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Department of Mechanical Engineering

**High-fidelity simulations and
data-driven modelling of turbulent
premixed jet flames**

Man Ching Dominic Ma

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Engineering

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Declaration of Authorship

I, Man-Ching Dominic Ma, declare that this thesis titled, ‘High-fidelity simulations and data-driven modelling of turbulent premixed jet flames’ and the work presented in it are my own. I confirm that:

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Abstract

In most practical premixed combustion devices, turbulence-flame interaction (TFI) is a key factor affecting flame structure, stability, and emissions. As a result, the overall aim of this thesis is to improve our fundamental understanding of the physical behaviour of TFI, as well as to develop models for TFI under various conditions. Direct Numerical Simulations (DNS) are used as a tool to address these goals.

This study investigates the effects of inflow turbulence on flame evolution and TFI, as well as the effect of Karlovitz number in turbulent premixed jet flames. This study also investigates the novel application of an evolutionary algorithm for developing algebraic Flame Surface Density (FSD) models. Three DNS cases of round jet methane/air flames are considered. Two of the jet flames are coupled to a long upstream pipe section to generate fully developed turbulent inflow conditions. The simulations are conducted with a modified version of the DNS solver HiPSTAR, extended in this study to include capabilities for combustion simulations. Single step chemistry was used to reduce the computational cost.

In the first two cases, the impact of turbulent inflow boundary conditions is investigated. The first flame is coupled with a fully developed turbulent inflow via simulation of the upstream pipe and the coflow region, while in the second flame a synthetic inflow boundary condition is generated with a digital filter-based method without including the upstream region. Differences in the turbulence kinetic energy resulted in a higher jet momentum and a longer flame for the case with the synthetic inflow compared to the flame with the fully developed turbulent inflow. The distributions of the flame front orientation in the near field are observed to differ between the two flames but differences decrease quickly downstream as distributions tend towards isotropy. While the difference between the inflow boundaries had a significant effect on global parameters such as flame length, the influence of the inflow conditions on local statistics related to turbulence-flame interaction appear to be limited to the near inflow region.

Next, DNS with fully developed inflow for two jets with different premixture temperatures are investigated. The difference in the laminar flame speed in these cases leads to different Karlovitz numbers. Comparison of the two flames shows differences in the jet and flame evolution. The scalar gradient, an important quantity in FSD modelling, is analysed by examining the tangential strain rate and curvature terms in its transport equation. The local Karlovitz number and mean shear are observed to influence the evolution of the terms in the transport equation. The common assumption of a balance

between the tangential strain rate and the flame curvature term made by existing algebraic models for the FSD is shown to be less applicable for the higher Karlovitz number flame.

Lastly, new algebraic models for the wrinkling factor in the context of Large-Eddy Simulation are developed using Gene-Expression Programming. The developed models are assessed a-priori and the performance of the models are found to be comparable or better than existing models.

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Nomenclature

a_t	tangential strain rate	α	heat release parameter
c	progress variable	β	Zel'dovich number
D	pipe diameter	Δ	filter size
Da	Damkohler number	δ_{th}	thermal flame thickness
$\mathbf{e}$	strain rate eigenvector	δ_z	Zel'dovich flame thickness
Ka	Karlovitz number	γ	specific heat ratio
k	wavenumber/Fourier mode	κ	flame stretch
k_m	flame curvature	λ	strain rate eigenvalues
l	length scale	λ_{ci}	swirling strength
Le	Lewis number	μ	dynamic viscosity
M	Mach number	ν	kinematic viscosity
$\mathbf{n}$	flame normal vector	$\dot{\Omega}$	chemical reaction rate
p	pressure	ω	vorticity
Pr	Prandtl number	Φ	equivalence ratio
R	pipe radius	ρ	density
Re	Reynolds number	Σ	Flame Surface Density
r	radial coordinate	τ	time scale
S_{ij}	strain rate tensor	Θ	normalised temperature
S_L	Laminar flame speed	θ	azimuthal coordinate
$\dot{Q}$	heat release rate	Ξ	Flame wrinkling factor
T	temperature	η	Kolmogorov length scale
t	time		
U	jet mean velocity		
u	velocity		
Y_R	reactant mass fraction		
z	streamwise coordinate		

List of Publications

Ma, M. C., Talei, M., and Sandberg, R. D. (2018). DNS of a Turbulent Premixed Jet Flame with Fully Developed Turbulent Inlet. *21st Australasian Fluid Mechanics Conference*.

Ma, M. C., Talei, M., and Sandberg, R. D. (In Press). Direct Numerical Simulation of turbulent premixed jet flames : Influence of inflow boundary conditions. *Combustion and Flame*.

Chapter 1

Introduction and Literature Review

1.1 Motivation

Computational Fluid Dynamics (CFD) of reacting flows plays a major role in the study of turbulent premixed combustion for practical applications and fundamental research. Over the last few decades, the use of Direct Numerical Simulations (DNS), which describes the reacting flows without the use of models for turbulence and turbulence-flame interactions, has been on the rise as computational power increased. A review of turbulent combustion DNS studies through the years shows an obvious trend of increasing scale and complexity of simulations (Poinsot et al., 1996; Chen, 2011; Im et al., 2016). Although DNS for practical applications is still not computationally feasible, the myriad of fundamental discoveries have no doubt contributed to improving the design of those practical systems. DNS has been used to further understand various phenomena such as turbulence-flame interactions (TFI) (Sankaran et al., 2007; Wang et al., 2016), ignition/extinction (Klein et al., 2008), flame-wall interaction (Gruber et al., 2010; Lai and Chakraborty, 2016).

In addition to improving the fundamental understanding of combustion physics, DNS has also aided in the difficult tasks of development and validation of models for lower order simulation methods such as Reynold-Averaged Navier-Stokes (RANS) calculations, and increasingly for Large-Eddy Simulations (LES) where larger scales are resolved while only the smaller scales are modelled. In particular, the increase in the availability of high-fidelity data in recent years has brought about the emergence of data-driven modelling approaches such as machine learning in turbulence modelling (Duraismy et al., 2019). Even more recently, the potential of data-driven approaches has been realised in the

combustion modelling community, such as the application of Neural Networks-based methods for modelling reaction rates (Blasco et al., 2000; Franke et al., 2017).

This thesis intends to contribute to the field of turbulent premixed combustion by introducing new toolsets for conducting and analysing DNS of turbulent premixed flames and modelling.

A review of the literature is presented in Section 1.2. At the end of the literature review, the research aims of this study are presented in Section 1.4. The numerical methods of this study are discussed in Chapter 2, including the implementation and validation of the reacting flow capabilities into the DNS solver. Post-processing tools and the machine learning algorithm are also discussed. At the end of the chapter, the computational setup of the DNS cases are presented. In Chapter 3, the influence of inflow turbulence generation methods on the flame and jet flow development and TFI is examined. Chapter 4 extends the analysis of global flame and jet flow characteristics and TFI to turbulent premixed jet flames with different Karlovitz numbers. The DNS datasets are then applied in a machine learning approach to develop LES models for TFI in Chapter 5. Finally, a summary of the research is provided in Chapter 6, as well as the recommendations for future work.

1.2 Literature Review

1.2.1 Fundamentals of premixed turbulence-flame interaction

Flames have been traditionally categorized into two groups: non-premixed and premixed. In non-premixed combustion, the fuel and the oxidizer are brought together from the opposite sides of the reaction zone. Non-premixed flames are also called diffusion flames, since reaction rates are influenced by micro-mixing within the flame front. In premixed combustion, the reaction zone separates the unburnt “fresh” mixture from the burnt mixture (Peters, 2000). A wide variety of engineering applications operate in the premixed combustion regime, such as spark ignition engines and premixed gas turbines. Figure 1.1 shows a sketch of some basics features of the structure of a laminar premixed flame. On the fresh mixture side, the mass fraction of the reactants Y_R is 1. A preheat zone observes an increase in the temperature of the mixture, indicated by the normalised temperature $\Theta = (T - T_u)/(T_b - T_u)$ where T_u is the fresh mixture temperature and T_b is the burnt mixture temperature, due to the diffusion of heat from the reaction zone. When the reactants reach sufficient temperatures for combustion to occur, the value of Y_R decreases as reactants are consumed in the reaction zone with a reaction rate $\dot{\Omega}$.

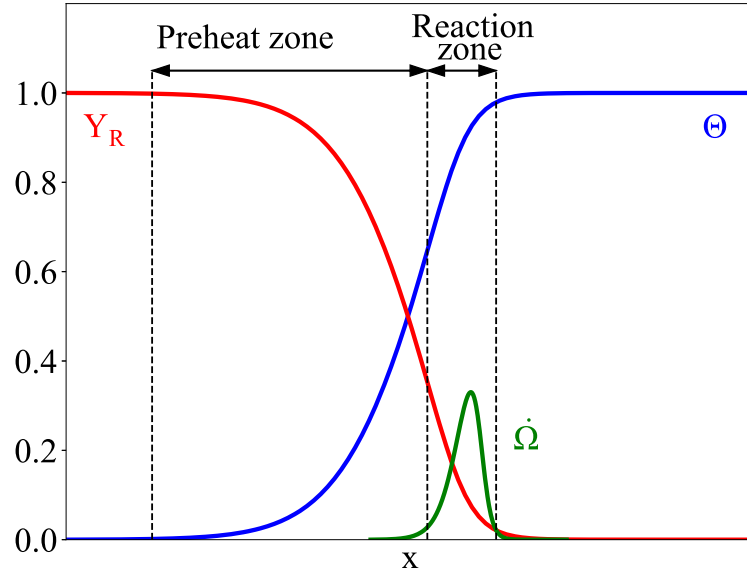


FIGURE 1.1: Sketch of laminar premixed flame structure.

In most combustion systems, flames in highly turbulent flow environments are encountered. The flame structure is stretched and distorted by turbulent structures, as depicted in Figure 1.2. At the same time, the turbulent structures are affected by thermodynamic effects, i.e. fluid expansion, from the combustion process (Clavin, 1985). It is clear that the coupling of turbulence and chemistry introduces a greater complexity to the already difficult problem of turbulence.

Turbulence is most often characterised by the turbulent Reynolds number,

$$Re_t = \frac{u' l_t}{\nu}, \quad (1.1)$$

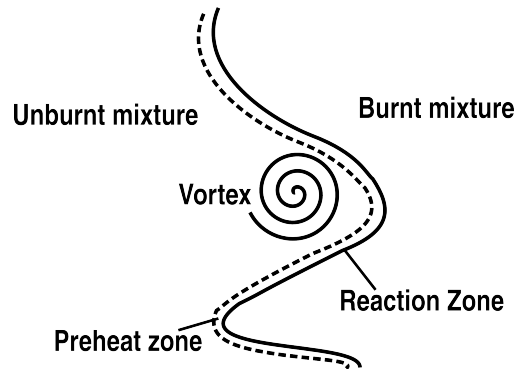


FIGURE 1.2: Interaction of vortex with flame front.

where u' is the velocity fluctuation, l_t is the integral length scale, and ν is the kinematic viscosity of the fluid. Premixed flames also possess an intrinsic characteristic flame speed due to their self-propagating nature, the laminar flame speed S_L . The presence of a laminar flame speed means that there is a single characteristic velocity scale. Turbulent premixed combustion regimes can be identified by a length scale ratio and a velocity scale ratio. The Damköhler number obtained from the turbulent integral length scale τ_t and the chemical time scale τ_c is defined as,

$$Da = \frac{\tau_t}{\tau_c} = \frac{S_L l_t}{u' \delta_l}, \quad (1.2)$$

where δ_l is the laminar flame thickness. For a high Damköhler number ($Da \gg 1$), the chemical time scale is short compared to the turbulent time scale, and the reaction zone is considered "thin". For a thin flame, the flame surface is distorted by the turbulent flow field, but the internal structure of the flame is not affected by turbulence.

