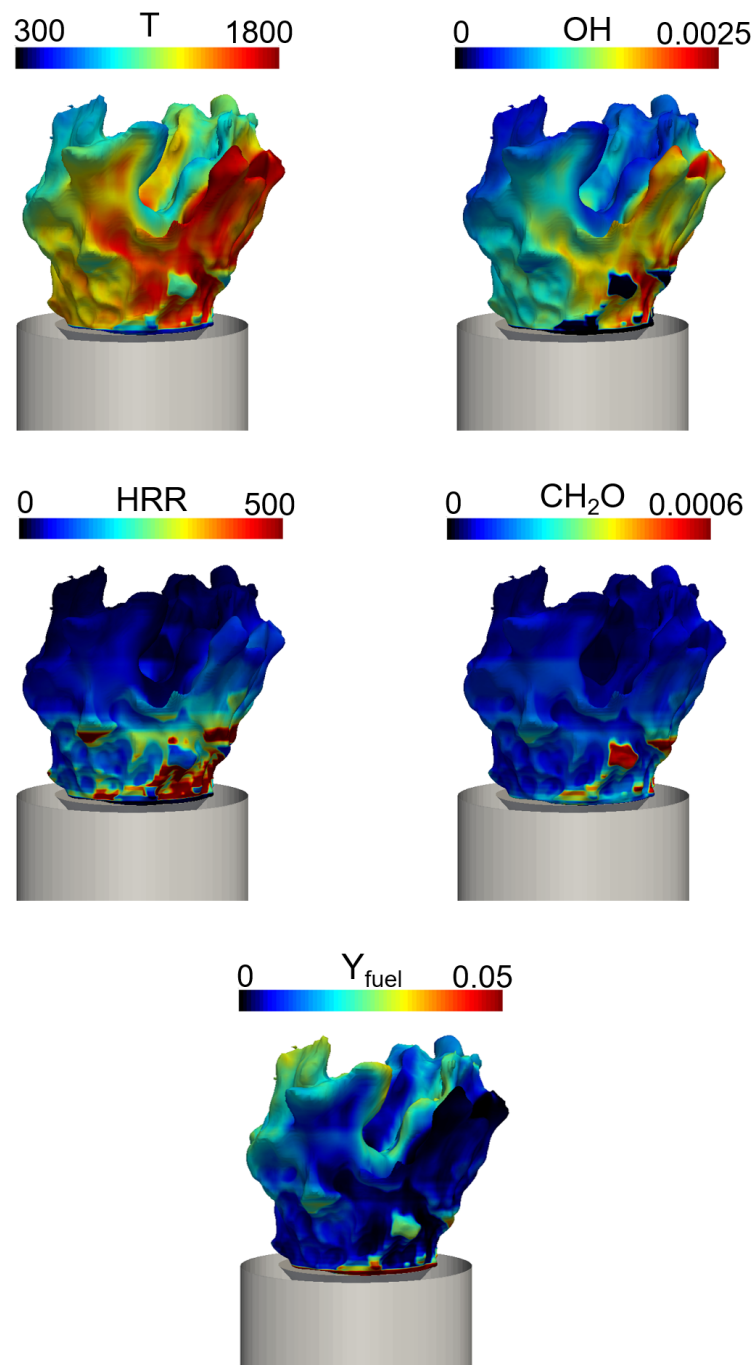


Fig. 5.7 3D ξ_{st} instantaneous isocontours of unconditional temperature (K), OH mass fraction, heat release rate (MW/m³), formaldehyde (CH_2O) mass fraction, and fuel mass fraction from the stable $\dot{m}_f = 0.27$ g/s flame.

2017], the Jet-A flame is much smaller in size and constrained between the annulus air of the shear layer and the bluff body edges. This is most likely due to the lower volatility of kerosene and heavy hydrocarbon flames. Dodecane and n-decane flames in [Yuan et al., 2018] were similarly constrained in size and location compared to n-heptane and ethanol.

Much of the isosurface is burning, with temperatures greater than 1600 K and OH mass fractions of 0.002 or higher. These regions correspond to low quantities of CH_2O and fuel mass fraction. However there are some small pockets along the isosurface where negligible OH is observed, and in these areas CH_2O and fuel mass fraction presences are significantly stronger. These regions indicate the presence of local extinctions in the stable burning flame.

5.3.2 Stoichiometric isosurface-averaged quantities

Using the stoichiometric isosurfaces shown in the previous section, quantities of interest are integrated across the surface area for every time solution. The resulting values are divided by the initial isosurface area to track how the surface-averaged quantities change in relation to the first instance over time. Surface-averaged quantities for the stable Jet-A flame are shown in Fig. 5.8. The OH mass fraction and temperature in Fig. 5.8a are conditional unfiltered quantities exported directly from CMC calculations and averaged over the stoichiometric isosurface, while Fig. 5.8b shows unconditional LES-filtered mass fractions averaged over the stoichiometric isosurface.

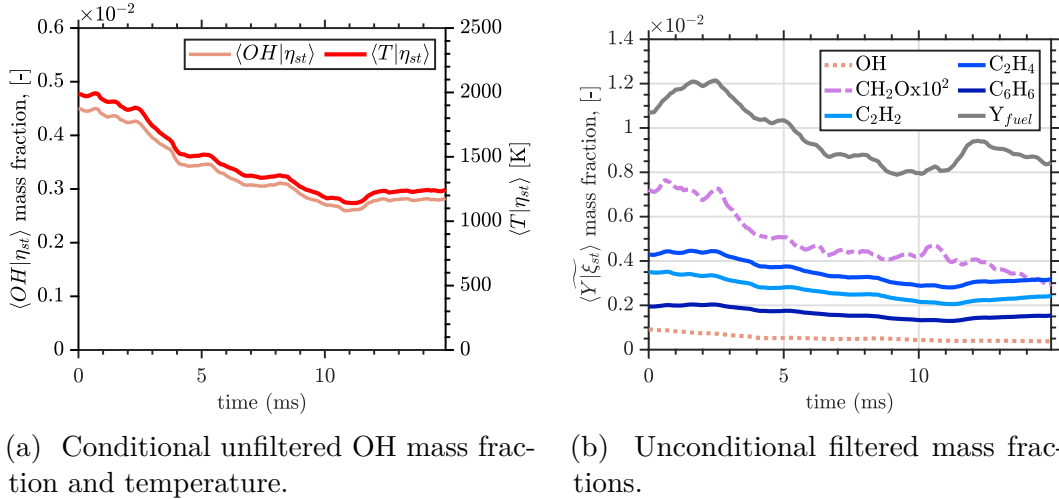


Fig. 5.8 Surface-averaged quantities of the stable condition $\dot{m}_f = 0.27$ g/s flame. The averaging is performed for each time instant based on the samples on the filtered $\xi_{st} = 0.0637$ isosurface.

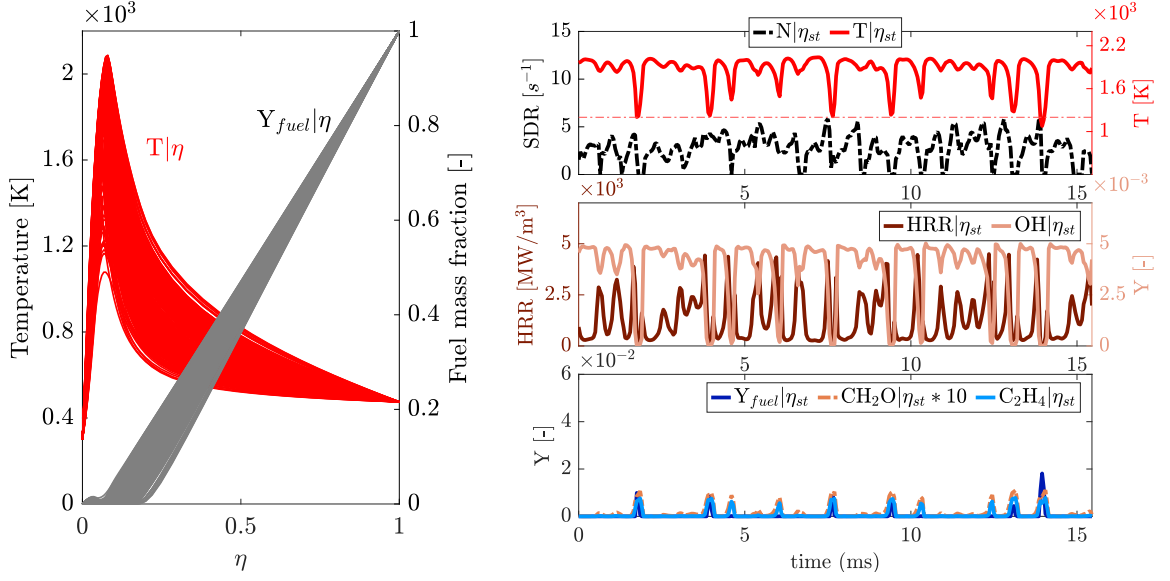
The temperature averaged across the entire isosurface in Fig. 5.8a is initially that of a hotly burning flame, but as the stable flame burns continuously there is a decrease in temperature and OH mass fraction. Certain parts of the isosurface are still experiencing temperatures of a burning flame, however there are significant parts of the $\xi_{st} = 0.0637$ surface which may be experiencing quenching or local extinctions, causing the average isosurface temperature to be relatively low. Intermediate species are shown over the same period of time in Fig. 5.8b. All the quantities decrease to some degree due to the corresponding reduction in temperature, but some species such as that of ethylene, acetylene and benzene mass fractions as well as the gaseous fuel increase after 11 ms.

5.3.3 Q probes: tracking extinctions in mixture fraction space

Moving from resolved scale to subgrid scale, the flame is analysed in mixture fraction space, denoted with η , directly from the CMC combustion equations. Q probes are used to track conditional species mass fractions, temperature, heat release rate and scalar dissipation rate (SDR) at predefined CMC cells over time. The probe results in Fig. 5.9 are located along the flame and air shear layer boundary at a radius of 14 mm and height of 4 mm above the bluff body, whereas those in Fig. 5.10 are located radially slightly inward at 13 mm, the same height above the bluff body. The Q probe locations are shown in the mixture fraction field in Fig. 5.6.

The cell along the air shear layer in Fig. 5.9 experiences a notable amount of intermittency and some very brief extinguishing of the flamelet. The temperature below which the flame is considered extinguished was determined from preliminary 0D-CMC simulations to be 1200 K, which is marked as a dash-dotted red line in the time series plots. This value was determined using the same methodology as in Zhang et al. [2015], using 70% of the temperature value in the solution prior to extinction. The range of states in the cell probe are expressed in mixture fraction space in Fig. 5.9a, with temperature peaks occasionally dropping below 1200 K and non-zero fuel mass fraction being present at $\eta_{st} = 0.0637$. These states at the low end of the temperature range are local extinction events. When temperature drops significantly, there is a corresponding drop in OH mass fraction and spikes in heat release rate, CH_2O , C_2H_4 and fuel mass fractions.

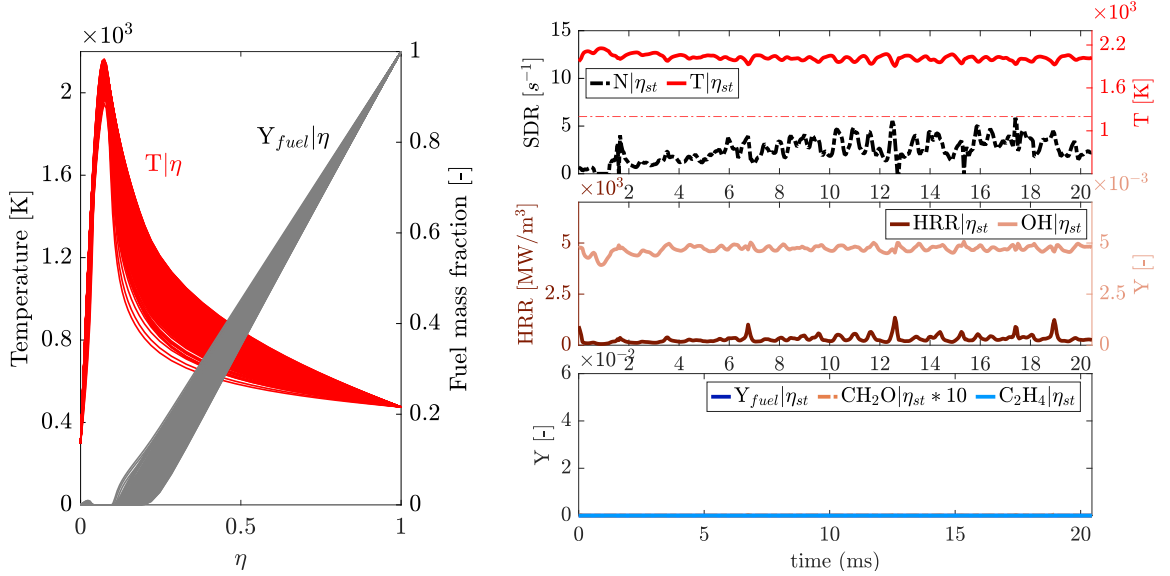
The cell in Fig. 5.10 just one millimetre closer to the centre of the bluff body experiences very different conditions, evident in Fig. 5.10a by the lack of spread in the temperature and fuel distributions at η_{st} . This cell is far enough from the air shear layer to not experience any local extinctions and to consistently experience fully burning states, although there are certainly still some fluctuations in the scalar dissipation rate



(a) Distributions of conditional filtered temperature and fuel mass fraction at many time instances in mixture fraction space

(b) Time series showing scalar dissipation rate N (s^{-1}), temperature (K), heat release rate (MW/m 3), OH, fuel, CH_2O and C_2H_4 mass fractions conditioned on stoichiometry

Fig. 5.9 Distributions of conditional quantities for a Q probe along the flame/air shear layer boundary in the stable $\dot{m}_f = 0.27$ g/s flame, $r/D = 0.56$, $y/D = 0.16$.



(a) Distributions of conditional filtered temperature and fuel mass fraction at many time instances in mixture fraction space

(b) Time series showing scalar dissipation rate N (s^{-1}), temperature (K), heat release rate (MW/m 3), OH, fuel, CH_2O and C_2H_4 mass fractions conditioned on stoichiometry

Fig. 5.10 Distributions of conditional quantities for a Q probe along the flame/air shear layer boundary in the stable $\dot{m}_f = 0.27$ g/s flame, $r/D = 0.52$, $y/D = 0.16$.

in Fig. 5.10b. There is a notable overall increase in the scalar dissipation rate over time, however the values are far from the critical scalar dissipation rate $N_{st,cr} \approx 25 \text{ s}^{-1}$ determined from the 0D-CMC extinction results discussed in Chapter 4 Fig. 4.14.

Along the air shear layer, the scalar dissipation rate in Fig. 5.9b reaches marginally larger values compared to the cell in Fig. 5.10b. The actual value of $N|\eta_{st}$ does not seem to cause local extinctions in this stable flame, however the gradient of change in $N|\eta_{st}$ certainly does. There are many more instances of sudden steep changes in the scalar dissipation rate in Fig. 5.9b, many times it drops to about zero. These instances can be correlated with the frequent drops in temperature and OH mass fraction. Scalar dissipation rate and changes in micromixing do have considerable effects on the flame, however as values are not reaching the critical extinction dissipation rate, this leaves room for other phenomena to be potential contributors to the extinguishing of spray flames.

5.3.4 Species markers of heat release rate (CH, $\text{CH}_2\text{O} \times \text{OH}$)

In McManus et al. [2020] recent experimental advancements in characterising liquid-fuel flame topology have been made using novel CH-PLIF imaging techniques. The CH radical has been identified as a useful marker for local extinctions and has been explored numerically in 0D simulations of methane and a kerosene surrogate in Paxton et al. [2019]. Using the detailed HyChem Jet-A mechanism with LES-CMC in this work allows for some additional analysis of the CH radical in the context of kerosene spray flames which may be useful for the experimentalist.

Results from the same probe in Fig. 5.9 are displayed in Fig. 5.11, comparing heat release rate to CH mass fraction and $\text{CH}_2\text{O} \times \text{OH}$ signal. The pixel by pixel products of CH_2O and OH signals is an accepted experimental technique to mark regions of peak heat release rate along the flame front [Kariuki et al., 2015; Yuan et al., 2015]. OH radical is a useful marker for the flame front, however particularly in non-premixed flames OH can be present in wider regions of the flame front than the CH radical due to its comparatively long lifetime, whereas CH has a relatively thin profile and rapidly decays [Grisch & Orain, 2009]. CH may provide a more definitive marker for the location of the flame front especially when large unsteady flame curvature is concerned.

The LES-CMC results of conditional quantities in Fig. 5.11 appear to corroborate the claims that CH can provide a good indication of the location of heat release rate and corresponding flame extinction behaviour in the context of Jet-A non-premixed spray flames. The CH mass fraction matches both HRR and $\text{CH}_2\text{O} \times \text{OH}$ signal fluctuations well, although the CH radical on its own does not peak quite as strongly during local

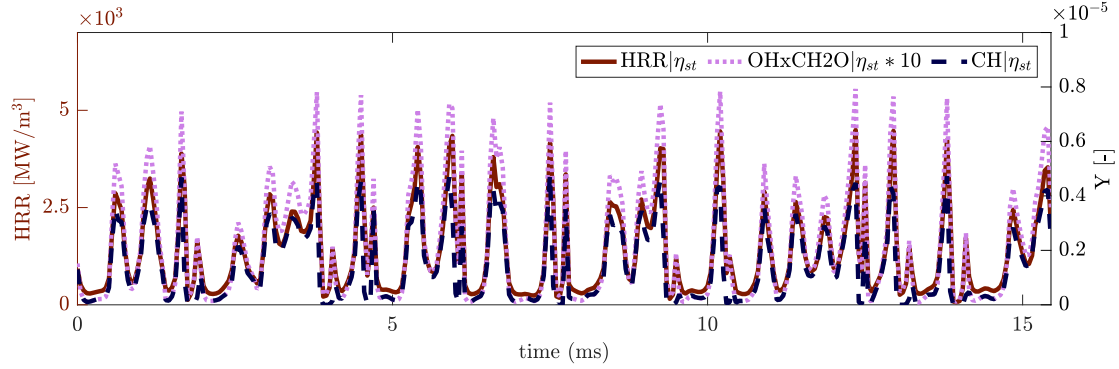


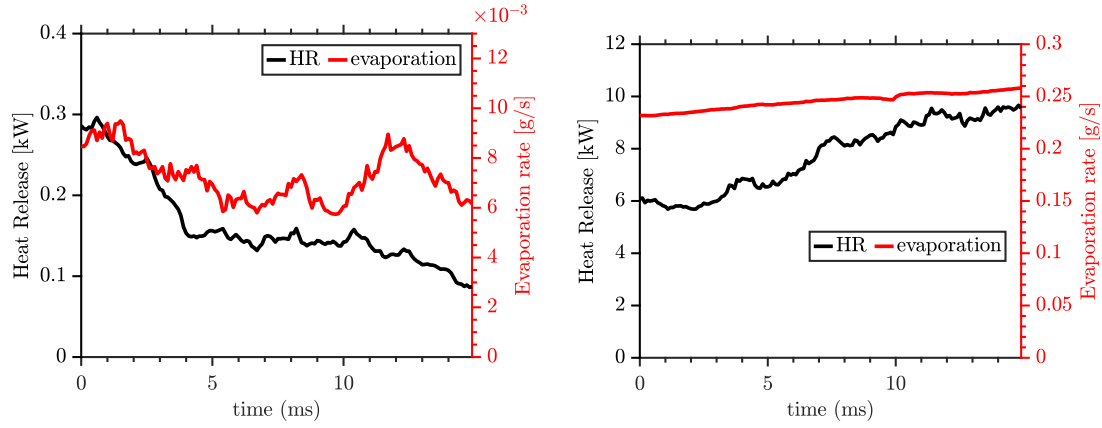
Fig. 5.11 Time series showing filtered heat release rate (MW/m^3), CH mass fraction, and $\text{CH}_2\text{O} \times \text{OH}$ signal conditioned on stoichiometry, $r/D = 0.56$, $y/D = 0.16$.

extinctions. Multiplying the CH_2O signal with CH instead of OH could give a more refined location of the flame front as well as accurate indications of instances of local extinction.