In addition to the Damköhler number, the Karlovitz number is often used to categorise premixed combustion regimes, and is defined as

$$Ka = \frac{\tau_c}{\tau_k} = \frac{u_k \delta_l}{S_L l_k}, \quad (1.3)$$

describing the ratio of the chemical time scale to the smallest turbulence time scales, Kolmogorov scales τ_k , where l_k is the Kolmogorov length scale and u_k is the velocity of the smallest turbulent structures. Based on Kolmogorov's theory, the length and velocity scales for isotropic turbulence can be described as (Pope, 1988),

$$l_k = (\nu^3/\epsilon)^{1/4}; \quad l_t = (u'^3/\epsilon); \quad u_k = (\nu\epsilon)^{1/4}, \quad (1.4)$$

where ϵ is the turbulent kinetic energy dissipation rate. Equation 1.3 can then be written as

$$Ka = \left(\frac{u'}{S_L}\right)^{3/2} \left(\frac{l_t}{\delta_l}\right)^{-1/2} = \sqrt{Re_t/Da^2}. \quad (1.5)$$

Figure 1.3 shows the categorisation of premixed flames into regimes (Peters, 2000). Four turbulent regimes have been identified:

- The wrinkled flamelet (WF) regime is characterised by a velocity ratio $u'/S_L < 1$. The turnover velocity of the largest turbulent eddies is smaller than the laminar flame speed, and the eddies cannot affect the inner structure of the flame. The flame is wrinkled, but propagates like a laminar flame.
- The corrugated flamelet (CF) regime is characterised by $u'/S_L > 1$, but with $Ka < 1$. The distortion of the flame is sufficient to increase the propagation

speed. The smallest eddies are still larger than the characteristic length scale of the flame, and therefore will not affect the internal structure of the flame.

- The thin reaction zone (TRZ) regime is characterized by $1 < Ka < 100$. The small eddies are able to penetrate into the preheat zone, resulting in greater thermodiffusivity. The structure of the preheat zone is affected by turbulence while the reaction zone is still unaffected.
- The broken reaction zone (BRZ) regime is characterised by $Ka > 100$. The Kolmogorov length scale is much smaller than the laminar flame thickness, small eddies are able to penetrate into the reaction zone, altering the inner structure of the flame. The intense straining by turbulence can lead to local extinction in the reaction zone of the flame. A consequence of these local extinction events is an increase of pollutant production.

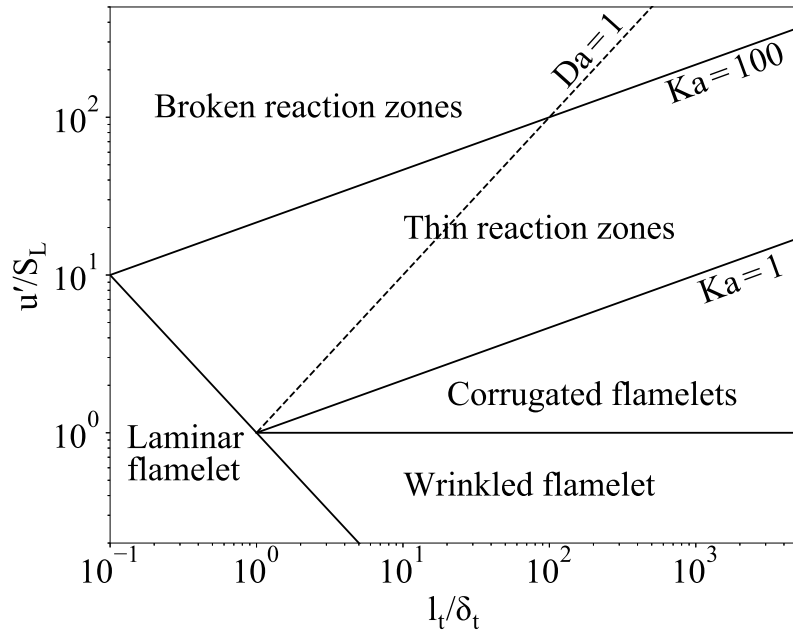


FIGURE 1.3: Turbulent premixed combustion diagram, adapted from (Peters, 2000).

The majority of turbulent premixed flames in engineering applications can be found in the CF and TRZ regimes and in most cases, these different regimes can be present at the same time (Peters, 2000).

1.2.2 Direct Numerical Simulation of turbulent premixed jet flames

1.2.2.1 Overview

DNS of turbulent flows is a high fidelity simulation approach that aims to solve the Navier-Stokes equations by resolving all the length and time scales of turbulence. The extension of DNS to reacting flows involves the consideration of how to represent the flame front and how it interacts with the turbulent fluctuations of the flow field. The presence of a flame poses another layer of complexity as the length and time scales associated with the flame often differ greatly from those of turbulence. This can further increase the resolution requirements of the simulations. The attractiveness of DNS is the ability to obtain fully resolved information, making it a useful tool for studying different aspects such as TFI (Sankaran et al., 2007; Cifuentes et al., 2014; Wang et al., 2017a), ignition/extinction (Klein et al., 2008), flame-wall interaction (Gruber et al., 2010; Lai and Chakraborty, 2016), flame acoustics (Liu et al., 2012; Jiménez et al., 2015; Haghiri et al., 2018), radiation effects (Wu et al., 2005), emissions (Hawkes and Chen, 2004), and model development (Chakraborty and Klein, 2008; Lipatnikov et al., 2015)

The turbulent premixed jet flame is an important configuration to study. The presence of a developing shear layer can affect the interaction between flame and turbulence. Since the dynamics of TFI are influenced by local fluid dynamics and chemical processes, spatial variations lead to changes in the local Karlovitz number (Hartung et al., 2008).

Figure 1.4 depicts a few examples of DNS studies of spatially developing jet flames and their approximate conditions on the regime diagram. It is interesting to see that a large majority of DNS studies of jet flames are in the TRZ regime. This is partly because traditional engineering devices tend to operate around the TRZ regime. The restrictions imposed by the turbulence and chemical scales is a major consideration, and one of the challenges is to push the use of DNS to study a wide variety of flames with different operating conditions.

1.2.2.2 Turbulence-flame interactions

The interactions between turbulence and premixed flames have been a topic of interest for decades. One of the main interests is the role of TFI in the production and dissipation of the scalar gradient, or progress variable gradient $|\nabla c|$. The quantity $|\nabla c|$ is an important parameter in turbulent premixed flame modelling.

The presence of the flame affects the turbulent flow through heat release induced pressure perturbations, often quantified by the dilatation rate. The effect of heat release

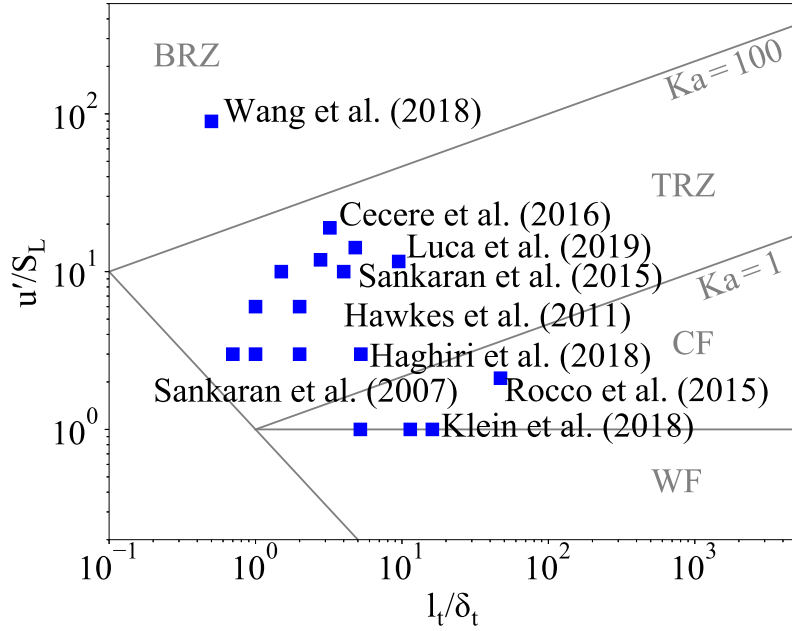


FIGURE 1.4: Turbulent premixed combustion diagram with examples of approximate conditions of jet flame DNS in literature.

is particularly evident for flames in the flamelet regime. Vortex stretching is the main mechanism for the transfer of turbulence kinetic energy to smaller scales where dissipation occurs. The alignment of the vorticity vector with the extensive principal strain rate is an indicator of an increase in vortex stretching, and thus dissipation. This has been observed for high Da flames (Chakraborty, 2014). However, in the presence of higher turbulence, such as in the broken reaction zone regime or even to various degrees in the thin reaction zone regime, turbulence effects can dominate the effect of the heat release. In this case, vorticity will preferentially align with the intermediate principal strain rate (Hamlington et al., 2011; Wang et al., 2016), similar to a non-reacting scalar surface (Ashurst et al., 1987; Nomura and Elghobashi, 1992).

In addition to the flame influence on turbulence, the opposite also occurs where turbulence influences the flame structure. In an unstrained laminar flame, $|\nabla c|$ is the result of a balance of gradient production by chemical processes and gradient dissipation by molecular diffusion. Under the influence of turbulence, the production/dissipation of $|\nabla c|$ is affected by the stretch rate of the flame surface and flame thickening, which are affected by local strain rates and curvature (Candel and Poinso, 1990). The flame tangential strain rate is often used to represent turbulent straining because the flame normal strain rate is affected by heat release across the flame brush. This is illustrated in Figure 1.5 (Steinberg and Driscoll, 2009), which depicts the effect of strain-rate and

vortical structures on a flame surface as it propagates through various times t . Strain-rate structures stretch the flame at t_1 , while vortical structures curves the flame front at t_2 .

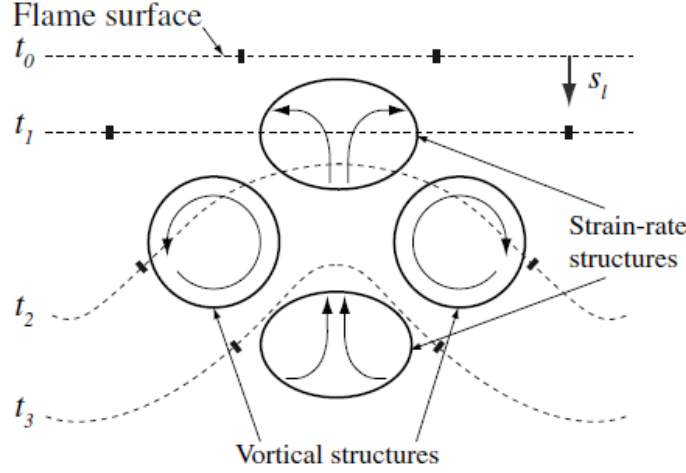


FIGURE 1.5: Illustration of the influence strain-rate and vortical structures on a flame surface by Steinberg and Driscoll (2009).

Steinberg and Driscoll (2009) showed that flame strain-rate is characterized by the fluid-dynamics strain-rate field rather than the vorticity field. Therefore, the flame strain rates are associated with the alignment of turbulence strain rates. For a passive scalar surface in a turbulent flow field, the surface normal aligns with the most compressive principal strain rate (Ashurst et al., 1987). The alignment of the surface normal with the compressive strain rate brings iso-surfaces together, contributing to the production of $|\nabla c|$.

Swaminathan and Grout (2006) analysed DNS of a turbulent premixed flame in the flamelet regime and found that the flame surface normal was preferentially aligned with the extensive principle strain rate instead, as shown in Figure 1.6. The effect of this alignment was the dissipation of $|\nabla c|$ as iso-surfaces are pulled apart. The difference in the alignment characteristics has been attributed to dilatation generated by high heat release rates. The heat release induced dilatation contributes to locally strong flow acceleration across the flame brush, acting in the direction normal to the flame surface. The preferential alignment of the flame surface normal with the extensive principal strain rate for flame with high heat release have been consistently observed in subsequent DNS studies (Chakraborty and Swaminathan, 2007a; Ahmed et al., 2014) and experiments (Hartung et al., 2008; Steinberg et al., 2012; Sponfeldner et al., 2015).

While it has been observed that turbulent premixed flames in the flamelet regime exhibit different alignment behaviour from passive scalar surfaces, studies have shown that this

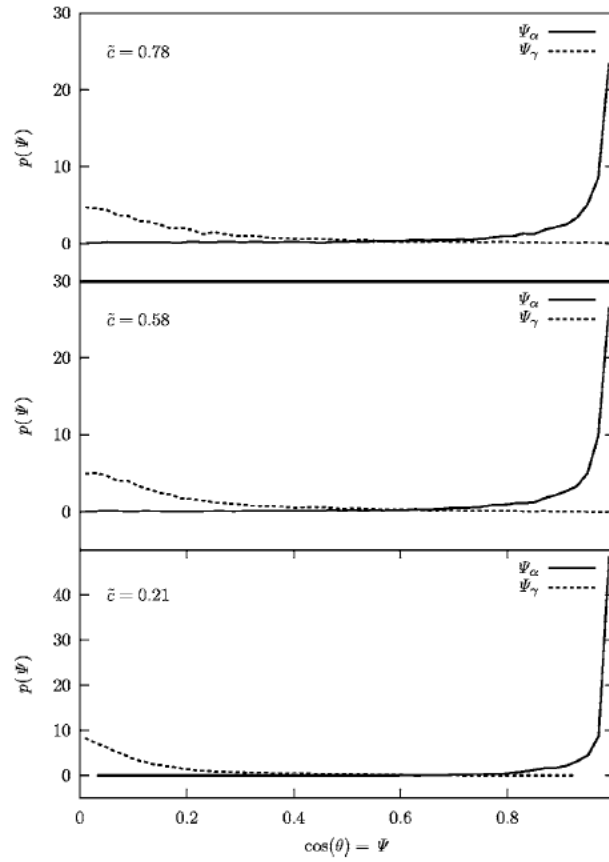


FIGURE 1.6: PDF of alignment between flame normal and the most extensive (α) and the most compressive (γ) principal strain rates by Swaminathan and Grout (2006).

is not necessarily applicable for flames outside the flamelet regime. Chakraborty and Swaminathan (2007a) observed that for a turbulent premixed flame front with $Ka > 1$ and $Da < 1$, the flame normal was preferentially aligned with the compressive principal strain rate for portions of the flame brush towards the fresh mixture, as shown in Figure 1.7. Although the generation of dilatation from heat release is persistent for flames in this regime, the effects were found to be locally competing with fluid dynamic processes, and alignment can vary across the flame brush (Chakraborty et al., 2009). In lower Damköhler number flames, the turbulence strain rates are stronger, overcoming the surface normal flow acceleration caused by heat release effects. As a result, the alignment characteristics are similar to those of a passive scalar surface. The preferential alignment between the flame normal and compressive strain rate for flames with lower Da and higher Ka have been reported in subsequent DNS studies (Kim and Pitsch, 2007; Chakraborty et al., 2010; Hamlington et al., 2011; Minamoto et al., 2011; Wang et al., 2016, 2017c; Nilsson et al., 2018)

DNS studies have also shown other factors that influence TFI. For example, Chakraborty et al. (2009) reported that the alignment with the extensive strain rate in the flamelet

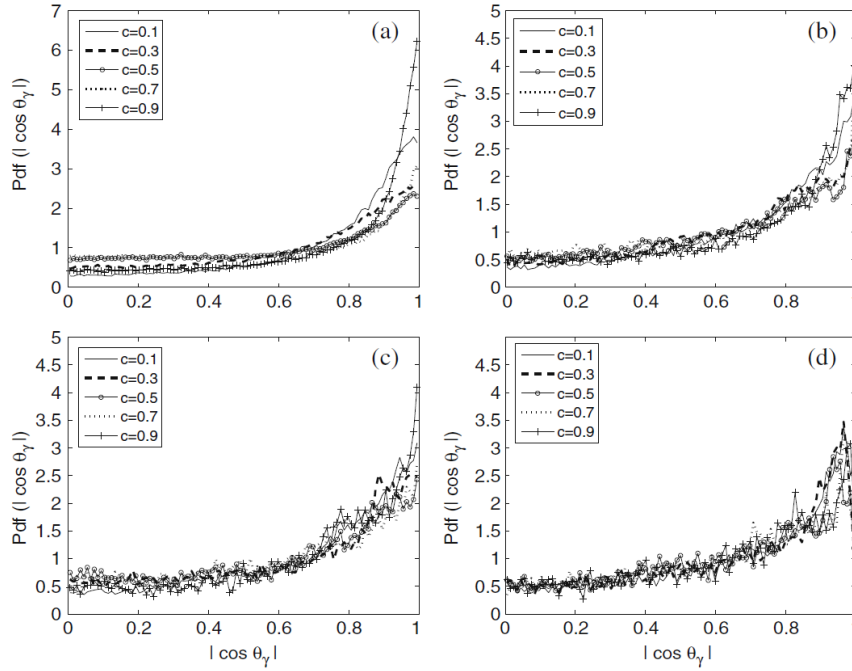


FIGURE 1.7: PDF of alignment between flame normal and the most compressive (γ) principal strain rates by Chakraborty et al. (2010).

regime increases with decreasing Lewis number.

Mean shear in the flow field has also been observed to influence TFI. Minamoto et al. (2011) compared statistically planar flames and V-flames, and attributed higher magnitudes of principal strain rates in the V-flames to the presence of the mean shear. They also found that the PDFs of the flame normal and principal compressive or extensive strain rates in the presence of strong mean shear does not peak at values of 1 or 0, but at intermediate values of $\cos \theta$. This alignment behaviour has also been observed in other DNS studies (Wang et al., 2016; Cecere et al., 2016). The contribution of strain rates imposed by the mean shear to the total flame tangential strain rate has been observed to have a significant influence on the mean flame (Wang et al., 2017b).

DNS studies have also examined the contribution of flame curvature to flame stretch. Dilatation was found to have a negative correlation with the curvature magnitude, resulting in a smaller influence of dilatation on TFI in regions of strong flame curvature (Chakraborty and Cant, 2005). Dopazo et al. (2015); Dopazo and Cifuentes (2016) analysed the production/dissipation of $|\nabla c|$ from the viewpoint of the normal strain rate using DNS. The effect of normal strain rate due to the fluid flow straining is balanced by contributions to normal strain rate induced by the variations of iso-surface propagation speeds, flame curvature, molecular diffusion, and chemical reactions.

It is clear that turbulence-scalar interactions, which are important in scalar gradient

production and dissipation, are influenced by many factors such as the level of turbulence, heat release, and mean flow. Chakraborty and Swaminathan (2007b) analysed the modelling of the TFI term in the scalar dissipation equation and noted the importance of capturing the effects of local Da on this term based on LES filter size and subgrid scale fluctuations. A review of flame surface density modelling will be given in Section 1.2.4.

1.2.3 Turbulent inflow boundary conditions

The challenge of the high computational cost of DNS was briefly discussed in Section 1.2.2.1. Reduction of the computational domain size can greatly decrease the total simulation cost, allowing the computational resources to be allocated to other areas such as the level of resolved turbulence length and time scales and the details of chemistry. Many canonical non-reacting flow simulations observe self-similarity in the flow direction, such as in a channel flow, enabling the use of periodic boundary conditions. These cases can exploit the periodicity to reducing the size of the computational domain. Additionally, these types of boundaries are also much simpler to define in comparison to boundary conditions such as inflow conditions. On the other hand, even the simplest canonical turbulent reacting cases often cannot exploit periodic boundary conditions as the separation of reactants and products on different sides of the flame front eliminates periodicity in the direction normal of the flame front. Due to this limitation, domain size are often confined to an area of interest. However, this will introduce another complication; the closer the boundaries of the domain are to the area of interest, the greater the influence of the boundary conditions on this region. Significant errors can be introduced due to the uncertainty of imposed boundary conditions in their ability to replicate the appropriate flow physics at the boundaries. Particularly, the inflow conditions which provides the turbulence feed data for spatially developing reacting flows, such as turbulent premixed jet flames, is important in flow and flame development.

The most common location to impose inflow boundary conditions in DNS is at the jet flame base (Sankaran et al., 2007; Lodato et al., 2008; Yoo et al., 2011; Wang et al., 2017a; Haghiri et al., 2018). In such cases, the inflow boundary conditions play a large role in turbulent flame simulations, i.e. the mean flow and fluctuations generated by the inflow boundary conditions can affect the flow development downstream. Dhamankar et al. (2015) recommended a list of criteria required for an ideal turbulent inflow boundary condition, including the ability to reconstruct all known turbulence information, requiring no adjustment length beyond the inflow boundary, not introducing non-physical artifacts into the field, minimising the cost of computation, storage, and data input, being independent of spatial discretisation and grid type, and being adjustable for a

wide range of flow problems. It is clear that achieving an ideal boundary condition is a tremendous task, and even the current methods fall short in some of these criteria. The most commonly used methods for generating turbulent inflow boundary conditions include library-based methods which use an outside dataset as an input for the inflow boundary, recycling methods in which the turbulent flow data from the domain is rescaled to be used as the inflow, or synthetic turbulence methods in which ad hoc fluctuations are generated in an attempt to replicate the inflow turbulence (Dhamankar et al., 2015). The synthetic turbulence methods can vary in complexity, cost, and accuracy. Examples include random noise (Passot and Pouquet, 1987), Fourier-transform methods (Lee et al., 1992), Proper Orthogonal Decomposition methods (Druault et al., 2004), diffusion-based methods (Kempf et al., 2005b), and digital filter (DF) methods (Klein et al., 2003).

Experimental studies have shown that the turbulent inflow boundary conditions have an impact on the jet development. Studies have used different nozzle geometries to generate the inflow boundary conditions for non-reacting free jets (Mi et al., 2001; Xu and Antonia, 2002; Langman et al., 2007). The nozzle geometries included a long pipe which resulted in small-scale turbulent structures emerging from a developed turbulent flow in a pipe dominating the near field only, and a contraction nozzle which resulted in a top-hat velocity profile leading to larger roll-up structures formed in the jet shear layer. The results showed that the classical view of universal self-similarity, where jets with different inflow profiles will converge to a universal spreading and decay rate in the downstream region, was incorrect. Xu and Antonia (2002) examined this effect on the velocity field and found that the spreading rate and the streamwise decay rate of the mean velocity were higher for the contracting nozzle jet in comparison with the long pipe jet due to large scale coherent structures formed by higher anisotropy in the mean flow. Similarly, temperature profiles examined by Mi et al. (2001) showed a higher spreading rate and streamwise decay rate for the contracting nozzle jet, though the long pipe jet exhibited higher molecular mixing due to fine-scale mixing. Burattini and Djenidi (2004) modified the inflow coherent structures by placing a grid at the nozzle exit, and similarly found lower decay rates for the inflow with weaker coherent structures.

The influence of the inflow boundary conditions is also highlighted in the numerical studies of non-reacting flows. For instance, the DNS study by Boersma et al. (1998) demonstrated that using two different mean velocity profiles does not lead to a universal self-similarity, leading to the question of the sensitivity of results in using synthetic turbulence generation methods in jet flow simulations. Glaze and Frankel (2003) showed that modelling the turbulent inflow has a crucial role in the correct prediction of jet development. As shown in Figure 1.8, it was found that Gaussian random forcing had a poor performance compared with an improved stochastic technique generating spectral

fluctuations. They showed that for the Gaussian random forcing method, the problem arises from a quick dissipation of turbulent fluctuations downstream of the inflow. Underprediction of turbulence kinetic energy due to the inflow boundary conditions was also observed in other studies (Herff et al., 2017; Bogey and Bailly, 2005), which have been attributed to missing azimuthal modes from the turbulent inflow boundary condition. In the DNS of a long pipe/jet configuration, Sandberg et al. (2012) observed a sharp increase in skin friction towards the trailing edge of the pipe, which caused a drop in the shear stress of the exiting flow. On the other hand, this effect was not observed in the simulations done by Bühler et al. (2014) where only a short pipe was used and the pipe flow had not yet become fully developed.