5.3.5 Heat release and evaporation rate

The volume-integrated heat release (HR) and evaporation rate from 3D cells located along the ξ_{st} isosurface threshold is shown in Fig. 5.12a whereas the volume integrated heat release and evaporation from the whole chamber volume is in Fig. 5.12b. Looking at the global evaporation rate in Fig. 5.12b, it reaches about 93% of the injected fuel mass flow rate. This indicates that about 7% of droplets are not fully vaporised even in a stable kerosene flame far from blow-off air velocity conditions. Global heat release in the chamber, which is strongly dependent on effective vaporisation of the fuel, ranges from 55% to 82% of the ideal heat of combustion for this case. Such large fluctuations of heat release were also observed in Zhang & Mastorakos [2016] in stable LES-CMC simulations of non-premixed methane flames.

The local heat release and evaporation rate along the stoichiometric mixture fraction isosurface in Fig. 5.12a is a bit more variable, especially the vaporisation rate. The heat release in the stoichiometric region experiences an initial sharp decrease up to about 4 ms, then levels out until after 10 ms have passed, after which heat release decreases further. Local heat release and evaporation are affected much more by the strength of the cold inlet air, which by reducing temperatures can reduce the the evaporation rate. The evaporation rate in the stoichiometric region appears to be overall stable.



(a) Integrated from cell volumes along the stoichiometric ($\xi_{st} = 0.0637$) isosurface.

(b) Integrated over entire chamber volume.

Fig. 5.12 Heat release (kW) and evaporation rate (g/s) for flame zone (left) and entire chamber volume (right)

5.4 Conclusions

The results presented in this section characterise the stable Jet-A flame modelled using LES-CMC and the detailed HyChem mechanism. The conditions are: $\dot{m}_f = 0.27$ g/s and $U_b = 0.74U_{BO,exp} = 15.9$ m/s, corresponding to stable experimental conditions. The simulation is compared against experimental time-averaged inverse Abel-transformed OH* and simultaneous instantaneous OH-PLIF and Mie scattering images.

The LES-CMC qualitative results compare decently against the experiments in the flame size and shape, however there are some significant discrepancies in the location of peak heat release rate, with the highest intensity observed along the shear layer in the simulation rather than near the spray cone in experiments. More attachment to the bluff body is also experienced in the simulation. These discrepancies have been observed in other LES of bluff body swirl spray flames. One reason for the discrepancy may be caused by inadequate near-wall modelling close to the bluff body surface. Another reason may be due to the nature of detailed chemical mechanisms, as previous studies with spray flames using LES-CMC and one-step chemistry were able to obtain good qualitative comparisons with high HRR along the spray at stable conditions [Giusti & Mastorakos, 2016; Tyliszczak et al., 2014]. The simulation may be exhibiting behaviour indicative of a flame at a near LBO condition rather than a low-air velocity stable flame. This may be due to aspects of the liquid fuel properties or the spray injection speed. This baseline case flame requires further validation against

experiments and testing of sensitivity to parameters such as the spray/evaporation modelling before strong confidence can be placed in these results.

The simulation results are analysed using time-averages of properties of interest, including mixture fraction, temperature, heat release rate, and various intermediate and pyrolysis species mass fractions. Local extinctions are identified along the 3D instantaneous stoichiometric mixture fraction isosurfaces, and brief extinction events are observed in conditional space. These conditional space extinctions correspond to low values of scalar dissipation rate well below the quenching value. These brief extinctions are likely caused by large fluctuations in the SDR, as well as convection from nearby inert CMC cells. CH is discussed in the context of local extinctions in mixture fraction space as a potential contender for marking heat release rate in experiments with increased accuracy over OH, although using $\text{CH} \times \text{CH}_2\text{O}$ is recommended over just CH.

Global and local (along stoichiometry) volume-integrated heat release and evaporation over time are discussed. When integrating over the volume of the whole chamber (global) heat release and evaporation are steadily increasing, whereas when integrated using the cell volumes along the stoichiometric isosurface (local) heat release and evaporation decrease and fluctuate, respectively. The global evaporation rate in the chamber is 93% of the injected fuel mass flow rate, indicating the presence of unburnt droplets. The global heat release rate of the flame reaches 82% of the ideal heat of combustion for these conditions. The flame overall exhibits stable characteristics, and is used to start the blow-off simulations in the next chapter.

Chapter 6

Lean Blow-off of Kerosene Swirl Spray Flames

This chapter builds on the work of Chapter 5. Using the stable LES-CMC solution, the air mass flow rate entering the inlet annulus of the bluff body swirl-stabilised spray burner is increased to induce lean blow-off. The stable solution is used to initialize two more simulations at different fuel mass flow rates, so as to have a set of three blow-off simulations at matching fuel flow rates to the middle three experimental Jet-A blow-off curve conditions presented in Allison et al. [2018]. The LES-CMC approach, which has had demonstrated success capturing local and global extinction for gaseous [Zhang, 2015; Zhang & Mastorakos, 2016] and spray flames [Giusti & Mastorakos, 2016, 2017], is used here with Lagrangian spray modelling and a detailed Hybrid Chemistry mechanism for Jet-A [Wang et al., 2018a; Xu et al., 2018]. The extinction transients of the three LBO simulations are disseminated in this chapter.

The objectives are: (i) to predict lean blow-off phenomena such as local extinction and fuel starvation, (ii) to investigate the flame structure, species and the interaction between turbulence and evaporation during global extinction, and (iii) to simulate the experimental blow-off curve of Jet-A spray flames. Through simulation of the blow-off curve, key physical phenomena can be identified which contribute to the blow-off of spray flames, which will help guide future engine designers in making spray combustion more resistant to flame blow-off.

The three final air bulk velocities causing LBO of the flames are compared with the experimental values. Methods for determining blow-off and duration of the transient are discussed, using both heat release and temperature as metrics. Blow-off times are reported. Local extinctions are identified in mixture fraction space, and the extinguished fraction of the flame stoichiometric isosurfaces is presented, quantified using metrics

generated from a 0D-CMC near-extinction solution in Chapter 4. Instantaneous images of the flame stoichiometric isosurfaces as they undergo the extinction transient are shown, and the relationships between fuel starvation, species, and temperature is explored to gain a deeper understanding of the physical mechanisms causing lean blow-off of spray flames. Unconditional quantities of species and temperature are presented in spatial visualizations unless explicitly stated otherwise.

6.1 Blow-off curve

After increasing the bulk air velocities to the experimental values via roughly 10% increases in air velocity, the simulations underwent the blow-off transient. In the three cases, the air velocity was increased beyond the experimental values to ensure blow-off within a feasible simulation time, to bulk air velocities 5–20% higher than those observed in experiments. The air velocity increases are tabulated in Table 3.9. Final U_b values for the LES-CMC simulations are recorded in Table 6.1 and graphical comparison with the experimental blow-off curve is in Fig. 6.1. The instance of blow-off was assessed using a reduction in heat release rate by 80% in the stoichiometric mixture region, which is discussed in more detail in the next section.

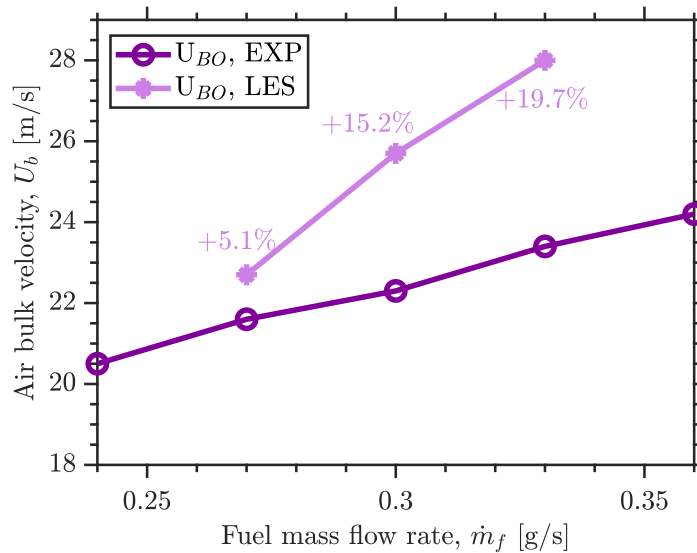


Fig. 6.1 LBO curve comparing LES-CMC blow-off bulk air velocities with experimental values for Jet-A from Allison et al. [2018].

The results of the simulated kerosene blow-off occurring within 5–20% of the experimental velocity value is in line with results in other studies for both gaseous and

6.2 Determining LBO: temperature, heat release, and evaporation rate

Table 6.1 Simulation fuel mass flow rates ($\dot{m}_f$), final blow-off bulk velocities (U_b), overall equivalence ratio ($\phi_{overall}$), and comparison with experimental blow-off velocities.

$\dot{m}_f$ (g/s)	Case	U_b (m/s)	$\phi_{overall}$	$U_b/U_{BO,exp}$
0.27	Stable	15.9	0.37	74%
0.30	Stable	18.6	0.35	83%
0.33	Stable	22.1	0.32	93%
0.27	Blow-off	22.7	0.26	105%
0.30	Blow-off	25.7	0.25	115%
0.33	Blow-off	28.0	0.25	120%

liquid fuels. Simulation of the blow-off curve for non-premixed methane in Zhang & Mastorakos [2016] (reproduced in Fig. 2.1) using the same burner configuration was achieved within 25% of the experimental air velocity values. Blow-off of an n-heptane spray flame using LEC-CMC with one-step chemistry in Tylliszczak et al. [2014] was obtained at the exact experimental conditions. The Jet-A LBO simulations in Escalpez et al. [2017] using LES-FPV experienced blow-off at a global equivalence ratio 9.5% higher than the blow-off value recorded for corresponding experiments. These results were obtained by reducing the fuel flow rate however, rather than increasing the air velocity. A similar discrepancy in LES blow-off global equivalence ratio for Jet-A was found in Hasti et al. [2018], with a difference of about 6% lower than those recorded in experiments.

The results of the simulated kerosene blow-off occurring within 5–20% of the experimental value reflects decently on the capability of LES-CMC, although improvements could be made. The variability of the over-prediction of the experimental air velocity by the LES is primarily dependent on equivalence ratio of the stable simulation used to start the blow-off transient. As shown in Table 6.1, when the starting stable equivalence ratio is leaner, the blow-off transient becomes longer and a higher air velocity is needed to extinguish the flame.

6.2 Determining LBO: temperature, heat release, and evaporation rate

The blow-off transients in the flame zone are visualised quantitatively using conditional stoichiometric temperature averaged over the stoichiometric mixture fraction isosurface

area in Fig. 6.2 and using the volume integrated heat release rate (HR) from 3D cells located along the stoichiometric mixture fraction isosurface in Fig. 6.3a. Figure 6.2

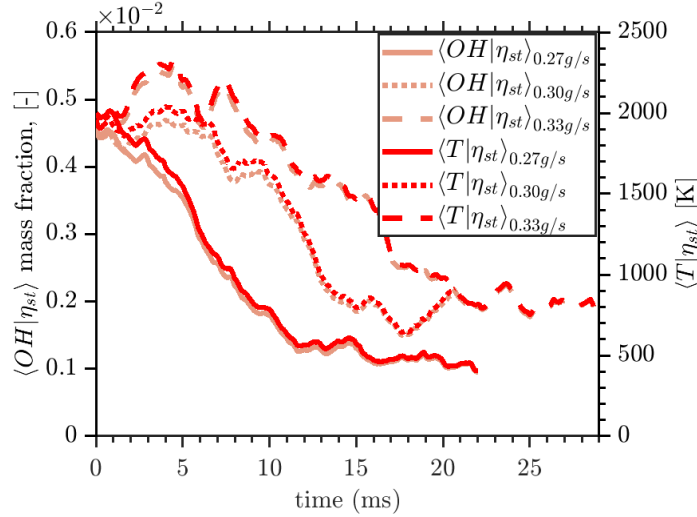
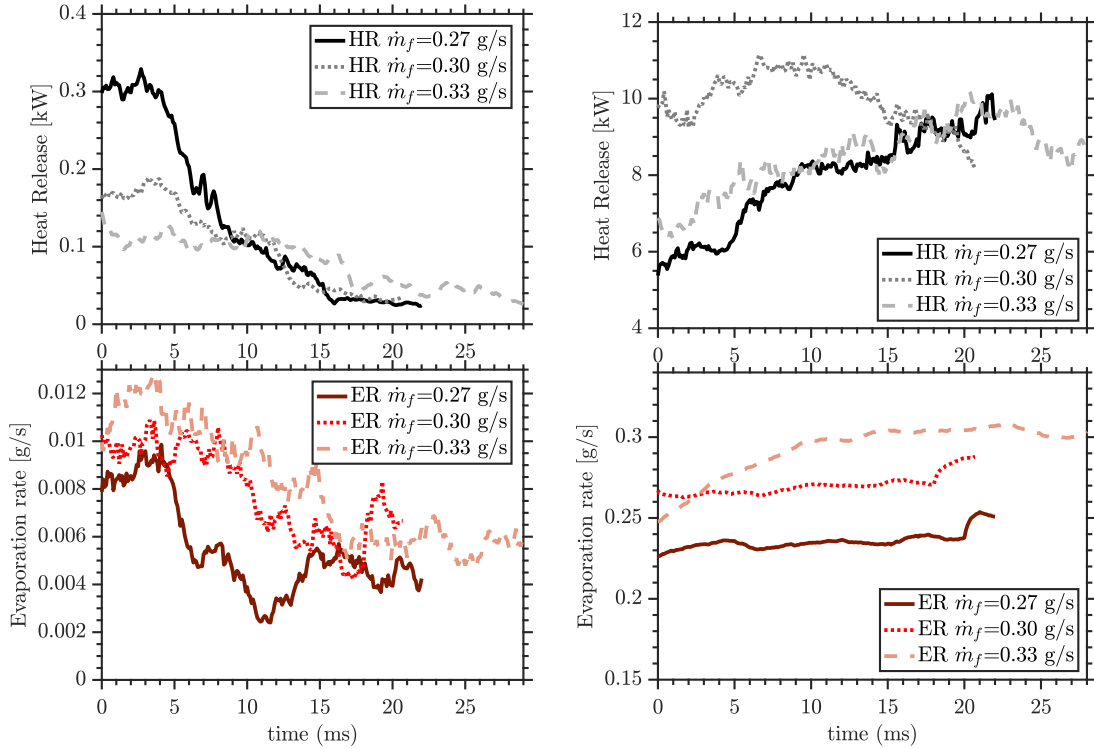


Fig. 6.2 Conditional OH mass fraction and temperature (K) averaged over the unconditional LES-resolved stoichiometric mixture fraction isosurface area ξ_{st} during LBO. $\xi_{st} = \eta_{st} = 0.0637$.

shows both the conditional stoichiometric isosurface-averaged temperature and OH mass fraction decrease fairly monotonically for the three cases, before levelling out to values indicative of an extinguished flame. The rates of decrease vary between the cases; the length of the blow-off transient appears to increase with increasing fuel mass flow rate.

Figure 6.3a shows the heat release and evaporation rate in the regions of stoichiometric mixture fraction for the three cases. The simulations in Fig. 6.3a experienced 89.5%, 80.3% and 81.2% reductions in heat release for $\dot{m}_f = 0.27$ g/s, 0.30 g/s and 0.33 g/s respectively. Reductions in the heat release in the flame stoichiometric region are linked to the evaporation rate, shown in the bottom of Fig. 6.3a. As evaporation rate decreases over time, so does heat release. However, even if after a certain point evaporation rate increases again, it does not necessarily mean the heat release will increase, as seen in the $\dot{m}_f = 0.27$ g/s flame. Evaporation rate at stoichiometry is higher at larger fuel mass flow rates. The physical understanding for the cause of LBO in non-premixed flames is that local extinctions, or holes, in the flame surface increase in size and duration until the flame is extinguished globally. In Foale et al. [2021] local extinctions of the $\dot{m}_f = 0.27$ g/s flame were identified to increase in number during LBO, however their influence did not appear to be the sole reason for blow-off

6.2 Determining LBO: temperature, heat release, and evaporation rate



(a) Integrated using cell volumes along the stoichiometric ($\xi_{st} = 0.0637$) isosurface. (b) Integrated over entire chamber volume.

Fig. 6.3 Volume-integrated heat release (kW) (top) and evaporation rate (g/s) (bottom) for flame zone (left) and entire chamber volume (right)

of the flame, as the flame isosurface shrank downward and inward toward the centre of the bluff body. Decreased presences of gaseous fuel and pyrolysis products were observed during blow-off. In Fig. 6.3a the evaporation rate in the flame zone decreases considerably, supporting the idea proposed in Cavaliere et al. [2013] that fuel starvation from reduced temperatures and evaporation is another cause for the blow-off of spray flames.