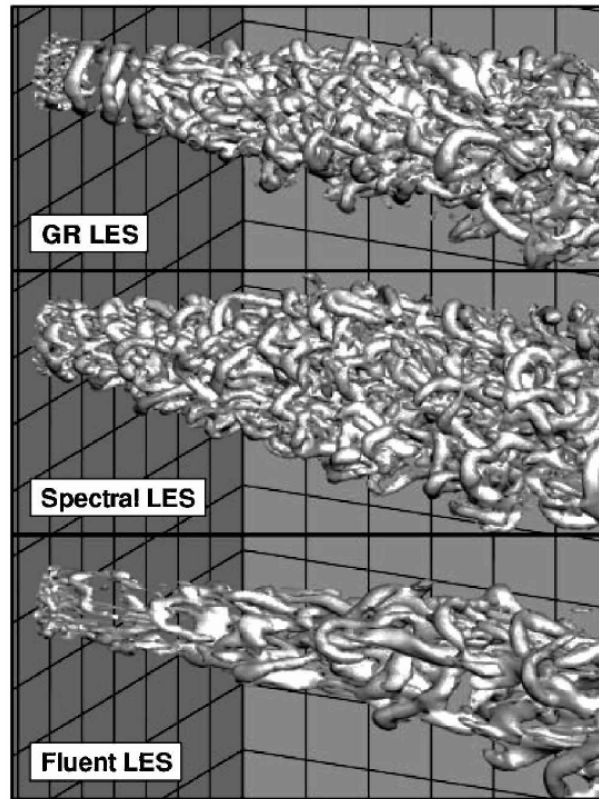


FIGURE 1.8: Visualization of instantaneous vortical structures in LES of turbulent jets with different turbulence inlet conditions by Glaze and Frankel (2003).

The impact of the inflow boundary conditions on turbulent flames has been relatively less studied. An experimental study in this context was performed by Langman et al. (2007). They examined the influence of the inflow boundary conditions on a non-premixed flame by injecting natural gas through a long pipe in one case and a contraction nozzle in the other case. Interestingly, they also found an important role of the boundary conditions on the global flame characteristics. The pipe case was found to feature a shorter flame due to a higher molecular mixing. Numerical studies of non-premixed flames have also

identified some issues related to the inflow boundary. For instance, Kempf et al. (2006) discussed the necessity for refining the grid at the inflow to avoid numerical diffusion and therefore artificial mixing. Furthermore, the effects of reaction on the flow upstream of the inflow boundary could not be captured when the inflow boundary conditions were specified. Furthermore, Prasad et al. (2013) suggested that a better representation of the velocity-scalar correlations at the inflow can be achieved by including the pipe in the upstream region. Differences in turbulence intensity at the inflow were found to cause differences in the scalar mixing, thereby affecting reaction rates and heat release (Afarin and Tabejamaat, 2013). Inflow conditions can also influence important flame physics such as flame base stability (Yoo et al., 2011) and differential diffusion (Nambully et al., 2014).

The above studies have shown that the setup of inflow boundary conditions is not trivial, as there is clearly a tradeoff between reduction of domain size to decrease computational cost and increase in influence of the boundary conditions. There is still a lack of DNS studies which focus on the effect of inflow boundary conditions on the flame and flow fields.

1.2.4 Turbulent Premixed Flame Modelling

1.2.4.1 Overview

The high computational cost of resolving all the scales in realistic turbulent reacting flows prohibit extensive use of DNS. Industrial design processes typically require a quick turnaround time in the design phase, where simulations would often be employed. Additionally, simulations in the design process would involve multiple iterations. These requirements drive the need for approximate simulation methods to reduce the simulation costs. At the heart of this problem is a reduction in the range of length and time scales that are to be solved.

Turbulent combustion modelling typically involves the introduction of models for the description of the flame front and its interaction with flow turbulence into existing turbulent flow modelling techniques. One traditional approach is the Reynolds-Averaged Navier-Stokes (RANS) modelling where the averaged governing equations are solved, which is a low cost approach. However, the lack of accuracy of RANS, especially in highly non-linear combustion phenomena, and the inability to capture transient effects, have necessitated the development of higher fidelity methods.

Large Eddy Simulations (LES) is an increasingly popular compromise between RANS and DNS, which resolves a range of scales from the integral scales to the scales in the

order of a cut-off scale, and models scales that are smaller. LES, unlike RANS, can capture transient effects which are often necessary for combustion phenomena.

The progress variable transport equation can be derived by applying a filtering operation to c such that

$$\bar{\rho}\tilde{c}(x) = \int \rho c(x^*) F(x - x^*) dx^*, \quad (1.6)$$

where F is the LES filter which suppresses the components greater than a cut-off frequency, and the integration is over the entire flow domain. The resulting Favre-filtered transport equation for c is

$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{c}}{\partial x_i} = -\frac{\partial}{\partial x_i} [\bar{\rho}(\tilde{u}_i\tilde{c} - \tilde{u}\tilde{c})] + \bar{\tilde{\Omega}}, \quad (1.7)$$

where the general quantities $\bar{\Phi}$ and $\tilde{\Phi}$ now denote LES filtered and Favre filtered quantities, respectively, rather than averaged quantities. Combustion modelling in LES is necessary at the scales below the filter scale to capture the chemical reactions (Peters, 2009). In Eq. 1.7, unclosed terms that appear as a result of the filtering operation are the unresolved scalar flux $(\tilde{u}_i\tilde{c} - \tilde{u}\tilde{c})$ and the filtered chemical reaction rate $\bar{\tilde{\Omega}}$. Models are needed to express the unclosed terms as functions of known quantities. The development of models is important as they affect the accuracy of the simulations.

Models for premixed combustion generally fall under one of two categories: statistical approaches and geometric approaches. The statistical approach describes the flame front internal structure by focusing on statistical properties of intermediate states within the flame front, i.e. using probability density functions (PDF). Examples of statistical approaches are the Bray-Libby-Moss model (BML) (Bray and Moss, 1977), Conditional Moment Closure (CMC) (Klimenko, 1990; Bilger, 1993), and transported PDF methods (Anand and Pope, 1987). Statistical approaches are more popular in the modelling of non-premixed flames due to their suitability for describing the micro-mixing during combustion.

In geometric approaches, the flame is described as a geometric surface. Geometric approaches are more useful in the modelling of premixed flames as opposed to non-premixed flames. The reason is that for a sufficiently thin flame, the flame front dynamics can be described as the propagation of a surface, rather than being described by the micro-mixing as is the case for non-premixed flames. As such, it is often not necessary to work out the statistics within the flame front. The evolution of scalar fields are represented by the dynamics and properties of iso-surfaces. Examples of geometric approaches are the G-field and flame surface density models.

The G -field models take a level-set approach to represent the flame front (Peters, 2000). In Eq. 1.7, where the flame front is described by the evolution of the iso- $\tilde{c}$ surfaces, a G field is introduced where the flame surface is represented by the level $G = G_0$, where G is a nonreacting scalar. The internal flame structure does not need to be resolved on the computational mesh, since only the G -field needs to be resolved. The equation for the evolution of G is then written as,

$$\frac{\partial \tilde{G}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \tilde{G} = \frac{\rho u}{\bar{\rho}} S_T \left| \nabla \tilde{G} \right|. \quad (1.8)$$

where $G(x)$ is the distance of the location x to the flame front. A model needs to be provided for the turbulent flame speed S_T . The variable S_T is not a fully well defined quantity. Experimental data exhibit a large scatter of S_T values depending on various parameters such as chemistry characteristics, turbulence scales, and flow geometry (Gouldin, 1996). Various approaches are presented in the literature for obtaining the progress variable c from the G -field. The most straightforward approach constructs the c field based on the distance normal to the G surface, though this approach suffers inaccuracy especially for high flame front curvature zones. Other approaches involve the modelling of the chemical source term as a function of the G -field (Schlimpert et al., 2017; Gicquel et al., 2012), or from reconstructing the temperature field (Kim et al., 1999).

In this study, the focus is the flame surface density modelling approach, which is discussed further in detail in Section 1.2.4.2.

1.2.4.2 Flame surface density models

1.2.4.3 Overview

Flame Surface Density (FSD) models are popular approaches in both RANS and LES modelling of turbulent premixed combustion, and two concepts for the different modelling strategies are closely related. These models are based on a geometric view of the flame. In particular, they are related to the properties of the local flame surface geometry (Pope, 1988). The geometric models are typically associated with the assumption of a sufficiently thin flame.

The averaged or filtered reaction rate of fuel can be expressed as

$$\bar{\dot{\Omega}} = \Omega_L \Sigma, \quad (1.9)$$

where Σ is the flame surface density, describing the flame surface area per unit volume and Ω_L is the fuel laminar mass consumption rate per unit surface. Equation 1.9 decouples the chemical contribution described by Ω_L from the TFI described by Σ . The flame surface density is defined for an iso-surface of c , c^* , as

$$\Sigma(c^*) = \left(\overline{|\nabla c| | c = c^*} \right) \bar{P}(c^*), \quad (1.10)$$

where $\left(\overline{|\nabla c| | c = c^*} \right)$ is the conditional average of $|\nabla c|$ for $c = c^*$ and $\bar{P}(c^*)$ is the probability to find $c = c^*$ at the given location. The quantity $|\nabla c|$ is known as the surface density function (SDF). Equation 1.10 is derived under an infinitely thin flame assumption, and is extended to flames which are not infinitely thin by integrating over iso-surface levels resulting in a generalized flame surface density:

$$\Sigma_{gen} = \int_0^1 \Sigma(c^*) dc^* = \overline{|\nabla c|}. \quad (1.11)$$

In the context of LES, the bar on the right term of Eq. 1.11 denotes filtered quantity (Boger et al., 1998), whereas in the context of RANS, it denotes ensemble averaging. Equation 1.9 can then be rewritten without the infinitely thin flame assumption as:

$$\bar{\dot{\Omega}} = \Omega_L \Sigma_{gen}. \quad (1.12)$$

The term Σ_{gen} can be described as the flame surface area per unit volume contained within the LES filtering volume, and its value approaches Σ as the filter size Δ approaches 0. The effect of filter size on Σ_{gen} can be seen in Figure 1.9, where it is clear that the level of detail in the flame structure decreases for larger filter sizes. In Eq 1.12, Σ_{gen} has to be estimated. The computation of Σ_{gen} is done either by the solution of a transport equation or by directly estimating it with an algebraic expression.

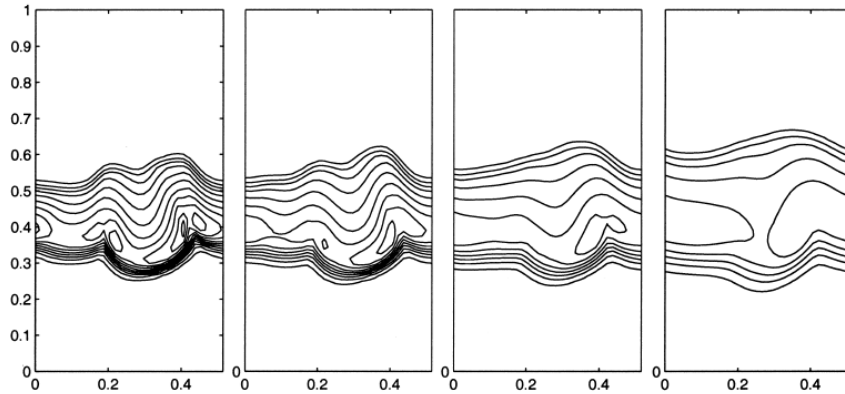


FIGURE 1.9: Flame surface density contours for increasing filter sizes from left to right by Hawkes and Cant (2001).

1.2.4.4 Flame wrinkling

Flame surface density can also be recast in terms of flame surface wrinkling, which is more often used in thickened flame modelling. The flame wrinkling factor Ξ is the ratio of the flame surface to its projection in the propagation direction, and is sometimes referred to as the flame surface area ratio. The flame wrinkling factor is related to the flame surface density by,

$$\Xi(c^*) = \frac{\Sigma(c^*)}{\left| \left(\overline{\nabla c} \right|_{c=c^*} \right) \bar{P}(c^*)}, \quad (1.13)$$

where $\bar{P}$ is the probability density function. Similar to Eq. 1.11, integrating over c iso-surface levels, results in the generalized flame surface wrinkling:

$$\Xi_{gen} = \Sigma_{gen} / |\nabla \bar{c}|. \quad (1.14)$$

The transport equation for Ξ is more complicated than the transport equation for Σ , but may have more convenient initial and boundary conditions since $\Xi \geq 1$ (Veynante and Vervisch, 2002). Various algebraic models have been proposed for the sub-grid flame wrinkling factor (Colin et al., 2000; Charlette et al., 2002; Fureby, 2005; Chatakonda et al., 2010).