The heat release and evaporation during the blow-off transients behave quite differently taking the whole combustion chamber volume into account, as seen in Fig. 6.3b. The mean evaporation rates in the chamber range between 87-90% of the injected fuel mass flow rates, indicating the presence of unburnt droplets in the system. Despite similar proportions of evaporated fuel in the three cases, the $\dot{m}_f = 0.30$ g/s chamber displays heat release close to the ideal heat of combustion for kerosene (≈ 11 kW) early on in the blow-off transient, while the other two cases release significantly less power initially. However as time progresses, the other two cases interestingly increase

in power during most of the transient, while the heat release of the $\dot{m}_f = 0.30$ g/s case decreases after about 10 ms. This increasing heat release behaviour can be attributed to increased strain rates and the presence of droplets downstream in the chamber, which continue to vaporise in the warm temperatures of the recirculation zone, producing gaseous fuel that reacts with increased quantities of fresh oxidants from the higher air mass flow rates.

It is recommended for future simulations to enact stronger step increases than 5% greater than experimental U_{BO} values, as it appears the heat release rate in simulations which experienced more gradual increments in velocity responded less quickly to the increase in air flow.

6.3 Blow-off time

Blow-off times for the duration of the extinction transients depending on which criterion is used are recorded in Table 6.2. Using an extinction temperature threshold of 1200 K, determined using 70% of the temperature value in the 0D-CMC solution prior to extinction (see Fig. 4.14 and accompanying discussion for details), Fig. 6.2 shows the flame blow-off event lasts between about 7 to 17 ms for the three mass flow rates.

Another way to estimate the blow-off transient time is through the change in heat release in the flame region. Using a threshold of 80% reduction in heat release to signify blow-off of the flame, the blow-off times from the data in Fig. 6.3a are 14.8 ms, 17.9 ms and 28.6 ms. These blow-off transient durations all fall within the expected range compared with n-decane and n-dodecane spray flame experiment blow-off times in Yuan et al. [2018], where transient durations ranged between 10 to 30 ms.

Table 6.2 Blow-off transient durations for the three flames. The columns are: simulation fuel mass flow rates ($\dot{m}_f$), blow-off duration based on temperature threshold $\tau_{ext,T}$, and LBO time based on heat release threshold $\tau_{ext,HR}$. These times fall in the expected range compared to experiments with non-volatile fuels [Yuan et al., 2018]. The $\tau_{ext,HR}$ values are used to quantify the blow-off transient of the flames for the remainder of the chapter.

$\dot{m}_f$ (g/s)	$\tau_{ext,T}$ (ms)	$\tau_{ext,HR}$ (ms)
0.27	7	14.8
0.30	12	17.9
0.33	17	28.6

6.4 Surface-averaged species over time

Surface-averaged species mass fractions over time for the three flames are shown in Fig. 6.4. Filtered species mass fractions of interest are integrated across the ξ_{st} isosurface area and divided by initial isosurface area Σ_0 (which can be seen in Fig. 6.10) for every time solution in the same manner as Fig. 5.8. All the species mass fractions decrease significantly in the stoichiometric region during blow-off in the three flames. Most of the species decrease gradually, however the fuel vapour mass fraction Y_{fuel} undergoes considerably drastic changes. Interestingly, the fuel mass fraction for the

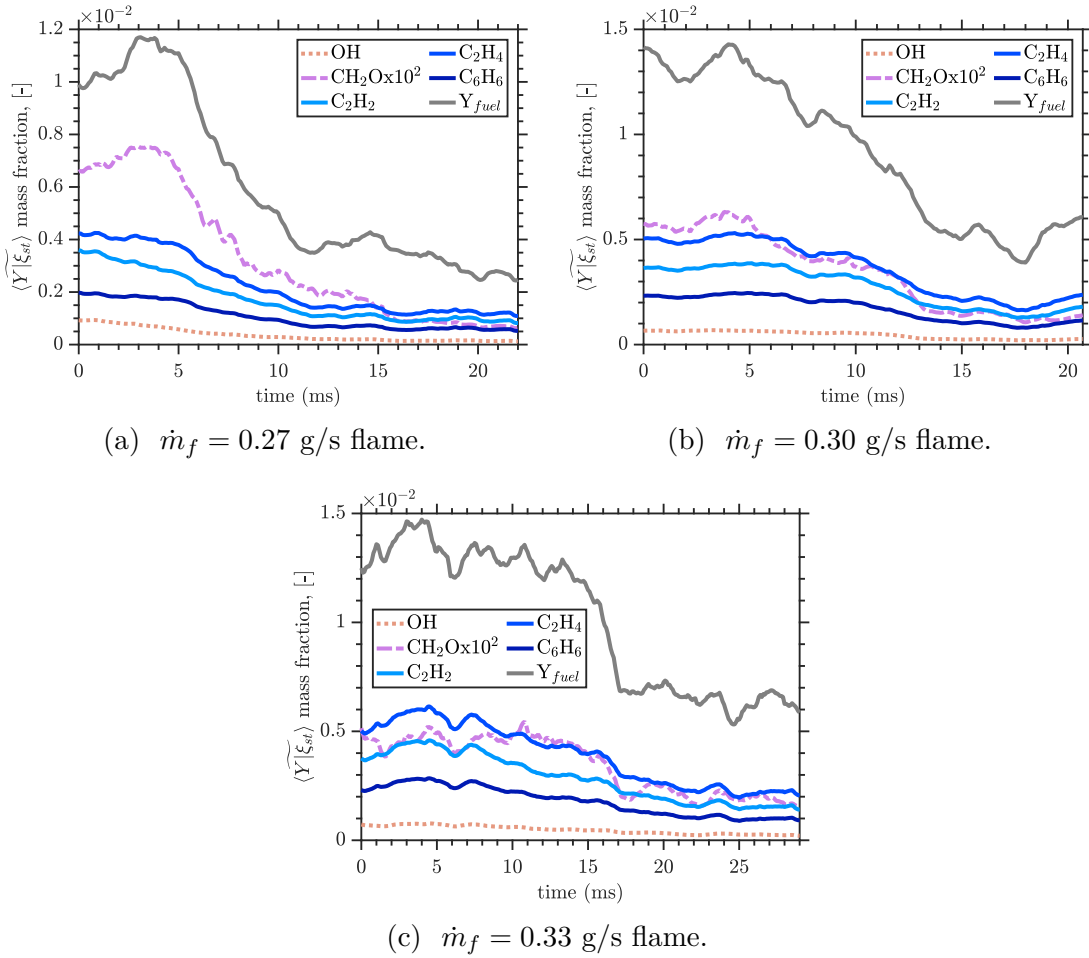


Fig. 6.4 Surface-averaged mass fractions during LBO. The averaging is performed for each time instant based on the samples on the filtered ξ_{st} iso-surfaces.

$\dot{m}_f = 0.30$ g/s flame is greater at the start than the $\dot{m}_f = 0.33$ g/s, although it begins to decrease earlier than the 0.33 g/s case. In Fig. 6.4a, Y_{fuel} increases for 5 ms due to the increased availability of fresh oxidants, but then falls steeply. U_b was increased

to $1.05U_{BO,exp}$ at $t = 8$ ms, however there is no discernible change from the slopes of the species due to this increase in air velocity. U_b for the $\dot{m}_f = 0.30$ g/s flame was increased to $1.15U_{BO,exp}$ at $t = 9$ ms, and this also did not make much of a discernible change. In the $\dot{m}_f = 0.33$ g/s flame, U_b was increased three times: to $1.05U_{BO,exp}$ at $t = 6$ ms, $1.10U_{BO,exp}$ at $t = 11$ ms, and $1.20U_{BO,exp}$ at $t = 25$ ms. The first and last increases in velocity do not appear associated with any change, but the increase at $t = 11$ ms perhaps contributed to the sudden steep drop off in Y_{fuel} in Fig. 6.4c.

The trends of the pyrolysis species C_2H_4 and C_6H_6 , as well as soot precursor C_2H_2 and incomplete combustion marker CH_2O follow the behaviour of Y_{fuel} fairly closely, typically levelling out after blow-off has occurred, although in Fig. 6.4b an up-tick is observed even after blow-off. The remaining fuel vapour mass fraction after blow-off increases with increasing fuel mass flow rate, as would be expected. As the mass flow rate was increased, the increased presence of fuel vapour likely contributed to the increasing length of time of the blow-off duration.

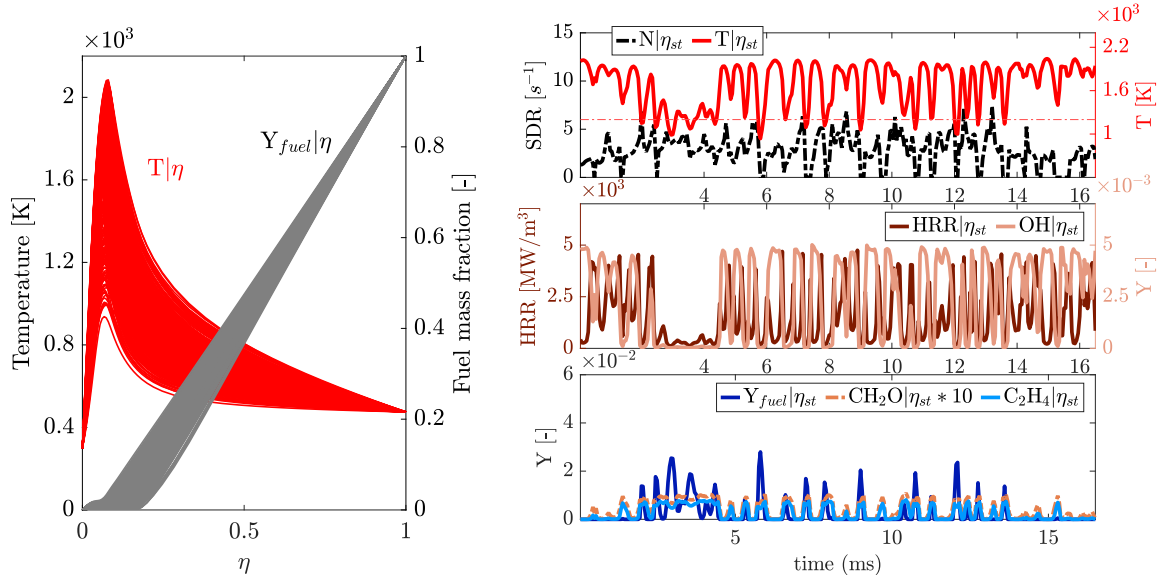
6.5 Q probes: extinction and reignition during LBO

Local extinctions of the $\dot{m}_f = 0.27$ g/s flame are analysed in conditional mixture fraction space, denoted with η , directly from the CMC combustion equations. Q probes were used to track species mass fractions, temperature, heat release rate and scalar dissipation rate at predefined CMC cells over time. The extinguished temperature, 1200 K, is marked as a dash-dotted red line. The probe results shown in Fig. 6.5 are located along the flame and air shear layer boundary (14 mm radially from the bluff body centre) and 4 mm above the bluff body, whereas those shown in Fig. 6.6 are located directly below at 3 mm above the bluff body. The probe in Fig. 6.5 is at the same location as the one in Fig. 5.9 analysed in Chapter 5 for the stable conditions flame. Figure 6.14 shows the probe locations.

Both probes experience a wide range of temperatures in η -space as well as unburned fuel present at $\eta_{st} = 0.0637$, demonstrating occurrences of fully burning and extinguished states at these two locations. The probe in Fig. 6.5a reaches overall higher temperatures, some peaking at over 2000 K, whereas in Fig. 6.6a that probe experiences a lower range of about 500 to 1900 K. The low range encompassing such low temperatures indicate the flame is strongly quenched at this point along the air shear layer.

In Fig. 6.5b, the time series showing quantities conditioned on stoichiometry display fully burning behaviour at the start, with high temperatures and OH mass fraction.

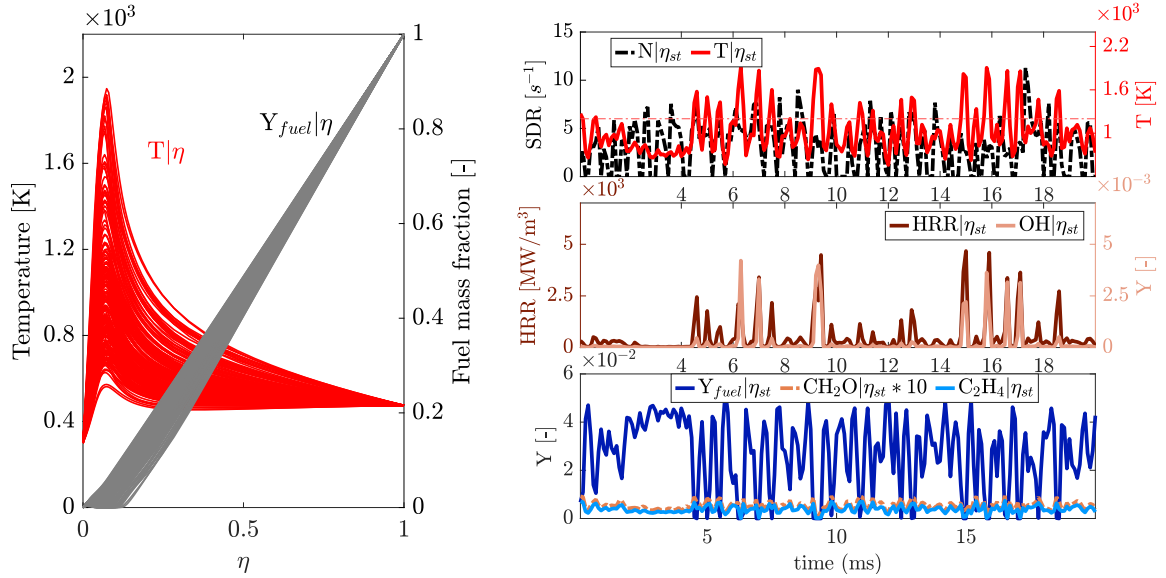
6.5 Q probes: extinction and reignition during LBO



(a) Distributions of conditional temperature and fuel mass fraction at many time instances in mixture fraction space

(b) Time series showing scalar dissipation rate N (s^{-1}), temperature (K), heat release rate (MW/m^3), OH, fuel, CH_2O and C_2H_4 mass fractions conditioned on stoichiometry

Fig. 6.5 Q probe along the flame/air shear layer boundary in the $\dot{m}_f = 0.27$ g/s flame during blow-off, $r/D = 0.56$, $y/D = 0.16$.



(a) Distributions of conditional temperature and fuel mass fraction at many time instances in mixture fraction space

(b) Time series showing scalar dissipation rate N (s^{-1}), temperature (K), heat release rate (MW/m^3), OH, fuel, CH_2O and C_2H_4 mass fractions conditioned on stoichiometry

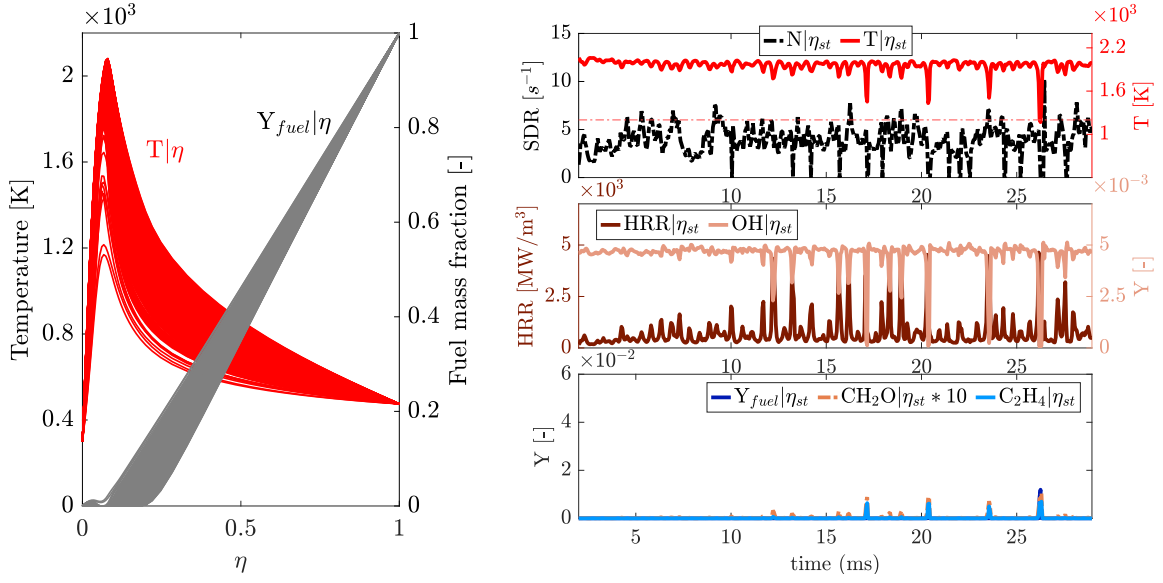
Fig. 6.6 Q probe along the flame/air shear layer boundary in the $\dot{m}_f = 0.27$ g/s flame during blow-off, $r/D = 0.56$, $y/D = 0.12$.

After the simulation air velocity was increased to $U_{BO,exp}$, we observe a local extinction occurring for nearly 2 ms starting at $t = 3$ ms, where OH mass fraction and heat releases rate drop to negligible quantities and temperature hovers around the extinguished threshold (indicated with a dashed horizontal line). The scalar dissipation rate during this event is relatively low and well below the $N_{st,cr}$ value of 25 s^{-1} . During this local extinction, peaks in unburnt fuel are evident and there is a constant presence of CH_2O and C_2H_4 . The mass fractions of formaldehyde and ethylene peak and then plateau during the extinction event, while the unburnt fuel mass fraction fluctuates to a much greater degree. After $t = 4$ ms, temperatures increase again to fully burning states, although interspersed with more frequent short extinction events, where temperature drops below the extinction threshold simultaneously as the scalar dissipation rate drops to zero. Probes above this one are observed to be fully burning, so this CMC cell's proximity to fully burning cells contributes to its ability to reignite, however with increased convection and scalar dissipation rate there is more intermittency observed as the flame experiences the transient fluctuating behaviour approaching blow-off.

In Fig. 6.6b, the cell is extinguished from the very beginning of initiating blow-off, coinciding with very intermittent and relatively high values of $N|\eta_{st}$. After the extinction event observed in the higher probe in Fig. 6.5b, the temperature in this probe too begins to experience higher peaks, as scalar dissipation does not drop to zero as regularly. As swirling air velocity is increased, pockets in physical space along the flame which are fully burning travel faster around the stoichiometric isosurface, passing nearby and interacting more frequently with regions more likely to be extinguished close to the bluff body. These interactions allow extinguished cells to be exposed to higher temperatures and increased presence of OH. Once OH is present, ethylene and formaldehyde mass fraction drop immediately as they are consumed momentarily before the temperature drops again.

Figures 6.7 and 6.8 show two probes from the $\dot{m}_f = 0.33 \text{ g/s}$ flame at radii of 13 and 14 mm respectively from the centre of the bluff body and at heights of 4 mm above the bluff body. The probe in Fig. 6.8 is at the same location as the probe for the $\dot{m}_f = 0.27 \text{ g/s}$ flame in Fig. 6.5. The Q probe locations are the same as those shown in Fig. 5.6. The temperature and fuel mass fraction in the probe shown in Fig. 6.7a indicate a reasonably well-burning flamelet, with only a few instances where the peak temperature drops below 1200 K. This probe sits just within the flame region, close to the air shear layer. The time series in Fig. 6.7b demonstrates the flame is burning very stably for the first 10 ms during LBO, but after this point dips in OH mass fraction begin to appear and the temperature begins to drop toward a quenched

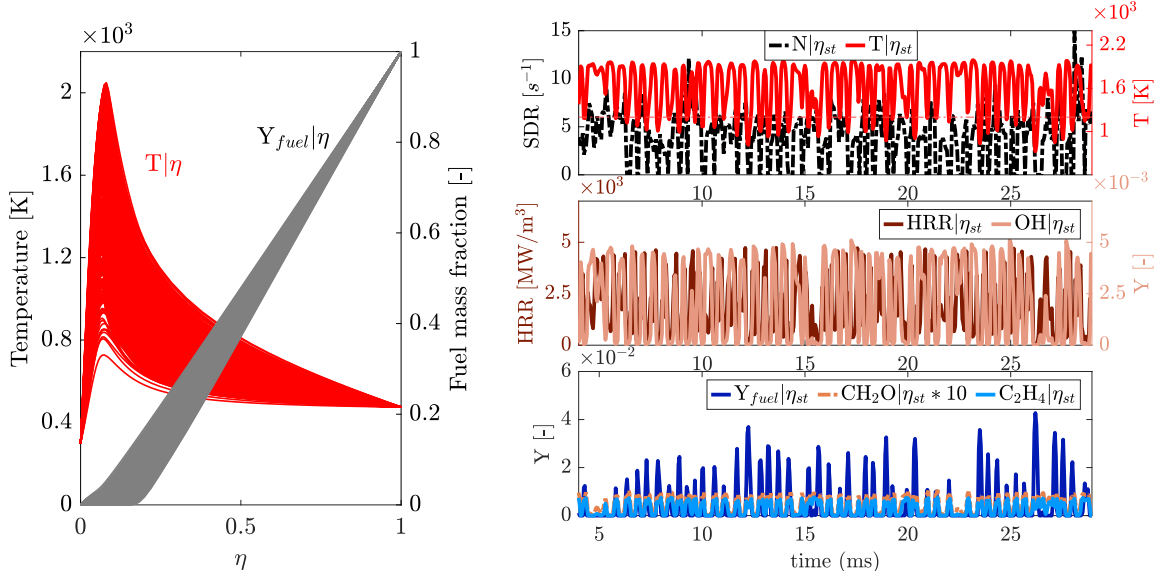
6.5 Q probes: extinction and reignition during LBO



(a) Distributions of conditional temperature and fuel mass fraction at many time instances in mixture fraction space

(b) Time series showing scalar dissipation rate N (s^{-1}), temperature (K), heat release rate (MW/m^3), OH, fuel, CH_2O and C_2H_4 mass fractions conditioned on stoichiometry

Fig. 6.7 Q probe along the flame/air shear layer boundary in the $\dot{m}_f = 0.33$ g/s flame, $r/D = 0.52$, $y/D = 0.16$.



(a) Distributions of conditional temperature and fuel mass fraction at many time instances in mixture fraction space

(b) Time series showing scalar dissipation rate N (s^{-1}), temperature (K), heat release rate (MW/m^3), OH, fuel, CH_2O and C_2H_4 mass fractions conditioned on stoichiometry

Fig. 6.8 Q probe along the flame/air shear layer boundary in the $\dot{m}_f = 0.33$ g/s flame, $r/D = 0.56$, $y/D = 0.16$.

state every 2 to 3 ms. This increase local extinction behaviour is likely caused by the increase in the bulk air velocity from $1.05U_{BO,exp}$ to $1.10U_{BO,exp}$ at $t = 11$ ms. Before this the SDR almost never dropped to negligible values, but after 11 ms the SDR displays increased instances of dropping to nothing. In the DNS study by Sripakagorn et al. [2004] fluctuations in the SDR were shown to contribute to local extinctions, which added to the understanding that local extinctions which led to global extinction of the flame were caused by the SDR reaching levels higher than the critical scalar dissipation rate $N_{st,cr}$. However, in Fig. 6.7b the scalar dissipation rate is still low overall, reaching only 10 s^{-1} at one point, 40% of the $N_{st,cr}$ determined from 0D-CMC calculations (see Fig. 4.14 and discussion for how $N_{st,cr}$ was calculated).

The probe in Fig. 6.8a is on the boundary of the flame and the air shear layer, resulting in a vast range of burning and extinguished instances. The time series in Fig. 6.8b shows the intermittency of the flame during the LBO transient. There are one or two instances of slightly longer local extinctions of 1 to 2 ms, however the majority are quite brief. The SDR in this CMC cell experiences higher peaks, such as the 15 s^{-1} one near the end of the blow-off transient, as well as many troughs.

In these probes tracking the conditional Q s from CMC we see some evidence of local extinctions during the blow-off transient. Brief extinctions occur more often with increasingly variable scalar dissipation rate, which is affected by the droplet evaporation rate. The SDR increases overall as fuel and air mass flow rates are increased, but still is well under the critical stoichiometric extinction SDR $N_{st,cr} \approx 25\text{ s}^{-1}$. Local extinctions increase in frequency and the burning states become more intermittent with short duration spikes, which matches the findings from experimental LBO studies of Jet-A spray flames in Muruganandam et al. [2004]. They attributed this increased intermittent behaviour to reductions in evaporation and mixing, causing spatial and temporal fluctuations in local fuel concentrations.

There are occasionally longer duration local extinctions (2 ms) observed in the Q probes, but in the end the probes are still returning to fully burning states rather than staying extinguished, even after the flame has fully blown-off. The extinguished cell in Fig. 6.6 actually began to see more frequent instances of fully burning conditions as time progressed, and long duration extinctions like the one seen in Fig. 6.5 were not observed again during the blow-off transient. The lack of fully extinguished Q probes during the blow-off transient is likely due to the values of $N|\eta_{st}$ remaining below the critical quenching rate. These simulation results support the notion that it is fuel starvation rather than increased local extinctions causing the extinction of the spray flames during LBO.

6.6 Extinguished fraction

In previous studies with non-premixed methane flames by Zhang & Mastorakos [2016] a method was developed to quantify the degree of extinction along the ξ_{st} isosurface as it evolves over time. This method uses the *extinguished fraction*, f_{ext} , dividing the extinguished isosurface area Σ_{ext} by the total area Σ . Its formulation is shown in Eq. 6.1.

$$f_{ext} = \frac{\Sigma |(\widetilde{Y_{OH}} < 0.00045)|}{\Sigma} \quad (6.1)$$

An f_{ext} equal to 0 means the isosurface experiences no extinctions, whereas when equal to 1 it means the entire isosurface is extinguished. To calculate the OH mass fraction threshold, preliminary 0D-CMC calculations at the highest scalar dissipation rate prior to extinction are utilized (see Fig. 4.14). In this extinguished fraction analysis, a threshold of 15% of the peak 0D-CMC OH mass fraction is used as the lower bound for unconditional filtered $\widetilde{Y_{OH}}$ along the f_{ext} isosurface, below which the region is considered extinct.

The top of Fig. 6.9 shows the f_{ext} and total ξ_{st} for the stable conditions flame analysed previously in Chapter 5, and the bottom of Fig. 6.9 shows how the stoichiometric isosurface changes as the flame progresses through lean blow-off.

The stable conditions flame experiences a decrease in isosurface area, until about 11 ms, after which the area stabilises. There is a peak in the extinguished fraction after about 12 ms, where 40% of the flame isosurface is considered extinguished, but the level of extinctions quickly reduces again and no further stoichiometric isosurface area is lost. The isosurface area of the stable flame is more than twice the area of the flame after LBO at 15 ms. Counter-intuitively, the stable flame experiences marginally higher levels of local extinctions in the first 10 ms than the flame at LBO conditions.

As for the flame undergoing LBO, the total surface area decreases at an approximately linear rate as air U_{bulk} is equal to $U_{BO,exp}$, while the fraction of the surface experiencing extinction remains fairly steady. Once U_{bulk} is increased by 5% at $t = 8$ ms, f_{ext} increases to 0.47, so nearly 50% of the isosurface is extinguished at $t = 16$ ms, but subsequently the f_{ext} decreases. This is because the isosurface has retreated from the bluff body edge as it lifts off (shown in Fig. 6.12), hence the OH on the isosurface is shielded from high scalar dissipation rates and strong convection. This f_{ext} result is quite different from the non-premixed methane flame blow-off in Zhang & Mastorakos [2016], where the isosurface was between 70-100% extinguished. The results in Fig. 6.9

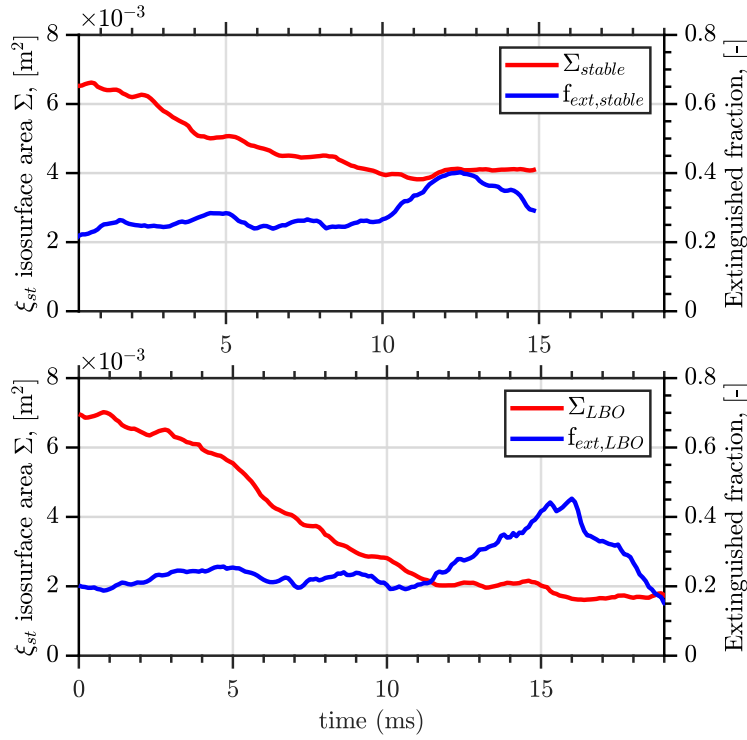


Fig. 6.9 Extinguished fraction and stoichiometric isosurface area (m²) for stable conditions (top) and LBO (bottom) for the $\dot{m}_f = 0.27$ g/s flame.

show that local extinctions do increase during the blow-off event, however they are not the only physical phenomena contributing to the death of the flame.

Figure 6.10 shows the ξ_{st} isosurface area on top and the f_{ext} on bottom, comparing the extinction behaviour of the three flames during LBO. All the flames demonstrate similar behaviour with respect to the isosurface area, decreasing fairly steadily over time to between 0.002 to 0.003 m². The variability in the isosurface area of these spray flames is considerably lower and more stable in comparison to gaseous non-premixed methane [Zhang & Mastorakos, 2016], which regularly experienced fluctuations as great as 0.012 m². These area fluctuations are greater than the maximum isosurface area of the stable Jet-A flame shown in Fig. 6.9, indicating the large size difference between non-premixed gaseous and spray flames. This difference is caused by the limiting factor of the vaporisation rate for the spray flames. The extra step of evaporation reduces the amount of fuel availability, causing shorter flames with smaller ξ_{st} isosurface areas.

The peak value of f_{ext} for the three flames typically occurs right around the $\tau_{ext,HR}$ blow-off time for each flame listed in Table 6.2. Neither the $\dot{m}_f = 0.30$ g/s nor 0.33 g/s flames have as large extinguished areas compared to the $\dot{m}_f = 0.27$ g/s flame, peaking at most to a 40% extinguished fraction value or lower. The differences between

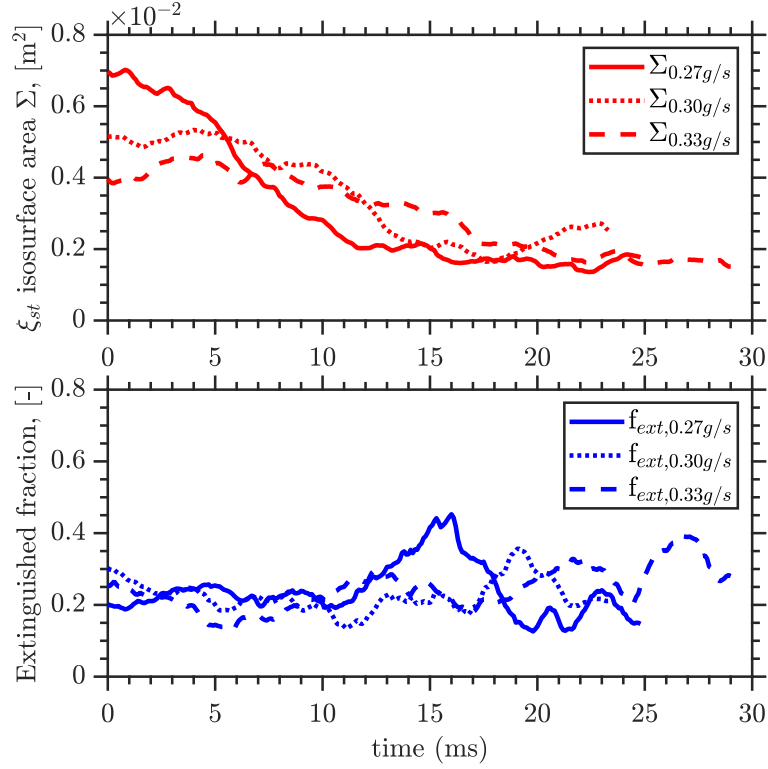


Fig. 6.10 Stoichiometric isosurface area (m^2) (top) and extinguished fraction (bottom) for the three flames during LBO.

non-premixed gaseous flames and these results further support the idea that fuel starvation is a significant factor in lean blow-off of spray flames. Local extinctions are likely not the primary driver of extinction in these flame simulations, as they account for less than half of the isosurface at the blow-off time $\tau_{ext,HR}$, whereas the reductions in isosurface area are much more significant, with areas diminishing by more than 50-75% from their initial values.

6.7 Spatial evolution of species during LBO

Moving on to qualitative results and the structure of kerosene spray flames during LBO, this section first provides OH^* chemiluminescence images from the blow-off transient of Jet-A in experiments as a visual reference for expected flame structures. The asymmetric nature of the wedge-shaped flames generated by fuels with low volatile matter content is emphasized. Then the qualitative results from the LBO simulations are presented, including three-dimensional stoichiometric mixture fraction isosurfaces and two-dimensional cross-sections of the domain.

6.7.1 LBO flame structure from experiments

Key structural features of low-volatility spray flame blow-off are presented as a qualitative references for the LBO simulations. Figure 6.11 shows instantaneous OH^* chemiluminescence images from experiments [Sidey et al., 2017] with the $\dot{m}_f = 0.27$ g/s flame during lean blow-off. This experimental visual data of the Jet-A flame lean blow-off event demonstrates some of the expected structural behaviour of spray flames during LBO.

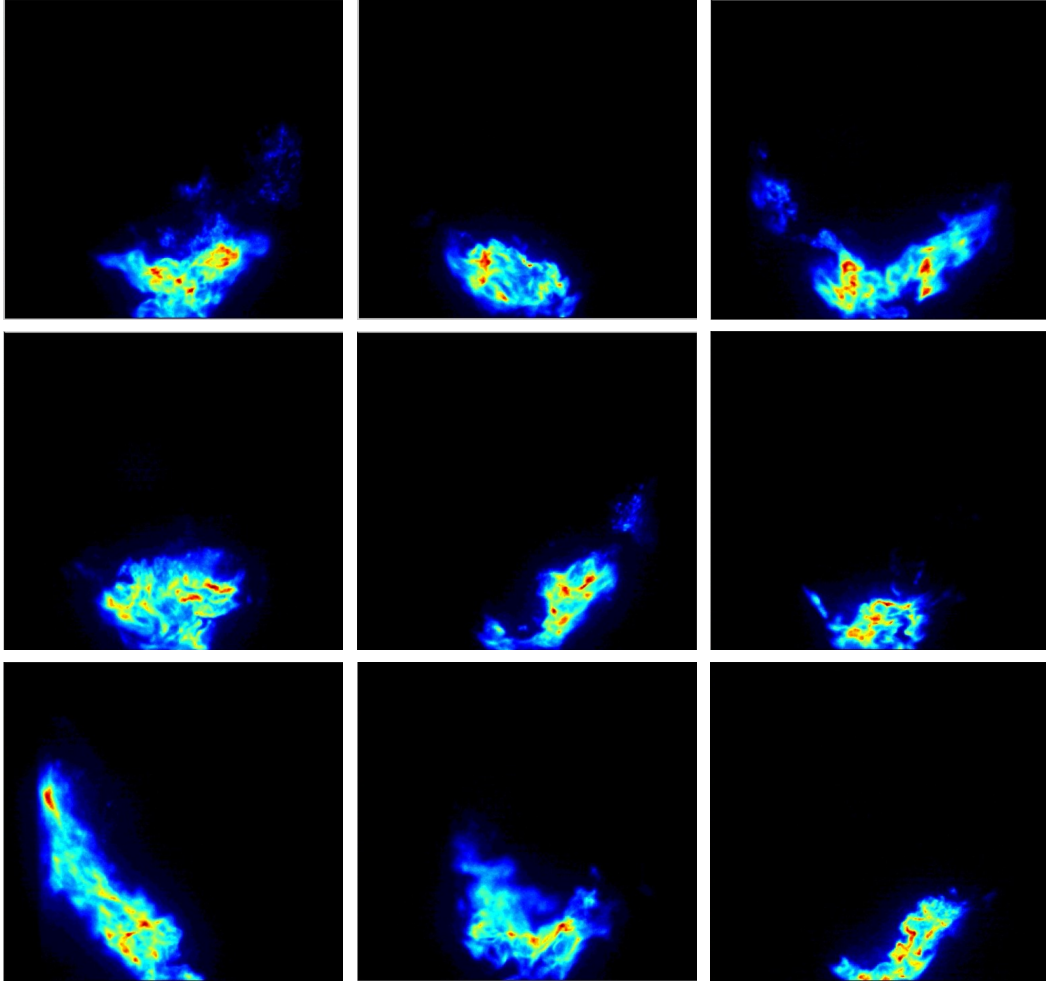


Fig. 6.11 Instantaneous OH^* chemiluminescence images of Jet-A experiments from the work of Sidey et al. [2017]. Fuel mass flow rate $\dot{m}_f = 0.27$ g/s, air velocity near blow-off. The asymmetric flame shapes are similar to low-volatility decane and dodecane spray flames during LBO in Yuan et al. [2018]. Domain window is 0.095 m x 0.10 m.