The wrinkling factor can also be related to the turbulent flame speed by the relation

$$\frac{S_T}{S_L} = \Xi_{gen}, \quad (1.15)$$

and likewise S_T is related to Σ_{gen} by

$$\Sigma_{gen} = \frac{S_T}{S_L} |\nabla \bar{c}|. \quad (1.16)$$

1.2.4.5 Σ_{gen} transport equation

The transport equation have been derived by Pope (Pope, 1988) by means of the rate of change of an infinitesimal area element, and Candel and Poinso (Candel and Poinso, 1990) by means of transport equations for area and volume elements, with both derivations leading to the same unclosed equation. The LES filtered Σ_{gen} equation is

$$\begin{aligned} \frac{\partial \Sigma_{gen}}{\partial t} + \frac{\partial u_j \Sigma_{gen}}{\partial x_j} = & - \frac{\partial}{\partial x_i} \left[\overline{(u_i)_s} - \tilde{u}_i \right] \Sigma_{gen} + \overline{\left((\delta_{ij} - N_i N_j) \frac{\partial u_i}{\partial x_j} \right)_s} \Sigma_{gen} \\ & - \frac{\partial}{\partial x_i} \left[\overline{(S_d N_i) \Sigma_{gen,s}} \right] + \overline{\left(S_d \frac{\partial N_i}{\partial x_i} \right)_s} \Sigma_{gen}, \end{aligned} \quad (1.17)$$

where $\overline{(N_i)}_s = -(1/\Sigma_{gen})(\partial\bar{c}/\partial x_i)$ is the surface averaged flame normal, and $\overline{(S_d)}_s = S_L(1 + \tau c^*)$ is the surface averaged displacement speed. Four unclosed terms appear on the right-hand side in Eq. 1.17 which require modelling, including terms for the subgrid turbulent flux, tangential strain rate, surface propagation velocity, and effects of curvature. One way to obtain Σ_{gen} in Eq. 1.12 is to solve Eq. 1.17. The solution of the additional equation adds to the computational cost of simulation, and is a major factor to consider when choosing to use this approach.

1.2.4.6 Algebraic Σ_{gen} models

Another popular approach to obtain Σ_{gen} in Eq. 1.12 is to directly model the term using algebraic models. Algebraic models do not require the solution of an additional transport equation for Σ_{gen} , and therefore are less computationally expensive. Numerous algebraic models, such as those listed in Table 1.1, are available in the literature. These models have been analysed in works such as Klein et al. (2008); Katragadda et al. (2012); Ma et al. (2013), and often serve as baseline models in the development of new models (Klein and Chakraborty, 2018). In particular, most of these models can be expressed in terms of the flame wrinkling factor by Eq. 1.14. While dynamic FSD models are also available, the focus of this study will be on development of static models, and so the discussion in this section will mainly be limited to static models. The models are expressed in terms of Σ_{gen} , though some of the models were originally developed in terms of Ξ_{gen} or S_T and the two definitions are interchangeable by Eqs. 1.14 or 1.16. It is important to realise the conditions under which these models are derived, and their accuracy in predictions and applicability to different conditions. It is also important to consider their complexity in terms of calculation speed and ease of implementation.

The basis of most algebraic FSD models is an assumption of equilibrium between the subgrid production and destruction of FSD. Many models appear to be sufficiently accurate when there is a local balance between FSD production and dissipation, but suffer in accuracy under response to strain rate and curvature. The models can suffer from a lack of flame thickness control that can lead to predictions of flame being too thin and overpredicting the wrinkling. Most algebraic models for Σ_{gen} have been proposed for flamelet regime where Lewis number effects are not accounted for (Katragadda et al., 2012). A brief discussion of selected models is now given, so as to highlight some of the premise for the derivation of the models and their potential performance. Models will be referred to by the name of the first author from the works in which they were proposed.

The model proposed by Boger et al. (1998) is based on the classical RANS Bray-Moss-Libby model (Bray et al., 1989), containing the term $\bar{c}(1 - \bar{c})$. The filter size and an

Source	Model
Angelberger et al. (1998)	$\Sigma_{gen} = \left[1 + a\Gamma \left(\frac{u'_\Delta}{S_L} \right) \right] \nabla \bar{c} \quad (1.18)$ where $a = 1$, $u'_\Delta = \sqrt{2\tilde{k}_\Delta/3}$, $\tilde{k}_\Delta = (\widetilde{u_i u_i} - \widetilde{u_i} \widetilde{u_i})/2$, $\Gamma = \text{efficiency function} = 0.75 \exp \left[-1.2 \left(\frac{u'_\Delta}{S_L} \right)^{-0.3} \right] \cdot \left(\frac{\Delta}{\delta_L} \right)^{2/3}$, $\Delta = \text{filter width}$
Colin et al. (2000)	$\Sigma_{gen} = \left[1 + \alpha\Gamma \left(\frac{u'_\Delta}{S_L} \right) \right] \nabla \bar{c} \quad (1.19)$ where $\alpha = \beta \cdot 2 \ln(2) / \left[3c_{ms} \left(Re_t^{1/2} - 1 \right) \right]$, $Re_t = \rho_0 u' l / \mu_0$, $\beta = 1$, $c_{ms} = 0.28$
Charlette et al. (2002)	$\Sigma_{gen} = \left(1 + \min \left[\frac{\Delta}{\delta_L}, \Gamma_\Delta \left(\frac{u'_\Delta}{S_L} \right) \right] \right)_1^\beta \nabla \bar{c} \quad (1.20)$ where $\Gamma_\Delta = \left[\left((f_u^{-a_1} + f_\Delta^{-a_1})^{-1/a_1} \right)^{-b_1} + f_{Re}^{-b_1} \right]^{-1/b_1}$, $Re_\Delta = \frac{u'_\Delta \Delta}{\nu}$, $b_1 = 1.4$, $\beta_1 = 0.5$, $C_k = 1.5$, $a_1 = 0.60 + 0.2 \exp \left[-0.1 \frac{u'_\Delta}{S_L} \right] - 0.20 \exp \left[-0.01 \frac{\Delta}{\delta_L} \right]$, $f_u = 4 \left(\frac{27}{110} C_k \right)^{1/2} \left(\frac{18}{55} C_k \right) \left(\frac{u'_\Delta}{S_L} \right)^2$, $f_\Delta = \left\{ \left(\frac{27}{110} C_k \pi^{4/3} \right) \left[\left(\frac{\Delta}{\delta_L} \right)^{4/3} - 1 \right] \right\}^{1/2}$, $f_{Re} = \left[\frac{9}{55} \exp \left(-1.5 C_k \pi^{4/3} Re_\Delta^{-1} \right) \right]^{1/2} Re_\Delta^{1/2}$
Weller et al. (1998)	$\Sigma_{gen} = [1 + 2\tilde{c}(\Theta - 1)] \nabla \bar{c} \quad (1.21)$ where $\Theta = 1 + 0.62 \sqrt{u'_\Delta / S_L} Re_\eta$ and $Re_\eta = u'_\Delta \cdot \eta / \nu$
Knikker et al. (2004)	$\Sigma_{gen} = \left(\frac{\Delta}{\eta_i} \right)^{\beta_k} \nabla \bar{c} \quad (1.22)$ where $\eta_i = 3\delta_L$, $\beta_k = [\log \langle \nabla \bar{c} \rangle - \log \langle \nabla \hat{c} \rangle] / \log \gamma$
Fureby (2005)	$\Sigma_{gen} = \left[\Gamma \left(\frac{u'_\Delta}{S_L} \right) \right]^{D-2} \cdot \nabla \bar{c} \quad (1.23)$ where $D = 2.05 / (u'_\Delta / S_L + 1) + 2.35 / (S_L / u'_\Delta + 1)$
Muppala et al. (2005)	$\Sigma_{gen} = \left[1 + \frac{0.46}{Le} Re_\Delta^{0.25} \left(\frac{u'_\Delta}{S_L} \right)^{0.3} \left(\frac{p}{p_o} \right)^2 \right] \nabla \bar{c} \quad (1.24)$

TABLE 1.1: Examples of algebraic models for Σ_{gen}

adjustable constant β was added for the context of LES. The simple model differs from the other models discussed here as it does not explicitly contain a term for the scalar gradient (i.e. $|\nabla \bar{c}|$). The model essentially approximates the shape of Σ_{gen} using $\bar{c}$, but contains no physical information about the combustion regime. The model does not take into account local values of flame strain and curvature.

The models of Angelberger et al. (1998), Colin et al. (2000), and Charlette et al. (1999) are derived using the DNS of flame vortex pair interaction. All three are of the form

$$\Sigma_{gen} = \left[1 + a\Gamma_n \left(\frac{u'_\Delta}{S_L} \right) \right] |\nabla \bar{c}|, \quad (1.25)$$

where Γ is an efficiency function. The Angelberger and Colin models use the following expression for the efficiency function:

$$\Gamma_n = 0.75 \exp \left[-\frac{1.2}{(u'_\Delta/S_L)^{0.3}} \right] (\Delta/\delta_t)^{(2/3)}. \quad (1.26)$$

In the Angelberger model, the constant $a = 1$ may lead to excessively high reaction rates. The Colin model changes the constant a such that it is a function of the global Re_t , which can improve flame wrinkling contribution of vortices at different length scales. However, the estimation of a global Re_t is difficult in LES since the local values of overall u' and integral length scale are unknown before the simulation is started. One approach is to approximate Re_t based on the inflow conditions of the experiment so that Re_t is treated as a constant. This model was found to under-predict Σ_{gen} for $Ka < 1$ and over-predict for $Ka > 1$ (Chakraborty and Klein, 2008). Charlette et al. (2002) proposed a model (referred to as Charlette2 model) that requires two input parameter ratios Δ/δ_L and u'_Δ/S_L , derived by formulating the efficiency function Γ in terms of the energy spectrum in homogeneous turbulence, and is designed to improve the behaviour of the limiting cases and avoid having to assume a value for Re_t . The efficiency function Γ accounts for the limited ability of smaller vortices to wrinkle the flame front.

Another popular basis which has been used to derive models is related to fractal theory. The concept is that the wrinkling factor can be expressed in a form such as:

$$\Xi = \left(\frac{\eta_o}{\eta_i} \right)^{D_f - 2}, \quad (1.27)$$

where D_f is the fractal dimension, η_o is the outer cut-off scale, and η_i is the inner cut-off scale. A typical approximation for η_o is the LES filter width. Some studies have shown that η_i appears to scale with the laminar flame thickness (Knikker et al., 2004; Gülder and Smallwood, 1995). The fractal dimension D_f has been shown to increase with increasing u'/S_L (Kerstein, 1988). With these parameters defined, the

fractal interpretation of the flame front can be seen as a manifestation of the dynamical self-similarity of the inertial range in high Reynolds number turbulent flows with an upper and lower cut-off. Examples include the models of Gülder (1991), Fureby (2005), Knikker et al. (2004), Tangermann et al. (2010), and Chakraborty and Klein (2008). The Fureby model neglects the resolved contribution in regions of zero turbulence, which may be more applicable for higher Reynolds number flows or for RANS. This leads to underpredictions of Σ_{gen} for lower turbulence levels (Chakraborty and Klein, 2008). Inaccuracies in the results from the model are generally due to the estimation of the efficiency function Γ for turbulent straining, fractal dimension D , and inner cut-off scale. The Knikker model calculates D_f through the application of a test filter. This additional filtering operation increases the computational cost. The accuracy of the Knikker model is also affected by the estimation of the inner cut-off scale. The Gülder model uses a constant value of $D_f = 7/3$. The Tangermann model, originally developed for RANS and extended for LES, also uses the value of $D_f = 7/3$. The model also contains $\tilde{c}(1 - \tilde{c})|\nabla\tilde{c}|$ obtained from integrating a Gaussian probability density function over a filter width. The integration of the probability function helps to account for the probability of the absence of the flame front in some regions of the domain and the probability of the flame brush spanning across several filter widths. However, the model does not recover the laminar flame speed in the limit of zero turbulence. Chakraborty and Klein (2008) proposed an expression for D_f which contains Ka . The fractal approach is likely to be inaccurate as the filter width decreases (Chakraborty and Klein, 2008).