The flame is short, often less than 30 mm tall, and hugs the bluff body surface. There are occasionally two stubby flame branches, but often the flame shape changes

from a small blob into the distinct and sometimes quite large asymmetric “half branch” or “wedge-like” flame shapes observed in the n-decane and n-dodecane flames in Yuan et al. [2018]. This is markedly different from ethanol or n-heptane spray flame LBO behaviour, where the flame is concentrated primarily as a blob above the bluff body and in the central recirculation zone [Cavaliere et al., 2013; Yuan et al., 2018]. Some smaller asymmetric branches are observed in these more volatile fuels, but not to the extent of decane and kerosene flames.

The missing flame branch in Yuan et al. [2018] is suggested to be a large precessing local extinction, where the flame has been quenched along the inner recirculation zone. The cause of this behaviour in fuels like decane and kerosene is thought to be linked to the low-volatility of the fuels. Cavaliere et al. [2013] describes the process as one where the flame shrinks due to the increased air flow and downward force of the central recirculation zone. The recirculation zone is cooled by the increased cold air and evaporation is correspondingly slowed. The flame is subsequently starved of fuel vapour and cannot sustain itself.

6.7.2 3D isosurface visualizations

Visualization of the flame blow-off event using LES-CMC for the $\dot{m}_f = 0.27$ g/s flame is shown in Fig. 6.12 from the start of blow-off at $t = 0.0$ s to $t = 0.015$ s using 3D isocontours of the stoichiometric mixture fraction ξ_{st} coloured with various quantities.

The flame at $t = 0$ s looks as it does during the stable flame configuration, extending to about 45 mm in height and nearly fully attached to the edge of the bluff body, which is visualized in the centre of the swirling air annulus. OH, as a chain-branching reaction species, shows where combustion is and is not occurring. There are numerous “holes” of negligible OH mass fraction along the isosurface, indicating local extinctions. These are caused by their proximity to the air shear layer, where high velocity and rates of scalar dissipation disrupt combustion reactions and cause these small pockets of local extinctions in the flame. In these holes, we can see there are higher presences of fuel mass fraction and formaldehyde, whereas temperature and heat release rate are lower than in surrounding regions. Unburnt fuel, increased CH_2O and low temperature together indicate incomplete combustion. Low heat release rate can indicate either fully burning, steady-state combustion or a lack of combustion reactions. Occurring simultaneously, these conditions provide sufficient evidence to conclude these regions on the flame isosurface are local extinction events.

As the time increases, the isosurface visibly begins shrinking. At time $t = 0.003$ s, there appear to be more local extinctions along the flame surface, particularly in close

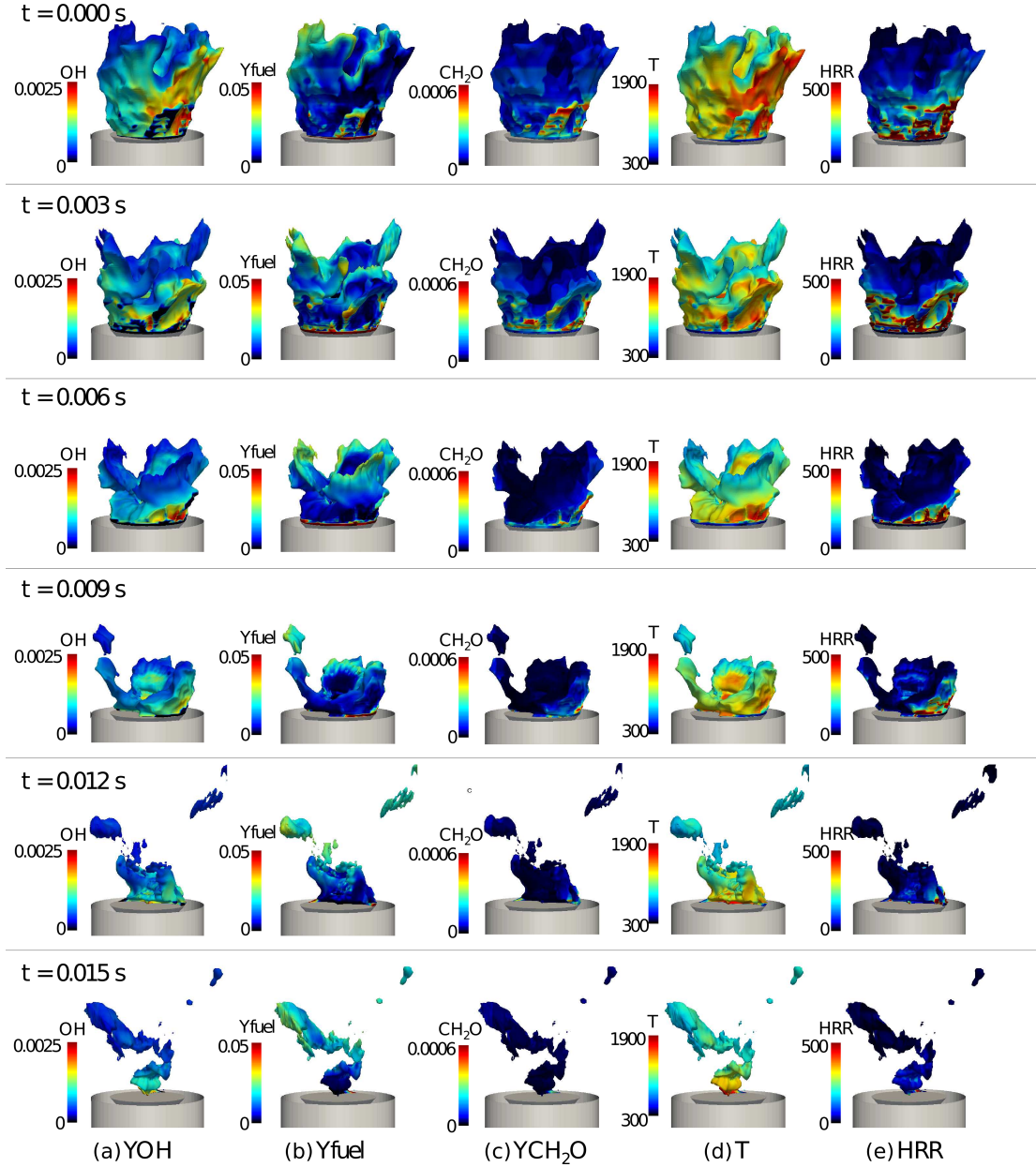


Fig. 6.12 Time sequence of 3D stoichiometric ($\xi_{st}=0.0637$) instantaneous isocontours of (a) OH mass fraction, (b) fuel mass fraction, (c) formaldehyde (CH₂O) mass fraction, (d) temperature (K), and (e) heat release rate (MW/m³) at six instances during the blow-off event for the $\dot{m}_f = 0.27$ g/s flame. Time is increasing from top to bottom, and $t = 0$ s indicates the first instance when the LES inlet air velocity $U_b = U_{BO,exp}$.

6.7 Spatial evolution of species during LBO

proximity to the bluff body. At the following time $t = 0.006$ s, the flame has shrunk considerably, with high temperature and OH mass fraction being concentrated only in the region near the bluff body. In the HyChem model, Jet-A is completely pyrolyzed at temperatures of 1250 K and above [Han et al., 2019], whereas the final instance of Fig. 6.12d shows much of the isosurface temperature is below 1200 K. Thus, less isosurface area is experiencing burning temperatures—the fuel mass fraction presence in 6.12b has spread down from the top of the isosurface to nearly half of the isosurface height, as reduced temperatures result in less parent fuel consumed by pyrolysis.

From $t = 0.009$ s onward the flame continues to shrink downward and the flame edges increasingly retreat from the bluff body edge. As the isosurface edge moves toward the centre of the bluff body, very few local extinctions with negligible OH are observed. Once away from the air shear layer, the OH presence on the ξ_{st} isosurface is shielded from total annihilation, though in some areas is still present only in low quantities. The temperature of the recirculation zone is still between 1000 to 1300 K (see Fig. 6.14), enabling fuel vaporization to continue at locations far downstream from the bluff body. This is evidenced by the appearance of blobs of ξ_{st} at times $t = 0.012$ s and 0.015 s with considerable quantities of unburnt fuel mass fraction. Fuel is still pyrolysed in the hot spray injection zone (evidenced by negligible fuel mass fraction), however the high temperature region is so small that it is unlikely the flame could recover. Once the isosurface is almost entirely detached from the bluff body edge, the isosurface is considered lifted-off. This corresponds with the global blow-off event for the flame at $\tau_{ext,HR} \approx 15$ ms.

Figure 6.13 shows the stoichiometric mixture fraction isosurface coloured with temperature of the $\dot{m}_f = 0.30$ g/s and $\dot{m}_f = 0.33$ g/s flames during the blow-off event. A small degree of flame lift-off is captured, notably at $t = 12$ ms in the top sequence and at $t = 4$ ms in the bottom sequence. The flame shapes are asymmetric with a single flame branch, which rotates around the bluff body edge. The $\dot{m}_f = 0.30$ g/s flame is stretched upward quite high during LBO, reaching over 50 mm. Then the flame fully detaches from the edge of the bluff body after 12 ms and the isosurface shrinks back down toward the spray injection point. The $\dot{m}_f = 0.33$ g/s flame is about half the height of the $\dot{m}_f = 0.30$ g/s flame and it morphs from a single flame branch into a blob that strays into the recirculation zone. Eventually the flame shrinks down into the bluff body and the flame along the bluff body edge lifts off, leaving stoichiometric isosurface only around parts of the spray cone.

These behaviours match well with the asymmetric spray flame structures discussed in Fig. 6.11 and observed in Yuan et al. [2018] for decane and dodecane, where low

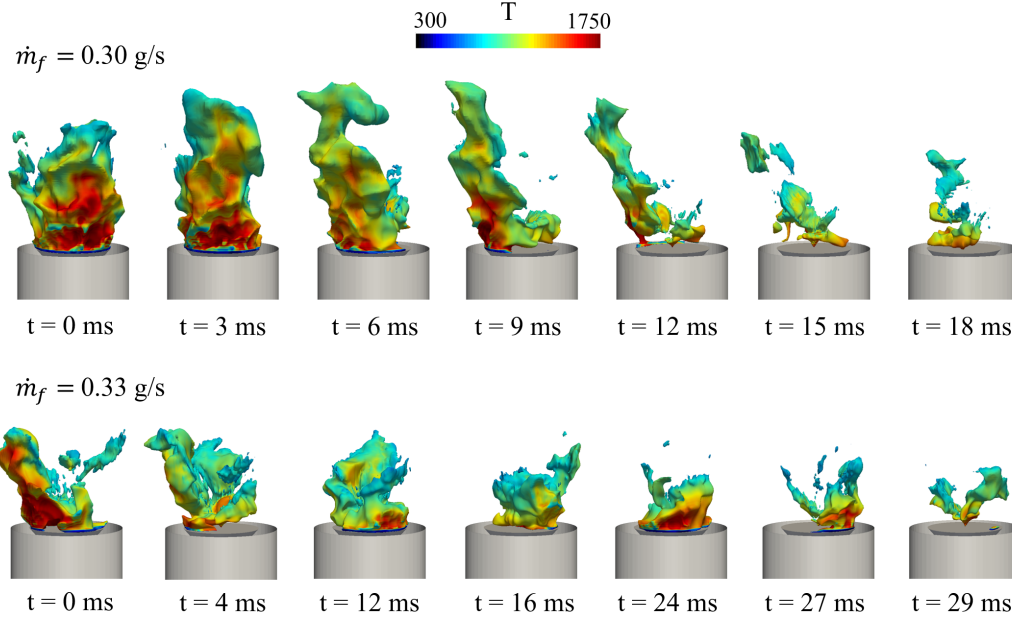


Fig. 6.13 LBO time sequence of the 3D stoichiometric isosurface ($\xi_{st} = 0.0637$) coloured with temperature (K) for the $\dot{m}_f = 0.30$ g/s and $\dot{m}_f = 0.33$ g/s flames displaying asymmetric flame shapes characteristic of low-volatility fuels close to blow-off.

fuel volatility was suggested to cause a lack of fuel vapour in the central recirculation zone. Significant quantities of unburnt fuel vapour (pre-pyrolysis) can also quench large regions of the flame, observed in the $\dot{m}_f = 0.27$ g/s results in Fig. 6.12, resulting in a large local extinction which can travel with the swirling air. Once the flame is extinguished at $t = 18$ ms in Fig. 6.13, stoichiometric mixture fraction isosurface still persists, although only in the vicinity of the spray.

6.7.3 2D cut-plane visualizations during blow-off

Various species, including pyrolysis products such as ethylene (C_2H_4) and benzene (C_6H_6), are explored during the blow-off transient. These particular species are important as they contribute strongly to the production of soot, the mitigation of which is the greatest challenge facing non-premixed flame regimes at this time. In Fig. 6.14 mass fractions of fuel, benzene, ethylene and formaldehyde are shown along with temperature at three instances during the blow-off process in cut-planes of the domain.

Pre-pyrolysis gaseous fuel is present along the spray cone, close to the stoichiometric isolines. These regions of unburnt fuel correspond to lower temperatures, even along the isolines, indicating that the gaseous fuel as well as the spray quenches parts of the flame along the isosurface. Peaks of CH_2O mass fraction are usually not too far

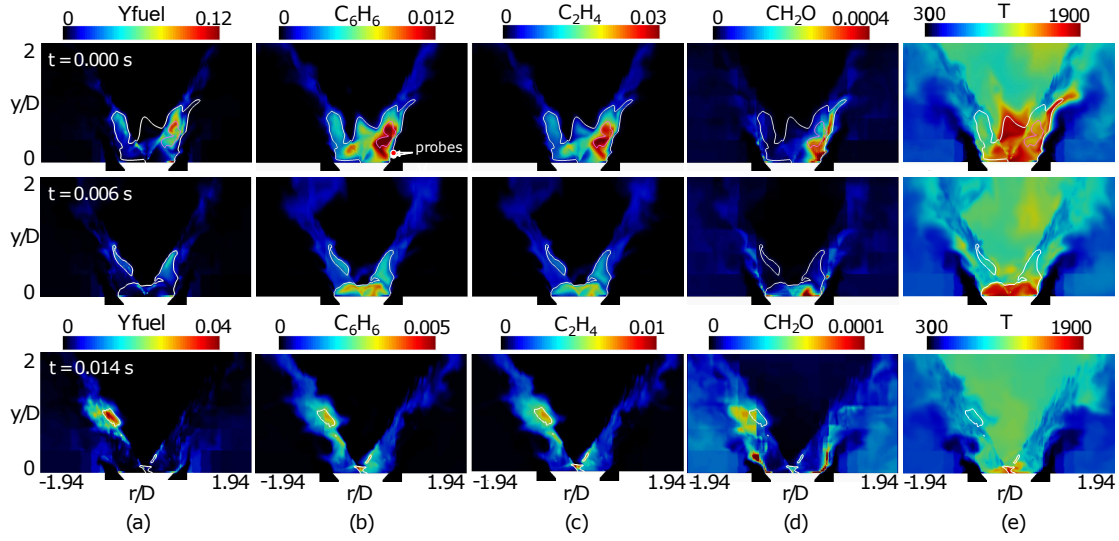


Fig. 6.14 Instantaneous 2D cut-planes of the combustor show mass fractions of (a) fuel, (b) benzene, (c) ethylene, (d) formaldehyde as well as (e) temperature (K) at three time instances during blow-off for the $\dot{m}_f = 0.27$ g/s flame. White isolines indicate stoichiometry $\xi_{st} = 0.0637$, pink isolines correspond to rich mixture fraction $\xi = 0.2$. Q probe locations are indicated along the air-shear layer with dots in the benzene field.

from the gaseous fuel, although there is also significant presence of CH_2O along the shear layer. CH_2O notably collects in areas away from the flame in smaller quantities around the corners of the chamber where temperatures are low, due to the motion of the side recirculation zones. The peak values of benzene and ethylene mass fraction are found in the same regions of rich mixture fraction between the spray cone and the swirling air. As the stoichiometric isoline shrinks toward the bluff body over time, the presence of benzene and ethylene decreases to very low quantities around the bluff body. It was shown in Chapter 4 that these species peak at rich mixture fractions around 0.2, thus they reduce in peak values as the mixture becomes increasingly lean. During the middle of the blow-off transient at $t = 0.006$ s, the presence of the pyrolysis products has increased slightly along the spray trajectory downstream of the flame as their consumption in the combustion zone is reduced. The temperature along the spray and in the recirculation zone decreases to below 1000 K in some areas, where the vaporized fuel can no longer pyrolyse [Han et al., 2019]. This leads to the reduction of critical pyrolysis products like C_2H_4 whose presence is necessary for providing fuel to sustain the flame. Without enough pyrolysis products the flame experiences fuel starvation, evidenced by the decreased ξ_{st} isosurface area during the blow-off transient. Local extinctions contribute to the fuel starvation by reducing the temperature and evaporation through increasing peak values and variability of the scalar dissipation

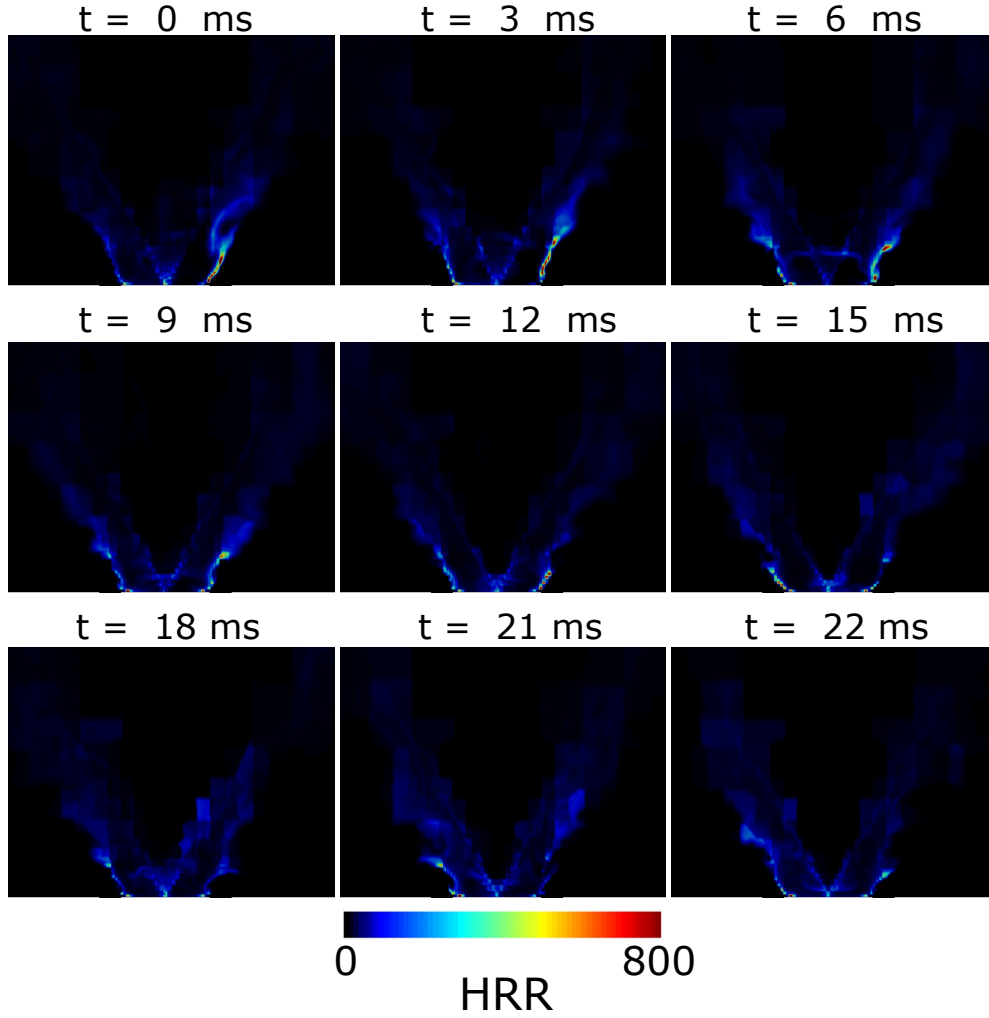


Fig. 6.15 2D cut-planes of the LBO sequence showing HRR (MW/m^3) for $\dot{m}_f = 0.27$ g/s flame. Domain window is $0.095 \text{ m} \times 0.075 \text{ m}$.

rate. Combined, local extinction and fuel starvation may cause the flame to approach blow-off.

Heat release rate during the blow-off event for the $\dot{m}_f = 0.27$ g/s case is displayed in Fig. 6.15. At first HRR is high along the shear layer and the flame is solidly attached to the bluff body edge. As the transient progresses the peak levels of HRR decrease and regions of very low HRR appear along both the inner and outer flame branches. These results are similar to OH-PLIF results for decane and dodecane [Yuan et al., 2018], where the inner and outer flame branches were also often disconnected and fragmented, especially near LBO.

The unconditional OH mass fraction sequence taken from LES in the same flame is shown in Fig. 6.16. Strong peaks of OH coincide with regions of high heat release

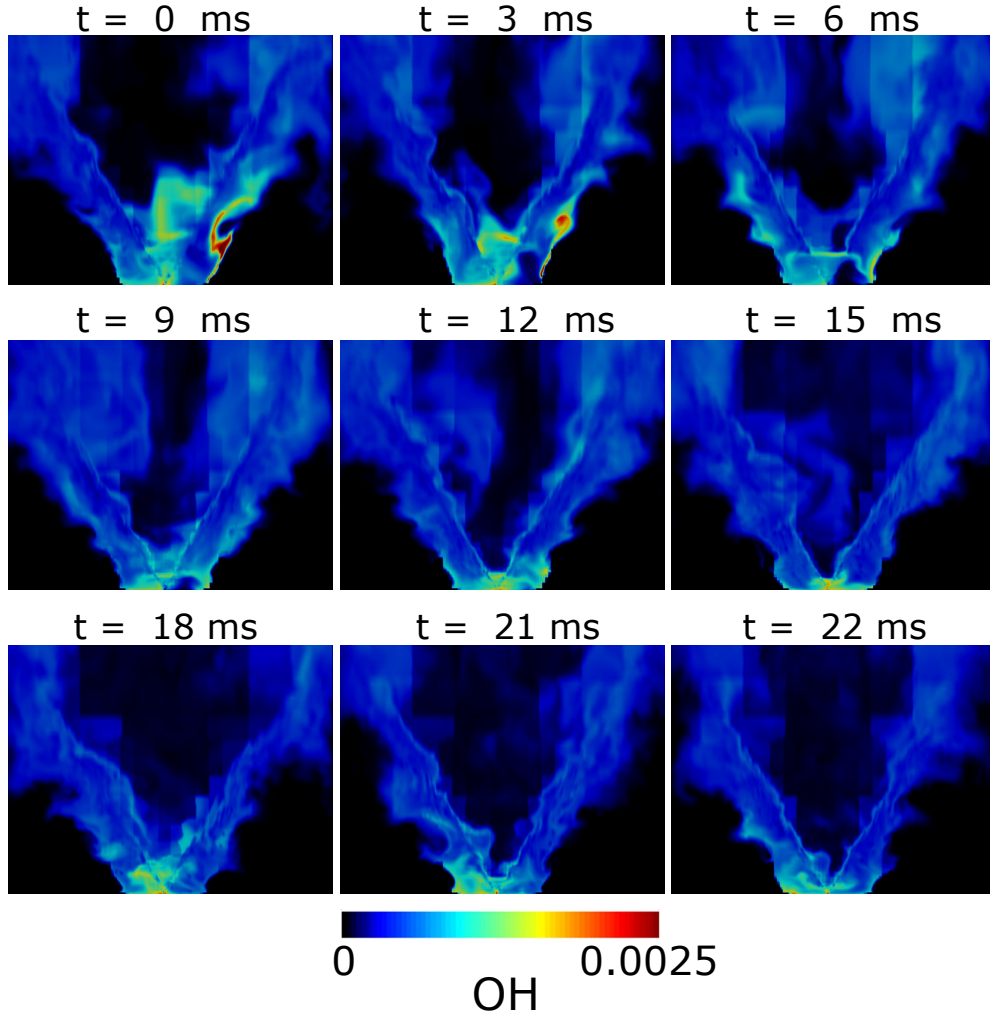


Fig. 6.16 2D cut-planes of the LBO sequence showing OH mass fraction for the $\dot{m}_f = 0.27$ g/s flame. Domain window is 0.095 m x 0.075 m.

rate in 6.15, although only along the air shear layer. There is significant presence of OH in the recirculation zone at the start of the transient, however this is not reflected in the heat release rate results. At these instances, part of the flame surface is in the recirculation zone, as seen in the temperature images in Fig. 6.14. It was noted in Chapter 5 that there are some discrepancies between OH* signal and HRR in simulations; HRR exhibits most strong responses along the shear layer, and a limited signal in the spray injection region, whereas OH* captures much greater signal along the spray. The OH in Fig. 6.16 is present in broad, thick layers around and inside the flame, whereas the HRR is typically confined to much thinner regions close to the steep velocity gradients along the flame-air boundary. OH is present in small quantities along the spray trajectory, where unburnt fuel has made its way a considerable distance

downstream of the flame. This may be an artefact of the HyChem lumped pyrolysis technique in the detailed chemical mechanism, caused by the presence of OH in the semi-global pyrolysis reaction equations. This causes small but visible quantities of OH to the fuel cracking process occurring near vaporising droplets, which persist even in regions far downstream of the combustion zone.

The LBO sequence of OH mass fraction in the same 2D plane for the $\dot{m}_f = 0.33$ g/s case is shown in Fig. 6.17. The asymmetric flame branch is visible with medium to high values of OH as the start of LBO, but as time increases the peak OH reduces and shrinks down toward the bluff body where peaks eventually reduce to extinguished flame values. At blow-off ($t = 28$ ms), very little OH is present in the conical central recirculation zone and none whatsoever is located around the outer corners of the chamber.

Figure 6.18 shows the temperature field for the same flame. The colour scale emphasises the intermediate temperature range, 1050 K being the temperature when pyrolysis of the parent fuel begins, according to shock tube experiments with Jet-A in Han et al. [2019]. From time $t = 0$ ms to about 11 ms the recirculation zone contains regions hot enough to enable the full pyrolysis of the evaporated fuel, and OH is present in these corresponding regions in Fig. 6.17. In Fig. 6.18 the temperature of the recirculation zone during blow-off decreases over time due the increased amount of cold air, to the point where its temperature is at the lower threshold 1000-1050 K, below which pyrolysis of the fuel does not occur. The stoichiometric isolines show how the flame shrinks during the transient, after $t = 28$ ms the only location stoichiometric mixture can be observed is along the fuel spray.

CH₂O mass fraction, a marker of incomplete combustion, is shown in Fig. 6.19. After noting its interesting tendency to gather in the low-temperature corners of the chamber, its relationship with temperature is investigated further. Prior to blow-off and between $t = 0$ to 11 ms, CH₂O peaks are near stoichiometry (white isolines) and the air shear layer. However as the blow-off transient progresses, peak CH₂O tends to appear more in regions of low to intermediate temperature, between the 500 K and 800 K temperature isolines, especially in regions of large gradients like the air shear layer where the isolines come close together. CH₂O presence gradually builds up both in the recirculation zone and the outer corners of the chamber during the blow-off transient, where temperatures are either low or decreasing from intermediate levels. This is due to the corresponding lack of OH presence in these regions, as reaction with OH is a primary CH₂O consumption pathway [Paxton et al., 2019]. Similar behaviour of CH₂O entering the recirculation zone from downstream during LBO was observed

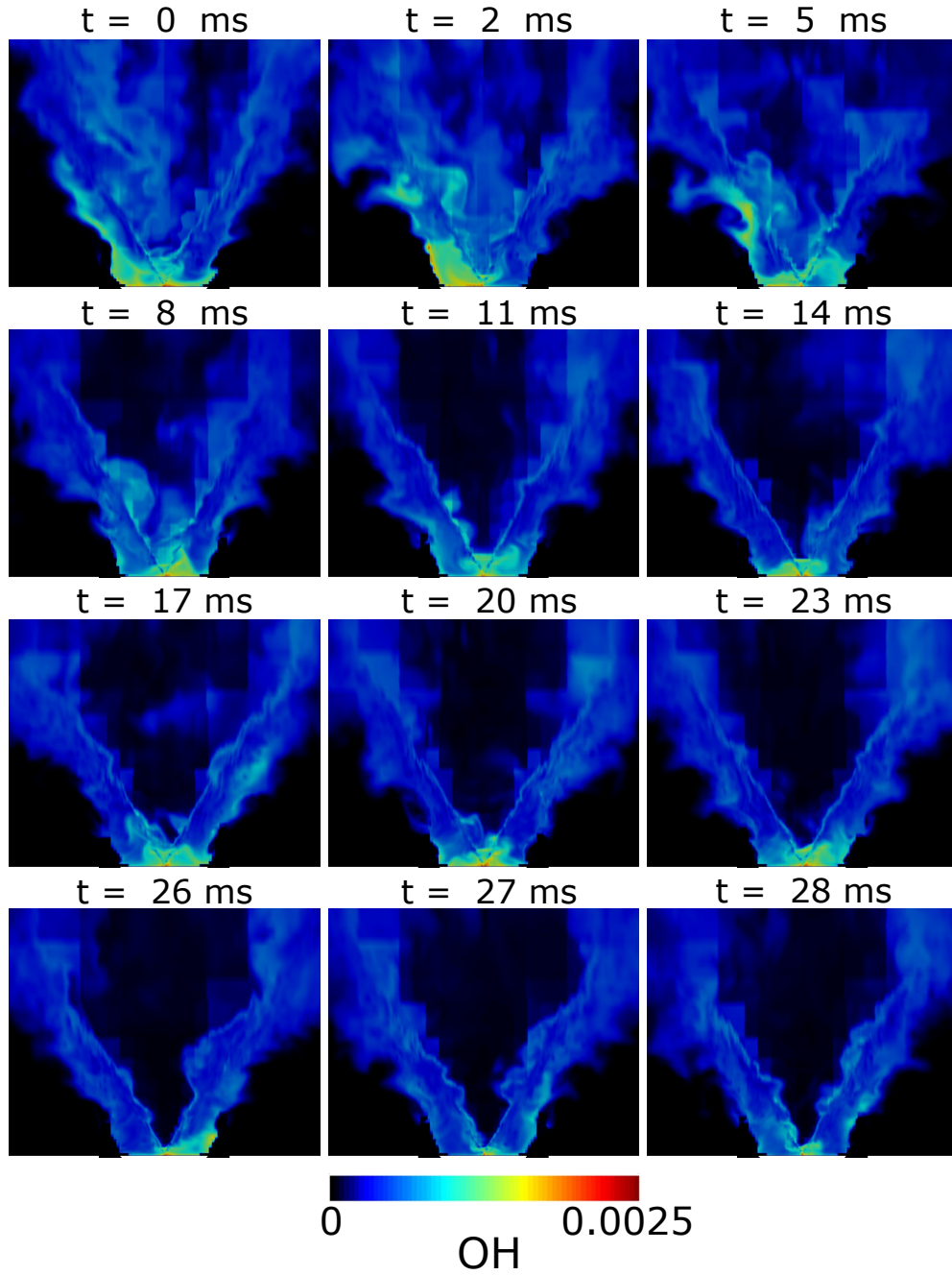


Fig. 6.17 2D cut-planes of the LBO time sequence showing OH mass fraction, $\dot{m}_f = 0.33$ g/s flame. Domain window is 0.095 m x 0.075 m.

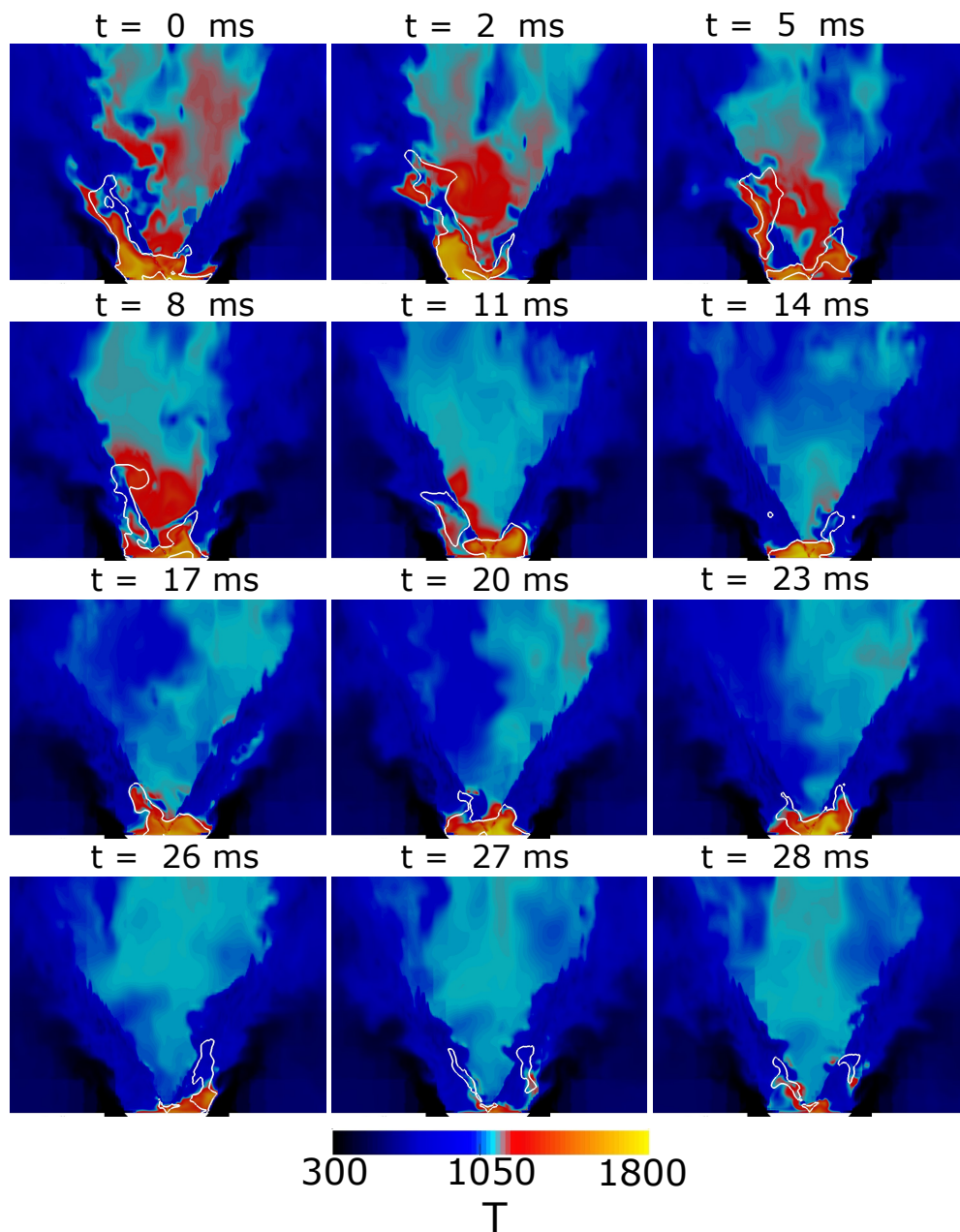


Fig. 6.18 2D cut-planes of the LBO time sequence of temperature (K), $\dot{m}_f = 0.33$ g/s. White isolines indicate stoichiometry ($\eta_{st} = 0.0637$). Domain window is 0.095 m x 0.075 m.