Muppala et al. (2005) derived a model originally for RANS which is based on a flame-surface-wrinkling factor ratio $A_T/\bar{A}$, which is the ratio of the turbulent flame surface per unit volume A_T and the average projected area per unit volume $\bar{A}$. The model expresses Σ_{gen} as the product of $A_T/\bar{A}$ and $|\tilde{c}|$, and provides the expression for estimating $A_T/\bar{A}$:

$$A_T/\bar{A} = 1 + aRe_{\Delta}^{0.25} \left(\frac{u'_{\Delta}}{S_L} \right)^{0.3} \left(\frac{p}{p_o} \right)^2. \quad (1.28)$$

where the factor $a = 0.46/Le$ is obtained from empirical fitting to experimental data of methane-air, ethylene-air, and propane-air Bunsen-type flames. The term also includes the pressure ratio $\frac{p}{p_o}$ which is not found in the other models.

The model of Weller et al. (1998) was found to over-predict Σ_{gen} and vary with different filter sizes. The model predicts a highly skewed profile of conditionally averaged Σ_{gen} on $\bar{c}$ across the flame brush, resulting in inaccurate prediction of conditionally averaged Σ_{gen} values.

The model derived by Zimont and Lipatnikov (1995), originally for RANS and high turbulence applications, approximates the turbulent flame speed S_T as a function u'_{Δ}

and Da .

A few more important general observations on the characteristics and performance of the different models are noted below.

As mentioned previously, one common observation for most models is the poor ability to account for effects of strain rate and curvature. As discussed in Section 1.2.2.2, these effects significantly vary for different premixed combustion regimes. It is evident from various studies that models which work in one combustion regime can poorly perform in other regimes (Chakraborty and Klein, 2008; Ma et al., 2013; Katragadda et al., 2012; Klein and Chakraborty, 2018). For example, Figure 1.10 from the study of Chakraborty and Klein (2008) shows that the Angelberger model had the best agreement with the DNS data in the CF regime, while the Chakraborty model had the best agreement in the TRZ regime. Works have been done attempting to improve the performance of models across regimes to varying degrees of success. For example, Chakraborty and Klein (2008) include Ka in their formulation. It is also difficult to parameterize the regime especially in more complex flow configuration, as seen in the simulation of Ma et al. (2013) where large-scale instabilities due to vortex shedding result in locally higher subgrid Karlovitz numbers, or flame-quenching near walls (Lai et al., 2017). Some other models simply rely on adjustable constants to account for these effects. It is evident that there is still potential work to be done to improve the performance of models for higher Ka regimes.

It is important to consider models such as the Angelberger, Boger, Colin, and Tangermann models contain adjustable constants, which can be tuned in each individual case to obtain satisfactory results. The use of adjustable constants in models provide some flexibility, as models can be manually adjusted to provide better results outside the operating regime for which the models were derived. However, the arbitrary nature of these constants can make the use of these models somewhat ambiguous, as it is difficult to determine the “best” value for these constants before the start of a simulation. This is evident in the *a-posteriori* simulations of Ma et al. (2013).

The *a-priori* study of Chakraborty and Klein (2008) showed that correlation between modelled Σ_{gen} and the actual Σ_{gen} decreases as the filter size increases, as illustrated in Figure 1.9. This is attributed to local strain rate and curvature effects that are lost with increasing filter sizes. This was also shown in the *a-posteriori* simulations by Ma et al. (2013). However, it is also interesting to note the effects observed by Klein and Chakraborty (2018) regarding numerical errors in the LES context. In their study, the Fureby model was found to give good predictions of volume averaged flame wrinkling factor $\langle \Xi_{gen} \rangle$ even with increasing filter sizes. However, $\langle \Sigma_{gen} \rangle$ was found to be increasingly underpredicted with higher filter sizes. By comparing the volume averaged resolved FSD $\langle |\nabla \bar{c}| \rangle$ on DNS and LES grids, increasing effects of truncation errors were

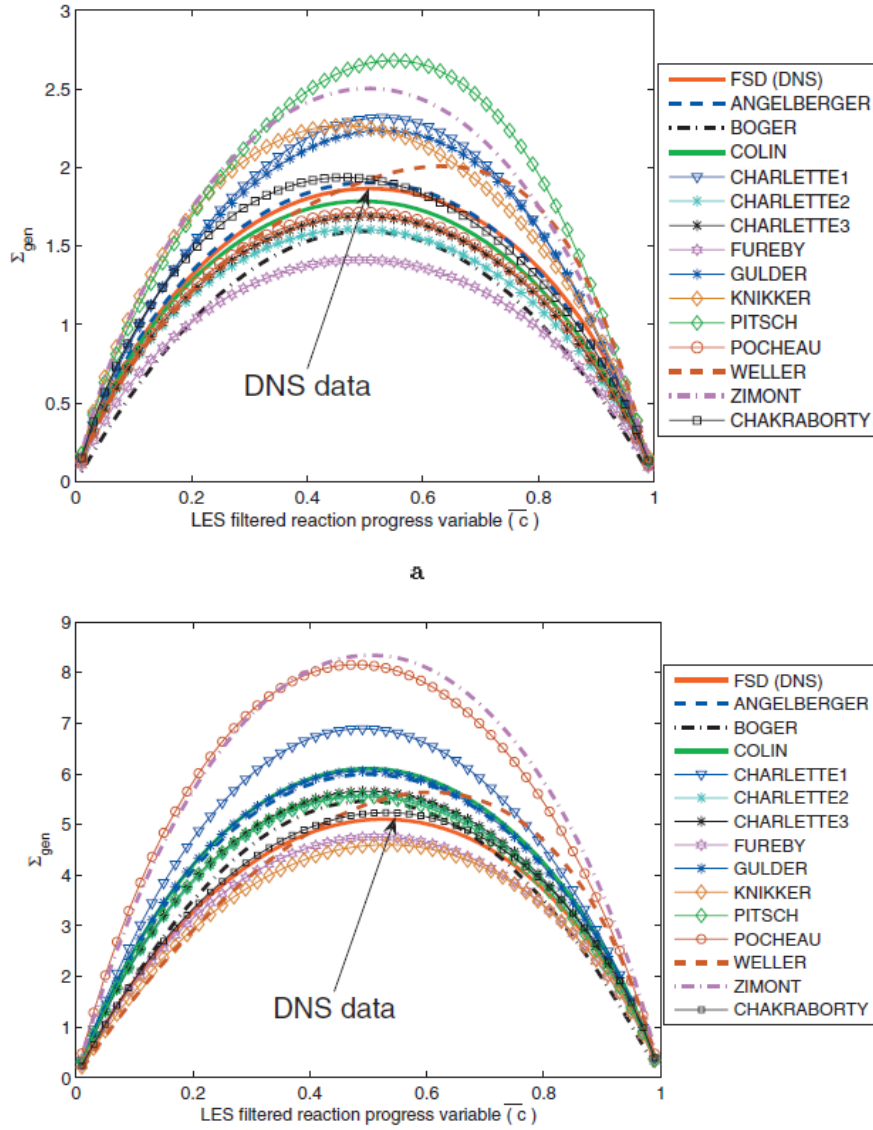


FIGURE 1.10: Conditionally averaged Σ_{gen} with $\bar{c}$ for a flame in the CF regime (top) and the TRZ regime (bottom) by Chakraborty and Klein (2008).

observed as filter size is increased, and they suggested that a well performing model might be one which moderately overpredicts flame wrinkling to offset truncation errors inherent in LES.

By comparing various formulations, it can be seen that some models are functions of the unweighted progress variable $\bar{c}$ while others are functions of the density-weighted progress variable $\tilde{c}$. In particular, there is a difference in the way the resolved component of the flame surface density is described. The quantity $\tilde{c}$ is closed and is calculated directly in a LES. On the other hand, the quantity $\bar{c}$ is unclosed, requiring an additional model, such as the most common BML formulation (Bray et al., 1989):

$$\bar{c} = \frac{(1 + \tau) \tilde{c}}{1 + \tau \tilde{c}}, \quad (1.29)$$

where $\tau = (T_b - T_u)/T_u$. A modified version of the formulation have also been proposed (Chakraborty and Cant, 2007) which weights the model with the filter size, such that $\bar{c} \rightarrow \tilde{c}$ for small filter sizes:

$$\bar{c} = \frac{(1 + \tau)\tilde{c}}{1 + \tau\tilde{c}} \left[1 - \exp\left(-\Theta \frac{\Delta}{\delta_L}\right) \right] + \tilde{c} \exp\left(-\Theta \frac{\Delta}{\delta_L}\right), \quad (1.30)$$

where Θ is an empirical constant. The additional closure problem for $\bar{c}$ contributes to another level of uncertainty, especially since the BML formulation is based on the validity of the thin flame assumption. Equations 1.29 and 1.30 have been found to result in steeper gradients near the unburnt side of the flame. As a result, overprediction of flame thickening have been observed when models use $|\nabla \bar{c}|$ with Eqs. 1.29 or 1.30. Ma et al. (2013) have suggested that explicit counter-gradient transport (CGT) models can be used to correct this. Alternatively, the usage of $\tilde{c}$ have been suggested to act as an implicit CGT model, negating the need to explicitly account for CGT in the subgrid scalar flux (Allaiddin et al., 2017). Klein and Chakraborty (2018) investigated the difference by applying existing models for flame wrinkling factor to both definitions of $\Sigma_{gen} = \Xi |\nabla \bar{c}|$ and $\Sigma_{gen} = \Xi |\nabla \tilde{c}|$. The shapes of the conditionally averaged Σ_{gen} and Ξ_{gen} were observed to be different for higher filter sizes. $\Sigma_{gen} = \Xi_{gen} |\nabla \bar{c}|$ profiles skewed towards the unburnt side of the flame, while $\Sigma_{gen} = \Xi |\nabla \tilde{c}|$ skewed towards the burnt side of the flame. These observations also reinforces one known shortcoming of the “gradient-type” model in the form of 1.14 is a lack of flame thickness control, as the shape of the $|\nabla \bar{c}|$ and $|\nabla \tilde{c}|$ largely influences the thickness of the flame.

1.2.5 Model Development from DNS: the use of data-driven approaches

1.2.5.1 Overview

The derivation of equations for RANS and LES generally involves the application of averaging which results in unclosed correlations. The motivation of model development is to express these unclosed quantities as a function of known quantities. This brings about two major considerations:

- What known quantities should be used in the model?
- What is the functional form between the model and the selected quantities?

As Raman and Hassanaly (2019) have noted, model form uncertainty is a dominant source of error in reacting flow simulations. This drives the need for innovation in model development techniques.

Early model development efforts used experimental data as the reference. However, as discussed in Section 1.2.2, the quality of DNS data provides an attractive tool for development of lower order combustion models, in frameworks such as RANS and LES.

The data from DNS provides a tool for evaluating model performance. Traditionally, this involves the derivation of models through some theoretical basis, after which the model output is assessed against the DNS data. This may involve comparison a-priori or a-posteriori, or both. This may also constitute the addition of adjustable constants to “tweak” the model to obtain results close to the DNS data. Numerous examples of studies of Σ_{gen} modelling have been discussed in Section 1.2.4.2, and many have used DNS data for fine tuning the models through empirical fitting (Chatakonda et al., 2010).

With the advent of high-fidelity dataset from DNS, opportunities for computational approaches have emerged in the context of combustion modelling. Specifically, data-driven approaches have been gaining much interest in the community. Data-driven approaches refer to tools that use data to obtain a desired solution for a system, without explicit knowledge of the physical behaviour of the system. It is then unsurprising that early applications tended towards fields that did not possess an underlying physical basis, but the extension to fields in physical sciences have been emerging.

A subset of data-driven approaches called machine learning has been gaining traction. Machine learning relies on the automation of the process of pattern recognition and statistical inference between inputs and outputs, by using computational algorithms to “learn” the training data. The technique can be applied to classification problems or regression problems. Examples of machine learning algorithms are shown in Figure 1.11 (Brunton et al., 2019), categorized under supervised, semi-supervised, and unsupervised algorithms, referring to the degree of external information about the training data.