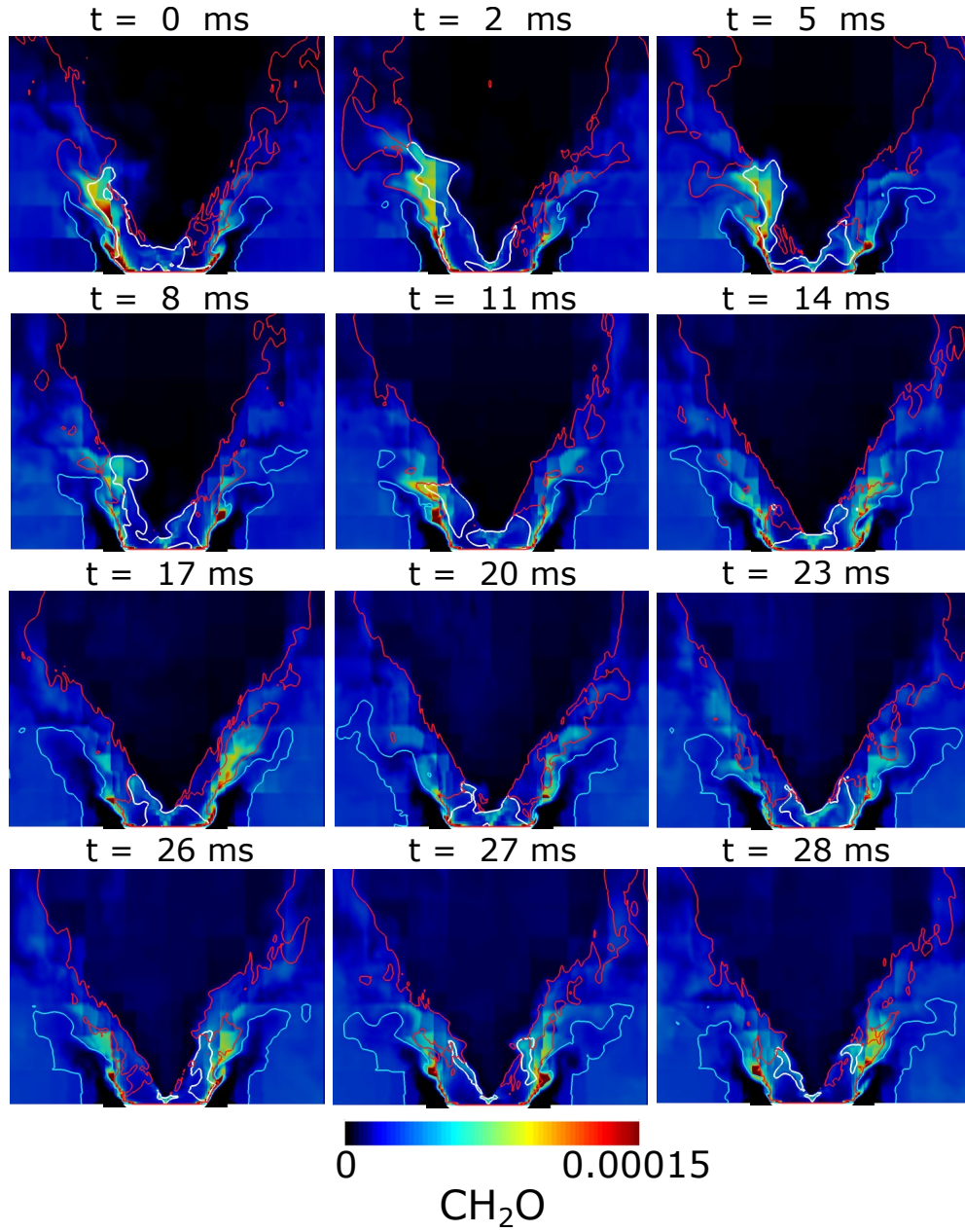


Fig. 6.19 2D cut-planes of the LBO time sequence of CH_2O mass fraction, $\dot{m}_f = 0.33$ g/s. White isoline contours indicate stoichiometry ($\eta_{st} = 0.0637$), cyan lines indicate $T = 500$ K, and red lines indicate $T = 800$ K. Domain window is 0.095 m x 0.075 m.

in pre-vaporised kerosene experiments by Pathania et al. [2020], where it was also suggested that CH_2O could act as a marker for low-temperature chemistry regions during LBO.

6.7.4 Conditional OH during blow-off transient

So far it has been suggested that local extinctions and fuel starvation may cause the flame to approach blow-off. Evidence for fuel starvation is shown through reduced evaporation rates and temperature in the recirculation zone, which results in smaller amounts of fuel species mass fractions and a shrinking ξ_{st} isosurface. There is however less evidence of strong local extinctions occurring in the flames, as the extinguished fraction never increases beyond 50% of the ξ_{st} isosurface and scalar dissipation rates $N|\eta_{st}$ never reach the $N_{st,cr}$ value in the Q probes, although SDR variability is noted to increase during the blow-off transient.

Looking at $\widetilde{\text{OH}}|\eta_{st}$ and the resolved mixture fraction ξ can help shed some light on the limited quantities of $N|\eta_{st}$ and local extinctions observed during the LBO simulations. The filtered conditional OH mass fraction from CMC is useful for assessing blow-off behaviour, as shown before in Fig. 6.2, averaged on the instantaneous isosurface area of the resolved stoichiometric mixture fraction. $\widetilde{\text{OH}}|\eta_{st}$ can also be analysed in physical space over time, shown in Fig. 6.20 for the blow-off transient of the $\dot{m}_f = 0.27$ g/s flame. Instantaneous snapshots well beyond the $\tau_{ext,HR} = 14.8$ ms value reported for blow-off of the flame are included. As $\widetilde{\text{OH}}|\eta_{st}$ is a species mass fraction conditioned on stoichiometric sample space mixture fraction ($\eta_{st} = 0.0637$) taken directly from CMC, the very coarse CMC grid resolution is visible. Isolines of the LES resolved mixture fraction ξ are also shown at lean, stoichiometric, and rich values.

Burning values of $\widetilde{\text{OH}}|\eta_{st}$ ranging between 0.004 to 0.005 during the transient are located in large regions between the spray and the air shear layer, and inert values are seen only in the air annulus and around the bluff body edge. The central and side recirculation zones contain middling values of $\widetilde{\text{OH}}|\eta_{st}$. The high values of $\widetilde{\text{OH}}|\eta_{st}$ shrink downward along the sides of the chamber as time progresses to well after $\tau_{ext,HR}$, but remain fully burning in the spray region. Regions of particularly high conditional OH appear to actually increase in size, extending further downstream, and only a few local extinctions are observed in the flame zone along ξ_{st} during the transient.

The isolines of the resolved mixture fraction ξ in Fig. 6.20 show that as the transient proceeds, peak values of mixture fraction are reduced. By 10 ms into the transient, rich values of ξ of 0.2 or larger no longer exist in this cut-plane of the domain. This is caused by reduced temperatures in the recirculation zone and reduced availability

6.7 Spatial evolution of species during LBO

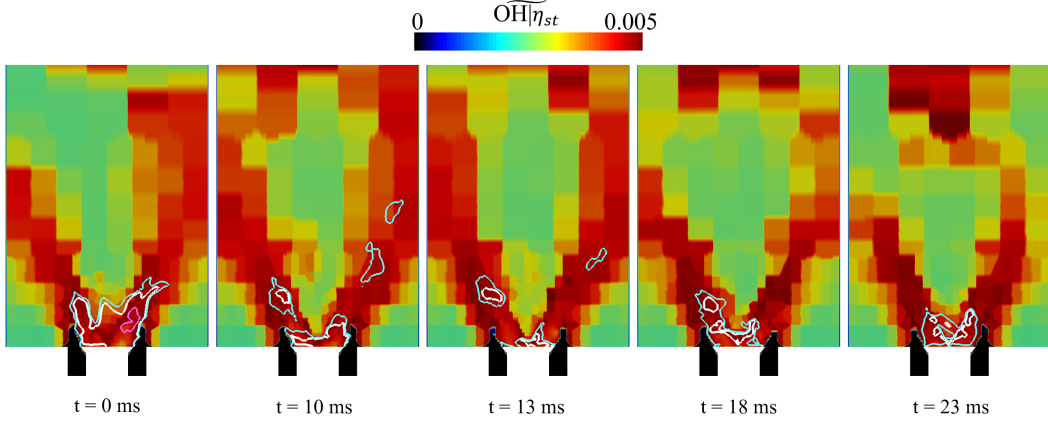


Fig. 6.20 2D cut-planes of the LBO sequence showing filtered conditional OH mass fraction from CMC η -space mapped onto physical space for the $\dot{m}_f = 0.27$ g/s flame. Isolines are resolved mixture fraction from LES: cyan is $\xi = 0.04$, white is $\xi_{st} = 0.0637$, pink is $\xi = 0.2$. Domain window is 0.095 m x 0.13 m.

of pyrolysed fuel products. After the transient duration $\tau_{ext,HR} \approx 15$ ms for this case, even the lean mixture fraction isolines have retreated downward to exist just above the bluff body. The domain mixture is almost entirely lean at this point in time.

This is an interesting contrast in behaviours. CMC Q s such as $\widetilde{OH|\eta_{st}}$ in the gaseous space remain chemically burning and active, while the spray evaporation and lower unconditional temperatures limit the presence of available fuel species and thus the resolved mixture fraction is drastically reduced, which is evidence of fuel starvation. This indicates that the PDF of the mixture fraction has become more narrow near the lean end ($\eta = 0$), and that rich mixture fractions hardly exist in these conditions. This causes most mixture fractions to occur in regions of low scalar dissipation rate, due to the fixed bell-shaped AMC distribution for $N|\eta$. There is evidence for this in the Q probes in Section 6.5, where scalar dissipation rates were well below the $N_{st,cr}$ value. This means that in conditional η -space local extinctions due to quenching scalar dissipation rates $N|\eta_{st} > N_{st,cr}$ are not observed, which allows for fully burning behaviour like that of $\widetilde{OH|\eta_{st}}$ in Fig. 6.20 well after the blow-off of the flame in unconditional space.

This behaviour is likely a weakness of using the AMC model at such lean conditions to close the conditional scalar dissipation rate. As the AMC model is fixed to be symmetric around the centre-line with the peak value at $\eta = 0.5$, it no longer corresponds the conditions in physical space where maximum mixture fractions are very low ($\xi_{max} < 0.2$), hence causing scalar dissipation rates that are too small. This also likely has an

effect on the blow-off velocity results for the three flames. With fewer local extinctions and low scalar dissipation rates, higher air velocity is required in simulations to extinguish the flame globally compared to experiments.

Thus, in these LBO simulations fuel starvation is almost entirely driving the blow-off of the flames. A spray flame during LBO should experience both local extinctions due to quenching scalar dissipation rates as well as fuel starvation. This could be achieved by using a more complex model to close the conditional scalar dissipation rate, such as the one developed in Devaud et al. [2004], which takes into account the mean and variance of the mixture fraction and their gradients, the turbulent scalar flux, and the mean velocity.

6.8 Conclusions

The LES-CMC approach is used to simulate kerosene spray flames in a bluff-body swirl burner for three fuel mass flow rates at lean blow-off conditions. A high-temperature detailed mechanism developed specifically for Jet-A using the HyChem methodology is deployed. LES-CMC is able to capture asymmetric flame structural behaviour and global blow-off events at multiple fuel mass flow rates within 5–20% of experimental blow-off velocities, which is in line with performance of other turbulence-combustion models.

Heat release varies in different regions of the chamber, but decreases by at least 80% in the flame stoichiometric zone. The evaporation rate decreases significantly in the flame region, but overall evaporation in the chamber remains fairly constant or even increases. Vaporising droplets are observed far downstream of the flame, where temperatures are still well above the boiling point for Jet-A. This contributes to the overall evaporation rate in the chamber. Between 87–90% of the spray is vaporised during the blow-off transients, indicating there are more unburnt droplets in the chamber compared to the stable flame.

The blow-off transient lasts between about 10–30 ms for the flames using the 80% HRR reduction to quantify the blow-off duration. These durations agree well with past experiments with low-volatility heavy hydrocarbon fuels. Species mass fractions, averaged along the flame isosurface, including that of the parent fuel, pyrolysis products, OH and CH₂O are observed to decrease over time in the stoichiometric region during blow-off. However, CH₂O builds up in low-temperature regions between 500–800 K in the bottom/upstream corners of the chamber, as well as in the recirculation zone, entering from downstream during LBO. These regions correspond to those

with negligible OH presence, thus allowing for the persistence of formaldehyde. This behaviour indicates that CH_2O may be used as a marker for low-temperature chemistry as well as a potential indicator for increased levels of flame extinctions.

Through analysis in mixture fraction space, local extinctions along the flame-air shear layer are observed to increase in frequency during the transient similarly to observations in past experiments, however complete extinguishing in conditional mixture fraction space is not observed during LBO. The instantaneous proportion of the flame isosurface area containing extinguished regions is quantified using the extinguished fraction. The extinguished fraction results for the three flames show that the proportion of extinctions along the isosurface does increase to a small discernible peak before the flame blows off, however less than 50% of the total isosurface area is extinguished during the transient. This is in contrast to behaviour in gaseous non-premixed flames, where the isosurface is nearly fully extinguished as the flame blows off. The lack of strong local extinctions is likely caused by the low scalar dissipation rates observed in conditional mixture fraction space, where $N|\eta_{st}$ values never reached higher than 60% of the critical quenching value $N_{st,cr}$.

In the LBO simulations, flame shape in three-dimensional space is shown to shrink downwards and inwards toward the bluff body during the transient. Some of the flames exhibit asymmetric flame shapes, where half of the flame appears to be missing as the isosurface rotates around the bluff body edge. The same asymmetric behaviour was observed in experiments with Jet-A as well as in experiments involving other low-volatility fuels such as n-decane and n-dodecane. This flame shape is postulated to be caused by the phenomena of fuel starvation, experienced by the flame when temperatures are not high enough to fully vaporise and burn the fuel, thus starving the flame to partial extinction. In a cross-sectional analysis of fuel mass fraction and temperature during the transient, unburnt gaseous fuel is observed in regions of lower temperature. This fuel, which has not yet undergone pyrolysis, quenches parts of the flame. Fuel starvation is proposed to play a significant part in the physical process of spray flame lean blow-off.

The effects of fuel starvation are shown to contribute to the blow-off of spray flames. Fuel starvation is caused by reduced temperatures in the recirculation zone, which both decreases evaporation rates as well as reduces pyrolysis of the vaporised fuel. Local extinctions contribute to the fuel starvation by reducing the temperature and evaporation and increasing the scalar dissipation rate. Combined, local extinction and fuel starvation can cause blow-off of the flame. However the lack of high scalar dissipation rates above the critical quenching value warranted further investigation

of the levels of extinction seen in conditional mixture fraction space. The OH mass fraction conditioned of the stoichiometric mixture fraction value filtered onto the physical domain is analysed during the LBO transient. $\widetilde{\text{OH}}|\eta_{st}$ is fully burning well beyond the flame zone during the entire LBO transient as well as long after the flame blows-off, indicating that the conditional space is not experiencing much local extinction whatsoever. In contrast, isolines of resolved mixture fraction ξ from the LES at rich, stoichiometric and lean values are shown to shrink and reduce down to just above the bluff body, and peak ξ values fall below 0.2 resulting in a very lean mixture in the chamber overall. This contrast in behaviours leads to the conclusion that in these LBO simulations fuel starvation is almost entirely driving the blow-off of the flames. It is likely a weakness of using the AMC model at such lean conditions to close the conditional scalar dissipation rate, as it is a bell-curve distribution with the ends fixed at $\eta = 0$ and $\eta = 1$. It is not able to shift the distribution toward the lean left side as peak resolved mixture fractions become very lean. This results in low scalar dissipation rates at the stoichiometric mixture fraction. It is recommended that a more complex model to close the conditional scalar dissipation rate is used at such lean conditions for spray flames which can take the narrowing mixture fraction PDF into account.

This work demonstrates that the LES-CMC approach is capable of modelling LBO phenomena of practical liquid fuels and paves the way for more research and modelling of alternative liquid fuels. LES-CMC predicted flame structural behaviour observed in experiments related to fuel starvation and a blow-off curve with similar accuracy to other studies. These results call attention to the importance of appropriate models for the conditional scalar dissipation rate when simulating spray flames at very lean conditions.

Chapter 7

Conclusions and Recommendations

7.1 General conclusions

The research questions and objectives of this work were addressed as best as possible given the complexity of the task and time constraints of the doctoral study.

Fuel starvation is determined to be the primary driver of spray flame lean blow-off in the LES-CMC simulations presented in this work. Larger quantities of cold air decrease the temperature in the recirculation zone. Lower temperatures cause reductions in evaporation rate near the flame, which results in reduced amounts of gaseous parent fuel and subsequent pyrolysed products, such as the flame-sustaining species ethylene. This fuel starvation causes the stoichiometric mixture fraction isosurface to shrink toward the bluff body and form asymmetric shapes like those observed in past experiments with LBO of non-volatile fuels. The quantity of local extinctions observed is lower than expected, and is linked to low values of the conditional scalar dissipation rate. Changing the model used to close the conditional scalar dissipation rate in the CMC equations is suggested as a potential way to improve the LBO results. A more complex model taking into account changes in the mixture fraction PDF could allow the simulations to experience higher values of conditional scalar dissipation rate and thus increased levels of local extinction. This could make the simulated blow-off curve results more accurate compared to experiments.

Fuel chemistry is an important factor in predicting extinction behaviour of different jet fuels. As C1 is chemically very distinct from A2 and C5, being composed only of paraffins, it is easier to replicate the experimental trend of C1 being most likely to blow-off at richer equivalence ratio or lower scalar dissipation rates. Greater availability of stable pyrolysis products like ethylene allows for flames like those of A2 and C5 which are more stable and robust to extinction via high scalar dissipation rate, although

Conclusions and Recommendations

this would come at the cost of a flame with increased sooting propensity. A larger presence of aromatic species, for example toluene in the C5 synthetic fuel, may provide additional chemical flame stability. Certain species such as CH_2O are found to be useful indicators in both laminar and turbulent flames to mark regions of low temperature and extinction events.