In the context of reacting CFD simulations, the machine learning approach which has been gaining attention is Artificial Neural Networks (ANN). The prime application of this has been for modelling reaction rates (Christo et al., 1996; Blasco et al., 2000; Franke et al., 2017; Sen et al., 2010), replacing the use of a stiff ordinary differential equation solver, which led to significant computational speed-up. The results were able to capture extinction and reignition to good accuracy. ANN has also been used for tabulation for flamelet methods (Kempf et al., 2005a; Ihme et al., 2009). A recent study by Nikolaou *et al.* (Nikolaou et al., 2018) showed the application of Deep Neural Networks (DNN), an extension of ANN, to obtain estimates of the unfiltered progress variable fields from filtered DNS fields. Using the deconvoluted progress variable and its variance, they obtained predictions of the reaction rate using two flamelet based models. The approach was found to recover good approximations of the unfiltered fields.

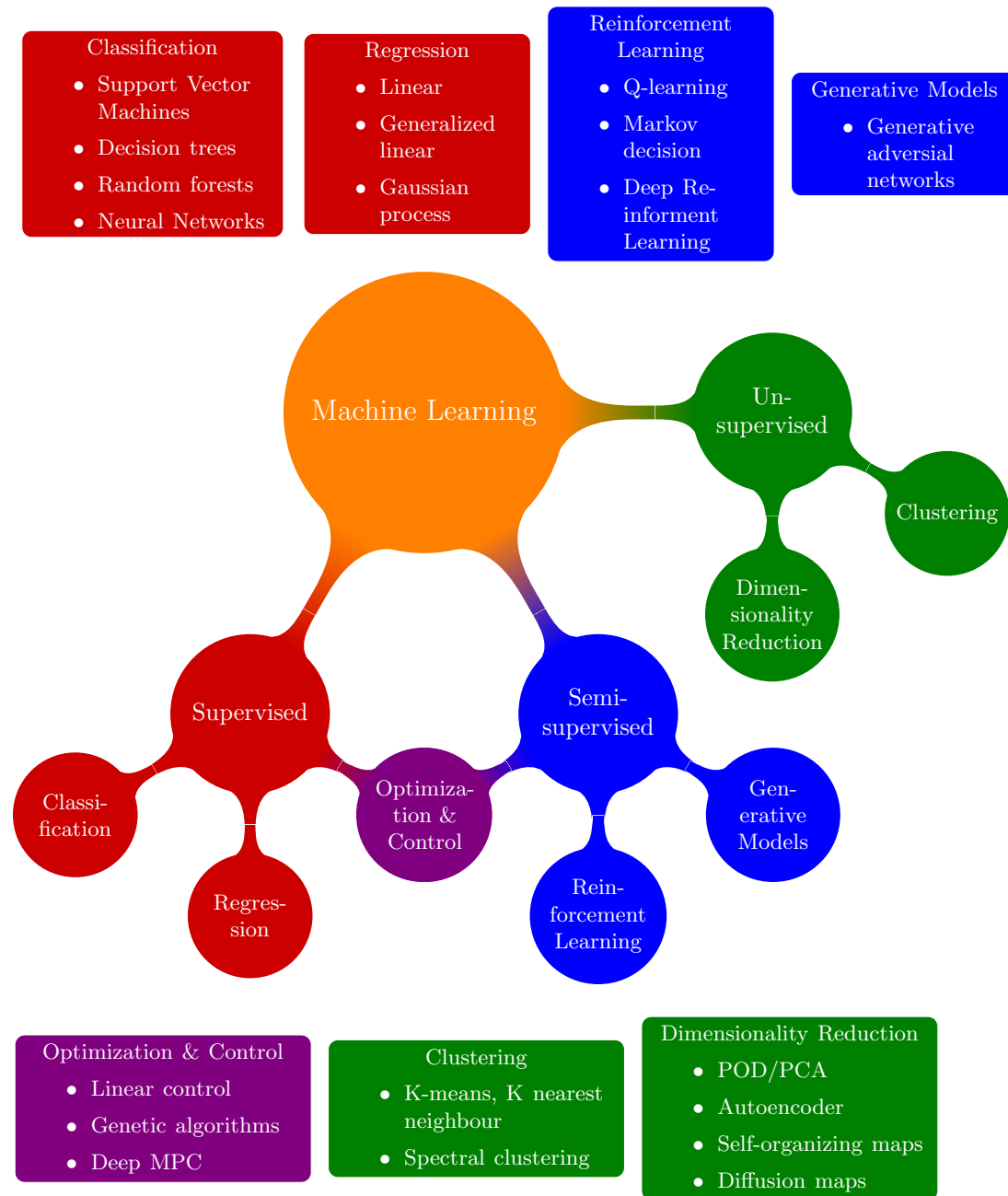


FIGURE 1.11: Examples of machine learning methods, adapted from Brunton et al. (2019).

Recently used machine learning approaches are based on neural networks and are therefore quite different from the traditional closure models in that neural networks do not directly provide functional forms. In the next section, machine learning methods called Evolutionary Algorithms are introduced which can be used to create functional forms for models in the LES or RANS context.

1.2.5.2 Evolutionary Algorithm and Gene Expression Programming

Evolutionary Algorithm (EA) is an adaptive system inspired by genetics and the processes of natural selection in biology. Akin to the process of evolution in biological populations, EA poses potential solutions to a problem as individuals/genes/chromosomes which make up a population. The concept of survival of the fittest is used to determine solutions that survive into the next iteration of individuals (generation). New individuals are introduced by replication to the new population. Genetic variations, such as the processes of mutation and genetic crossover, are introduced to produce a diverse population, where individuals are once again set to compete against each other in an iterative process, creating the cycle depicted in Figure 1.12. EAs are in principle a probabilistic search algorithm, where the best solutions are found by retaining the better variations over successive iterations in a trail and error process. Gene Expression Programming (GEP) is a certain branch of EA which differs from other branches by the way that the individuals are represented. A more detailed description of the GEP methodology is described in Section 2.5.

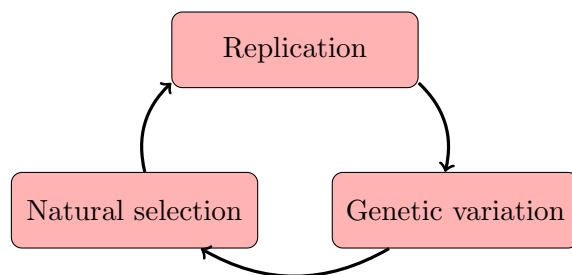


FIGURE 1.12: The cycle of evolution

The difference between the GEP approach and methods such as ANN is the ability to obtain functional forms that can be used directly as a model in the governing equations. Like most optimization approaches, GEP is robust and has been applied to a range of problems in different fields. However, in the context of CFD modelling, the application of this approach is still fresh, and many avenues are still unexplored. Recently, a number of works have delved into the application of the GEP framework, outlined in Weatheritt (2015), for turbulence modelling.

Reynolds stress modelling in the context of RANS has received most attention. This is motivated by the fact that the stress tensor is a proven source of error in RANS modelling. The first attempt was done in the work of Weatheritt and Sandberg (Weatheritt and Sandberg, 2016a), which served as a proof of concept for the GEP-based Reynolds stress tensor modelling. Using DNS training data of the reattachment region behind a backward facing step flow, which consists of the adverse pressure gradient region in the separated flow, algebraic models were developed for the anisotropy tensor of the Reynolds

stress. The trained anisotropy tensor model was used in the baseline shear-stress transport model and was evaluated *a posteriori* on backward facing step and periodic hills flows. The anisotropy and normal stress ratios predictions with the trained models were found to be generally improved over existing results which used the linear Boussinesq approximation and an established non-linear model. However, the near wall anisotropy was still not correctly represented compared to reference LES, which suggested further studies were needed for near wall regions. Another interesting result was that while improvements over baseline models were made under “on-design” conditions (similar conditions to the training data), results in the favourable pressure gradient region of the periodic hills simulation, which were “off-design” from the adverse pressure gradient of the training data, were found to perform worst than the baseline models. Though this result is not entirely surprising, it does show the sensitivity of the approach to the choice of the training data. Subsequent works by the same group have extended on this work by applying the approach to a number of different configurations, which are described below.

Weatheritt et al. (2017b) applied the GEP approach to the jet-in-crossflow configuration, using incompressible LES data of this configuration for training, and tested the GEP generated model on a frozen RANS simulation (freezing the mean LES flow field) with an altered cross flow angle. The new model was found to perform better than the linear Boussinesq solution, though was not able to obtain accurate anisotropy in the regions of strongest streamwise vorticity. One interesting analysis from this study is a comparison of the application of GEP and Neural Network approaches to the same problem. Both approaches showed promising improvement over the linear model, though it was recognised that the two approaches greatly differ in their methodology and philosophy.

In Weatheritt et al. (2017a), a model for the anisotropy of the Reynolds stress tensor was produced by training on the LES data of a region in the wake of a linear high-pressure turbine cascade which was above a certain threshold of turbulence kinetic energy. The model was expressed as a function of a set of tensor basis functions and scalar invariants. In this study, the final model was obtained using the ensemble average of the models over the different runs. However, it was found that the ensemble averaged model resulted in numerical instabilities in regions with no turbulence. One interesting analysis conducted in this study was to determine the frequency of appearance of each term (basis function or scalar invariant) through 100 runs of the non-deterministic GEP algorithm, which led to implications of which terms best modelled the physics of the problem. This analysis is quite significant, since it shows that even though the GEP approach is at heart based in mathematics, the interpretation of the results to real physics is important to validate the models. This concept is further illustrated in Weatheritt and Sandberg (2017a)

where GEP was also able to predict functional relationship for vortex creation which were consistent with the underlying physics.

The GEP algorithm was likewise applied to a low-pressure turbine cascade by Akolekar *et al.* (Akolekar et al., 2019) with Reynolds stresses in the wake region extracted from DNS, once again showing improvement in the Reynolds stresses and TKE production predictions in the wake region.

While the above studies were applied for modelling in steady RANS, Lav *et al.* (Lav et al., 2019) investigated the application of the approach to an unsteady flow, specially the wake of a flat plate, in the context of unsteady RANS (URANS) modelling. In this context, the preparation of the training data was different from the previous studies, dealing with the unsteadiness by decomposing the target anisotropy tensor by removing the vortex shedding frequency.

The approach for tensor modelling was extended from RANS closure to the modelling of subgrid scale (SGS) stresses in the context of LES (Schoepplein et al., 2018). The models were trained on a DNS dataset of freely propagating statistically planar turbulent premixed flames, marking the first time this approach was applied to a reacting flow configuration. This was motivated by the fact that SGS models have mostly been derived in the context of constant density flows, whereas heat release in reacting flows can affect the turbulent flux. Interestingly, the GEP algorithm was able to produce a model which matched a well known existing model in the literature (Clark model).

A heat flux model was also developed using GEP by Sandberg et al. (2018), using the LES training data of the wake region of a trailing edge slot flow. The resulting model showed improvement in the prediction of adiabatic wall effectiveness over commonly used gradient diffusion hypothesis.

A different application of GEP is the development of damping functions for hybrid RANS/LES (Weatheritt and Sandberg, 2015, 2016b, 2017b), which describes the amount of resolved stress over total stress so that the contribution of the modelled stress is dependent on the local grid spacing. In other words, as the local grid becomes finer, the damping function decreases the amount of modelling that is used. In this case, the result is a scalar expression, and an additional operation is added to bound the function between values of 0 and 1. The damping functions were found to perform well even when applied to *a-posteriori* simulations of configurations different from the configurations of the training data. Weatheritt and Sandberg (2016b) trained a damping function on the DNS data of a backward facing step flow, specifically in two regions of the flow: the first region was just before the flow reattachment, where normal stress components are significant, and the second region was the recovering boundary layer. The damping

function was applied with the hybrid RANS/LES methodology to a periodic hills flow, and generally good agreement with reference LES data was found in the predictions of first order statistics, examining predictions of mean velocity, TKE, shear stress, and friction coefficient. In the study of Weatheritt and Sandberg (2017b), a damping function was trained on the DNS data of a turbulent pipe flow. The damping function was tested in the simulation of a periodic hills flow which exhibits separation and reattachment of the flow, as well as in the simulation of flow past tandem cylinders with wake interference patterns. The results were promising providing good agreement of first- and second-order statistics with reference results from highly resolved LES, as well as improved predictions over delayed detached-eddy simulations results. Mesh independence was also achieved between two grids that were tested. In particular, the results were shown to perform well even for grids coarser than typical for those cases, which meant that simulations using the GEP-based damping functions produced comparable results for a lower cost.