The laminar flamelet based model 0D-CMC is able to replicate experimental global extinction trends with the HyChem A2 and C1 fuels, whereas the C5 chemistry bucks the trend and is extinguished at the highest scalar dissipation rate. This indicates that simulations incorporating chemistry alone cannot necessarily predict trends of fuels with unusual physical properties such as low viscosity and a flat-boiling curve. 0D-CMC is also able to predict flamelet extinction and reignition transients with a blow-off transient duration of 5.6 ms for Jet-A, which actually is not too different from the full LES-CMC blow-off transient durations, particularly when compared against the case with lower fuel mass flow rate. LES-CMC is able to predict the LBO curve of Jet-A with similar accuracy to other turbulence-combustion approaches, although further validation against experiments is required to conclude that LES-CMC is fully capable of replicating kerosene spray flame behaviour regarding locations of peak heat release rate. Some simulations of n-heptane and ethanol spray flames with LES-CMC in the past were able to achieve good qualitative comparison with experiments regarding peak HRR along the spray when using one-step chemical mechanisms, whereas detailed chemistry for ethanol spray flames resulted in higher peaks along the air-flame shear layer at stable conditions like the kerosene results observed here. Detailed chemical mechanisms may require further study regarding locations of peak HRR in comparison to experiments and simpler chemical mechanisms. However, other qualitative flame behaviours such as precessing asymmetric flame shapes and unburnt droplets are well-captured in the LES-CMC detailed chemistry simulations.

7.2 Laminar flamelet 0D-CMC results

In Chapter 4, laminar counterflow flames are run at various pressures and scalar dissipation rates using 0D-CMC. Four detailed chemical mechanisms are used: the Dagaut surrogate mechanism for Jet A-1, and the HyChem lumped-pyrolysis mechanisms A2, C1 and C5, which represent standard Jet-A and two synthetic fuels.

Increasing the scalar dissipation rate typically decreases temperature and peak species mass fractions, with some notable exceptions (CH_2O , CH_3 and HCO). The Dagaut surrogate and HyChem Jet-A results compare favourably with each other.

Differences between the Dagaut surrogate and the HyChem mechanisms are generally reduced with increases in scalar dissipation rate and pressure. The HyChem C1 fuel has some distinctly different trends concerning ethylene and iso-butene, due to its very different chemical composition. The mechanisms follow very similar trends overall at atmospheric and high pressure, especially as the scalar dissipation rate is increased toward extinction. Increasing pressure from atmospheric to 10 atm does not strongly affect large species behaviour, however small radical species are more significantly affected in peak levels of mass fraction. Ethylene is not sensitive to pressure change or molecular mixing, even when nearing extinction. Benzene and methane on the contrary are very sensitive to both pressure and SDR, exhibiting the most variability between the different fuels.

Scalar dissipation rates are increased to the point of flame extinction and the different extinction rates for the four fuels are compared at 1 atm and 10 atm. At 1 atm the C1 flame extinguishes at the lowest SDR, making it most susceptible to blow-off, which follows experimental observations. The most resistant fuel to blow-off however is C5, rather than the HyChem A2 fuel as observed in experiments. Small differences in the chain-branch reaction species like CH_3 which affect CH_2O and subsequently OH production may be the reason for robustness of the C5 fuel. Its extinction scalar dissipation rate is 5.6% greater the HyChem A2 value and 3.3% greater than the Dagaut surrogate extinction rate. At 10 atm the C1 fuel is still most prone to extinction, and amongst the HyChem fuels C5 is again the most robust against extinction. The Dagaut Jet-A1 surrogate extinguished at the highest value of scalar dissipation rate. This result indicates that it is the liquid fuel physical properties of C5 which caused it to blow-off at richer equivalence ratio than A2 in experiments, rather than chemical differences.

The extinction transients for the HyChem A2 fuel at 1 atm and 10 atm are explored through observation of several radical species, heat release rate markers as well as ethylene and acetylene mass fractions. OH^* and $\text{CH}_2\text{O} \times \text{OH}$ appear to correlate well as indicators of heat release rate. At 1 atm, HCO matches relatively well against these heat release rate markers, however at 10 atm there are larger discrepancies between HCO and the other heat release rate markers. Increasing the extinction scalar dissipation rate correspondingly reduces the duration of the extinction transient. CH is the first species to fall to zero, reaffirming it as a marker for the potential occurrence of an extinction event. CH_2O steadily increases during the extinction transient, reaching a distinct peak just after the flame is extinguished. This is linked to its primary consumption pathway involving OH; as OH is reduced, more and more

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CH_2O builds up. Once OH and other radical species are lost, CH_2O begins to decrease monotonically as its rate of production becomes smaller than its rate of consumption by other species. Reignition during the extinction transient is successfully attempted up to a point in the transient, after which radical species mass fractions are too small to allow for recovery of the flame. 0D-CMC is able to predict flamelet extinction and reignition transients with a blow-off transient duration of 5.6 ms for Jet-A at atmospheric conditions. This extinction transient duration is only about 40% of the LES-CMC blow-off duration using heat release rate as a metric in the $\dot{m}_f = 0.27$ g/s, but compared with the temperature-based time duration the 0D-CMC duration is about 80% of the LES-CMC value. These are not bad results given how much simpler the laminar flamelet simulations are compared to LES-CMC, although direct comparisons with the LES-CMC results should be made with reservation especially given the need to increase the air velocity beyond experimental values by some degree to induce LBO.

7.3 LES-CMC of Jet-A spray flame: Stable condition

In Chapter 5, a stable Jet-A flame is modelled using LES-CMC and the detailed HyChem A2 mechanism in the Cambridge bluff body swirl burner. The conditions are: $\dot{m}_f = 0.27$ g/s and $U_b = 0.74U_{BO,exp} = 15.9$ m/s, corresponding to stable experimental conditions. The simulation is compared against experimental time-averaged inverse Abel-transformed OH* and simultaneous instantaneous OH-PLIF and Mie scattering images. Limited quantitative data were available for the analysis of the experimental results, thus the focus is primarily on qualitative comparisons.

The LES-CMC results are comparable against the experiments in the flame size and shape, however there are significant discrepancies in the location of peak heat release rate, with the highest intensity observed along the shear layer in the simulation rather than near the spray cone in experiments. More attachment to the bluff body is also observed for the simulation. These discrepancies are common among LES of bluff body swirl spray flames, and may be caused by inadequate near-wall modelling close to the bluff body surface. The simulation appears to be exhibiting behaviour indicative of a flame at a near LBO condition rather than a low-air velocity stable flame. This may be due to aspects of the liquid fuel properties or the spray injection, or could be due to the detailed chemical mechanism. Some simulations of other spray flames with LES-CMC were able to achieve good comparison with experiments regarding peak HRR along the

spray when using one-step chemical mechanisms, whereas detailed chemistry resulted in higher peaks along the air-flame shear layer. Further simulations at different conditions are needed to validate the LES-CMC results against the experimental data.

The simulation results are analysed using time-averages of properties of interest, including mixture fraction, temperature, heat release rate, and various intermediate and pyrolysis species mass fractions. Some brief local extinctions are identified along the 3D instantaneous stoichiometric mixture fraction isosurfaces and in conditional mixture fraction space, although at scalar dissipation rates much lower than the critical quenching value. CH is discussed in the context of local extinctions in mixture fraction space as a potential contender for marking location of heat release rate and local extinction in experiments with increased accuracy over OH, although using $\text{CH} \times \text{CH}_2\text{O}$ may be recommended over just CH.

Global and local (along stoichiometry) volume-integrated heat release rate and evaporation rate over time are discussed. When integrating over the volume of the whole chamber (global) heat release and evaporation are steadily increasing, whereas when integrated along the cell volumes along the stoichiometric isosurface (local) heat release and evaporation decrease and fluctuate, respectively. The global evaporation rate in the chamber is 93% of the injected fuel mass flow rate, indicating the presence of unburnt droplets. The global heat release rate of the flame reaches 82% of the ideal heat of combustion for these conditions.

7.4 LES-CMC of Jet-A spray flames: LBO

In Chapter 6, the LES-CMC approach is used to simulate three fuel mass flow rates at lean blow-off conditions in the Cambridge bluff body swirl burner. The high-temperature detailed mechanism for Jet-A using the HyChem methodology is deployed. LES-CMC is able to capture asymmetric flame structural behaviour associated with the approach to global blow-off at multiple fuel mass flow rates using bulk air velocities 5–20% greater than experimental blow-off velocities. This range is commensurate with previous LES-CMC LBO studies with non-premixed gaseous flames which achieved LBO at bulk air velocities 25% greater than experimental U_{BO} . Other studies of liquid kerosene LBO also reported similar or lower amounts of discrepancy in ϕ_{BO} compared with experiments.

Heat release varies in different regions of the chamber, but decreases by at least 80% in the flame stoichiometric zone. The evaporation rate decreases significantly in the flame region, but overall evaporation in the chamber is constant or even increases

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towards the end of the transient. Between 87–90% of the spray is vaporised during the blow-off transients, indicating there are more unburnt droplets in the chamber compared to the stable flame. Vaporising droplets are observed far downstream of the flame, where temperatures are well above the boiling point for Jet-A. These vaporising droplets contribute to the overall steady evaporation rate in the whole chamber.

The blow-off transient lasts between 15 to 30 ms for the three flames using the 80% HRR reduction to quantify the blow-off duration. These durations agree well with past experiments with low-volatility heavy hydrocarbon fuels. Flames which were at a stable initial condition with a lower equivalence ratio had longer blow-off transients. Species mass fractions averaged along the flame isosurface are observed to decrease over time in the stoichiometric region during blow-off. However, CH_2O builds up in low-temperature regions between 500–800 K in the bottom corners of the chamber, as well as in the recirculation zone, entering from downstream during LBO. These regions correspond to those with low OH, which is a primary consumer of CH_2O , and are often areas experiencing high gradients and shear. This behaviour indicates that CH_2O may be useful as a marker for low-temperature chemistry as well as a potential indicator for increased levels of flame extinctions.

In conditional mixture fraction space, extinctions along the flame-air shear layer are observed to increase in frequency during the transient similarly to observations in past experiments, however complete extinguishing in η -space is not observed during LBO. The instantaneous proportion of the flame isosurface area containing extinguished regions is quantified using the extinguished fraction. The extinguished fraction results for the three flames show that the proportion of extinctions along the isosurface does increase to a discernible peak, although less than 50% of the total isosurface area is extinguished during the transient. This is in contrast to behaviour in gaseous non-premixed flames, where the stoichiometric isosurface is nearly fully extinguished as the flame blows off. The lack of strong local extinctions is likely caused by the low scalar dissipation rates observed in conditional mixture fraction space, where $N|\eta_{st}$ values never reached higher than 60% of the critical quenching value $N_{st,cr}$.

In the LBO simulations, flame shape in three-dimensional space using isosurfaces of ξ_{st} is shown to shrink downwards and inwards toward the bluff body during the transient. Some of the flames exhibit asymmetry, where half of the flame appears to be missing as the isosurface rotates around the bluff body edge in a wedge-like shape. The same asymmetric behaviour was observed in experiments with Jet-A as well as in experiments involving other low-volatility fuels such as n-decane and n-dodecane. This flame asymmetry is postulated to be caused by the phenomena of fuel starvation, which

is experienced by the flame when temperatures are not high enough to fully vaporise and burn the fuel, thus starving the flame to partial extinction. In a cross-sectional analysis of fuel mass fraction and temperature during the transient, unburnt gaseous fuel is observed in regions of lower temperature. This fuel, which has not yet undergone pyrolysis, quenches parts of the flame. Peak quantities of the parent fuel also decrease during LBO. Fuel starvation is proposed to play a significant part in the physical process of spray flame lean blow-off.

The effects of fuel starvation are shown to contribute to the blow-off of spray flames. Fuel starvation is caused by reduced temperatures in the recirculation zone, which both decreases evaporation rates as well as reduces pyrolysis of the vaporised fuel. Local extinctions contribute to the fuel starvation by reducing the temperature and evaporation and increasing the scalar dissipation rate. Combined, local extinction and fuel starvation can cause blow-off of the flame.

However the lack of high scalar dissipation rates above the critical quenching value warranted further investigation of the levels of extinction seen in conditional mixture fraction space. The OH mass fraction conditioned of the stoichiometric mixture fraction value filtered onto the physical domain is analysed during the LBO transient. $\widetilde{\text{OH}}|\eta_{st}$ is fully burning well beyond the flame zone during the entire LBO transient as well as long after the flame blows-off, indicating that the conditional space is not experiencing local extinctions. In contrast, isolines of resolved mixture fraction ξ from the LES at rich, stoichiometric and lean values are shown to shrink and reduce down to just above the bluff body, and peak ξ values fall below 0.2 resulting in a very lean mixture in the chamber overall.

This contrast in behaviours leads to the conclusion that in these LBO simulations fuel starvation is driving the blow-off of these spray flames. It is likely a weakness of using the AMC model to close the conditional scalar dissipation rate at such lean conditions, as it is a bell-curve distribution with the ends fixed at $\eta = 0$ and $\eta = 1$. It is not able to shift the distribution toward the lean left side as peak resolved mixture fractions become very lean. This results in low scalar dissipation rates at the stoichiometric mixture fraction. This also likely has an effect on the blow-off velocity results for the three flames. With few local extinctions and low scalar dissipation rates, higher air velocity is required in simulations to extinguish the flame globally compared to experiments. It is recommended for spray flames that a more complex model to close the conditional scalar dissipation rate is used at such lean conditions so that it can take the narrowing mixture fraction PDF into account.

7.5 Key Contributions

This work demonstrates that the LES-CMC approach is capable of modelling LBO phenomena of liquid aviation fuel and paves the way for more research and modelling of alternative liquid fuels. This is a step toward future computational models which can assist the combustion engineer in assessing flame stability and tendency to blow-off in the jet engine at the design stage.

The key contributions include:

- detailed analysis of intermediate species, including soot precursors and markers of extinction, and their response to varying amounts of scalar dissipation, pressure, and air velocity.
- the first known attempt to simulate the blow-off curve of a practical fuel, which was achieved within 5–20% of experimental air velocity values.
- emphasizing the role of fuel starvation as a driving cause of LBO in spray flames.
- evidence of fuel starvation phenomena, such as asymmetric flame shapes, presence of unburnt droplets, and shrinking flame isosurfaces, which are replicated against experiments.

7.6 Recommendations and future work

The objectives of this thesis were to characterise extinction and blow-off behaviour of conventional and alternative kerosene fuels, as well as to investigate causes of LBO in spray flames using numerical simulations. Based on the findings of this work, the following suggestions are made:

- Looking at conditional values directly from CMC, local extinctions due to high scalar dissipation rate above the critical extinction value are not observed, and fully burning behaviour of $\widetilde{\text{OH}}|\eta_{st}$ is shown to remain even after the blow-off event has ended for the flame. This may be a weakness of the fixed AMC distribution used to close the conditional scalar dissipation rate. This could be improved by using a more complex model to close the conditional scalar dissipation rate, such as the one developed in Devaud et al. [2004], which takes into account the mean and variance of the mixture fraction and their gradients, the turbulent scalar flux, and the mean velocity.

- The stable LES-CMC simulation for Jet-A should be examined more deeply with regard to the spray characteristics and tests should be made to assess the effects of droplet injection velocity and coarseness of the CMC mesh on the flame structure. Analysis should be made between detailed chemistry and simpler mechanisms to determine why in some cases of past studies one-step chemistry appears better able to predict the location of peak HRR along the spray at stable conditions when compared to experiments.
- LES-CMC simulations of the alternative C1 and C5 fuels should be run at stable and near-blow-off conditions to analyse the effects of liquid fuel properties and unusual chemistry on local extinction and blow-off behaviour. Extinction transient and reignition behaviour of the alternative fuels should be investigated in the 0D-CMC context.
- The spatial presence of CH mass fraction in the combustor should be investigated for its relevance to identification of heat release rate and extinction locations in experiments. Studies of $\text{CH} \times \text{CH}_2\text{O}$ profiles should also be made to assess whether it is an improvement on the $\text{OH} \times \text{CH}_2\text{O}$ correlation.
- Quick and efficient soot modelling using the methodology developed recently in Gkantonas et al. [2020] should be used to attempt prediction of the sooting propensity of the jet fuels LES-CMC results.

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Appendix A

Liquid fuel properties for Jet-A

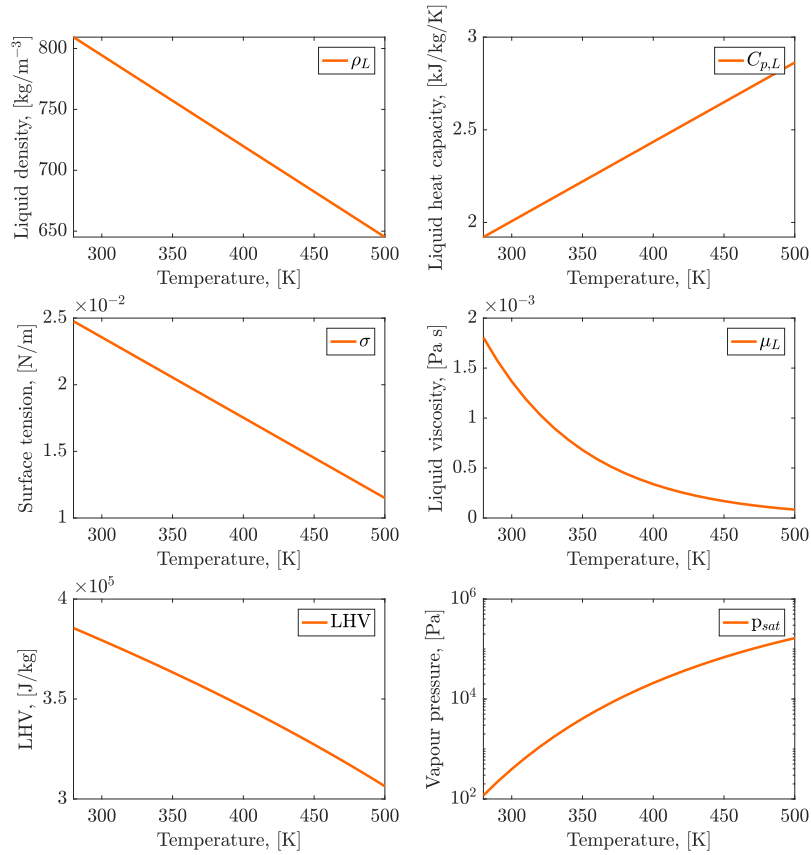


Fig. A.1 Liquid fuel property fits for OpenFOAM functions based on those reported for Jet-A (HyChem A2) in Esclapez et al. [2017].