This review highlighted the potential of GEP to produce a variety of functional forms (Reynolds stress models, heat flux models, sub-grid models, damping functions) by symbolic regression. It is also important to recognise the limitations of these models. For example, one of the key observations from the above studies is that the choice of the training region has a large impact on the performance of the models. Most importantly, it was recognised that further exploration was needed to understand the full potential of the approach in turbulence modelling. The encouraging results of the studies also suggest that GEP may be equally applicable to the development of other types of closure models not yet explored in these studies.

1.3 Summary

This chapter provided a review of the literature on using DNS of turbulent premixed jet flames to study and model Turbulence Flame Interaction (TFI). TFI plays a major role in the production and dissipation of the scalar gradient, an important parameter in turbulent premixed flame modelling. DNS studies have shown to be useful in quantifying the influence of the flame on vortex stretching and turbulence dissipation (Chakraborty, 2014; Hamlington et al., 2011; Wang et al., 2016), as well as the influence of turbulence on flame stretching and thickening (Swaminathan and Grout, 2006; Chakraborty and Swaminathan, 2007a; Hamlington et al., 2011; Dopazo et al., 2015). In the context of turbulent premixed jet flames, the mean shear was observed to be a major contributor to flame strain rates (Wang et al., 2017b).

The impact of turbulent inflow boundary condition was discussed in this chapter. For turbulent premixed jet flames, the inflow conditions is important for flow and flame

development. Synthetic turbulence generation methods are often used for the inflow boundary conditions with little to no development length (Veynante et al., 2010; Hara et al., 2015; Kerkemeier et al., 2013; Klein et al., 2018; Cecere et al., 2016; Wang et al., 2010), relying on the numerical algorithms to generate proper turbulent flows. However, as Dhamankar et al. (2015) noted, these methods cannot fully replicate a realistic turbulent flow. Studies of non-reacting jets have shown that the spreading rate of the jets are greatly affected by the inflow turbulence (Boersma et al., 1998; Glaze and Frankel, 2003; Herff et al., 2017). Inflow turbulence has also been found to affect flame development in the experimental study of Langman et al. (2007), and has been recognised as a source of error in some numerical studies (Kempf et al., 2006; Afarin and Tabejamaat, 2013). However, there is a lack of high-fidelity studies which directly focus on the effect of turbulent inflow boundary conditions on turbulent premixed jet flames.

A review of algebraic Flame Surface Density (FSD) modelling in the context of Large Eddy Simulation (LES) was also presented. Results from various studies (Chakraborty and Klein, 2008; Katragadda et al., 2012; Ma et al., 2013; Klein and Chakraborty, 2018) showed that the performance of the models were not consistent across different combustion regimes and flow configurations. This highlights the potential for further development of algebraic FSD models.

Machine learning algorithms were introduced as an alternative approach for modelling. In particular, the Gene Expression Programming (GEP) approach was introduced in the context of turbulence modelling. The algorithm has shown promise for turbulence modelling (Weatheritt and Sandberg, 2016a, 2017b; Akolekar et al., 2019; Lav et al., 2019). While the study of Schoepplein et al. (2018) applied the GEP algorithm to develop sub-grid stress model for reacting flows, GEP has not yet been used for modelling unclosed terms in the reactive scalar transport equation.

1.4 Research aims

The three research aims for this thesis are:

1. **to investigate the effect of the inflow turbulence generation method on flame characteristics in premixed jet flames**

The effects of the inflow turbulence generation method on turbulent premixed jet flames are investigated by considering two DNS cases with different inflow boundary conditions. The first simulation consists of an upstream pipe and coflow region to provide the flame with a fully-developed turbulent inflow,

while the second simulation uses a synthetic turbulence inflow. The results of the global evolution of the flame and the jet flow, and the local statistics at the flame front are analysed.

2. to examine the effects of Karlovitz number in premixed jet flames

The key parameters pertaining to TFI in premixed jet flames are analysed at two different inlet Karlovitz numbers. The Karlovitz number was varied by changing the premixture temperature, while the Reynolds number of the jet was kept the same. The statistics related to TFI were directly compared between the two flames. The global parameters related to the flow field and flame are compared. The scalar gradient, which is related to FSD modelling, is analysed by examining the local strain rates and curvature. The relationship between the terms of the scalar gradient transport equation are determined to assess the validity of common assumptions in algebraic FSD models.

3. to develop algebraic flame surface density models using machine learning

New algebraic FSD models for LES are developed using the GEP approach. The DNS conducted in this study as the training data. The performance of the models are then evaluated *a priori* and compared to existing models. Several models are trained based on individual flames while some others are based on the data of both flames. This is done to determine the sensitivity of the choice of the training data on the quality of the trained models. This work will be the first study to apply the GEP approach for combustion modelling.

Chapter 2

Numerical Methods

2.1 Introduction

This chapter presents the numerical methods and the configurations of the turbulent premixed jet flame DNS conducted in this study. Firstly, the DNS solver is described, including the implementation of reacting flow feature into the solver. Laminar flame simulations and their results, which were conducted to validate the implementation, are also presented. Next, the numerical setup of the DNS of the turbulent premixed jet flames are provided. Relevant post-processing algorithms which were used are also briefly discussed. The methodology of the Gene-Expression Programming algorithm is presented, including the implementation of parallelisation to improve computational performance.

2.2 DNS solver (HiPSTAR)

2.2.1 Overview

The simulations were conducted using the High Performance Solver for Turbulence and Aero-acoustic Research (HiPSTAR). HiPSTAR is a compressible high-fidelity simulation solver developed at University of Melbourne and University of Southampton. HiPSTAR was originally developed to simulate compressible non-reacting turbulent flows, and has resulted in numerous studies for configurations such as boundary layer flows (Bechlars and Sandberg, 2017), jets (Sandberg et al., 2012; Sandberg and Tester, 2016; Shin et al., 2017), wakes (Lav et al., 2019), and turbine blades (Sandberg et al., 2015; Leggett et al., 2018; Pichler et al., 2018). HiPSTAR is a Fortran code parallelized for

central processing units (CPU) using Message Passing Interface (MPI) and Open Multi-Processing (OpenMP) frameworks, and for graphics processing units (GPU) using OpenACC framework. In this study, HiPSTAR was modified to extend its capabilities to simulate reacting flows.

2.2.2 Governing Equations

In the non-reacting version of HiPSTAR, the cylindrical forms of the non-dimensionalised compressible Navier-Stokes equations are solved. The non-dimensional variables are defined as:

$$x_j = \frac{x_j^*}{L_{ref}}, \quad t = \frac{t^* u_{ref}}{L_{ref}}, \quad \rho = \frac{\rho^*}{\rho_{ref}}, \quad u_j = \frac{u_j^*}{u_{ref}}, \quad T = \frac{T^*}{T_{ref}}, \quad . \quad (2.1)$$

where $x_j = z, r, \theta$ are the streamwise, radial, and azimuthal spatial coordinates, respectively, t is the time, u_j are the velocity components, ρ is the density, T is the temperature, L_{ref} is the reference length, $*$ denotes the dimensional values, and $_{ref}$ denotes the reference values. The non-dimensionalized governing equations for the flow field are written as:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_1}{\partial z} + \frac{\partial \mathbf{F}_2}{\partial r} + \frac{1}{r} \frac{\partial \mathbf{F}_3}{\partial \theta} = \frac{\partial \mathbf{G}_1}{\partial z} + \frac{\partial \mathbf{G}_2}{\partial r} + \frac{1}{r} \frac{\partial \mathbf{G}_3}{\partial \theta} - \frac{1}{r} \mathbf{H}, \quad (2.2)$$

where $\mathbf{Q}$ are the conservative variables, $\mathbf{F}_{1,2,3}$ are the convective flux terms, $\mathbf{G}_{1,2,3}$ are the diffusive flux terms, and $\mathbf{H}$ are the terms which account for the cylindrical coordinate system:

$$\begin{aligned} \mathbf{Q} &= [\rho, \rho u_z, \rho u_r, \rho u_\theta, \rho E_t]^T, \\ \mathbf{F}_1 &= [\rho, \rho u_z u_z + p, \rho u_z u_r, \rho u_z u_\theta, u_z (\rho E_t + p)]^T, \\ \mathbf{F}_2 &= [\rho, \rho u_z u_r, \rho u_r u_r + p, \rho u_r u_\theta, u_r (\rho E_t + p)]^T, \\ \mathbf{F}_3 &= [\rho, \rho u_z u_\theta, \rho u_r u_\theta, \rho u_\theta u_\theta + p, u_\theta (\rho E_t + p)]^T, \\ \mathbf{G}_1 &= [0, \tau_{zz}, \tau_{zr}, \tau_{z\theta}, -q_z + u_z \tau_{zz} + u_r \tau_{zr} + u_\theta \tau_{z\theta}]^T, \\ \mathbf{G}_2 &= [0, \tau_{rz}, \tau_{rr}, \tau_{r\theta}, -q_r + u_z \tau_{rz} + u_r \tau_{rr} + u_\theta \tau_{r\theta}]^T, \\ \mathbf{G}_3 &= [0, \tau_{\theta z}, \tau_{\theta r}, \tau_{\theta\theta}, -q_\theta + u_z \tau_{\theta z} + u_r \tau_{\theta r} + u_\theta \tau_{\theta\theta}]^T, \\ \mathbf{H} &= [\rho u_r, \rho u_z u_r - \tau_{zr}, \rho u_r u_r - \rho u_\theta u_\theta - \tau_{rr} + \tau_{\theta\theta}, 2\rho u_r u_\theta - 2\tau_{r\theta}, \\ &\quad u_r (\rho E_t + p) + q_r - u_z \tau_{rz} - u_r \tau_{rr} - u_\theta \tau_{r\theta}]^T, \end{aligned} \quad (2.3)$$

In Equation 2.3, the pressure p , the total energy E_t , the viscous stress tensor components τ_{ij} , and the heat flux components q_j are:

$$p = \frac{\rho T}{\gamma M^2}, \quad (2.4a)$$

$$E_t = \frac{T}{\gamma(\gamma-1)M^2} + \frac{1}{2}u_i u_i, \quad (2.4b)$$

$$\begin{aligned} \tau_{zz} &= \frac{2\mu}{3Re} \left[2\frac{\partial u_z}{\partial z} - \frac{\partial u_r}{\partial r} - \frac{1}{r} \left(\frac{\partial u_\theta}{\partial \theta} + u_r \right) \right], & \tau_{\theta z} &= \frac{\mu}{Re} \left[\frac{\partial u_\theta}{\partial z} + \frac{1}{r} \frac{\partial u_z}{\partial \theta} \right], \\ \tau_{rr} &= \frac{2\mu}{3Re} \left[-\frac{\partial u_z}{\partial z} + 2\frac{\partial u_r}{\partial r} - \frac{1}{r} \left(\frac{\partial u_\theta}{\partial \theta} + u_r \right) \right], & \tau_{rz} &= \frac{\mu}{Re} \left[\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z} \right], \\ \tau_{\theta\theta} &= \frac{2\mu}{3Re} \left[-\frac{\partial u_z}{\partial z} - \frac{\partial u_r}{\partial r} + \frac{2}{r} \left(\frac{\partial u_\theta}{\partial \theta} + u_r \right) \right], & \tau_{\theta r} &= \frac{\mu}{Re} \left[\frac{1}{r} \left(\frac{\partial u_r}{\partial \theta} - u_\theta \right) + \frac{\partial u_\theta}{\partial r} \right], \end{aligned} \quad (2.4c)$$

$$\begin{aligned} q_z &= \frac{-\mu}{Pr(\gamma-1)M^2 Re} \frac{\partial T}{\partial z}, & q_r &= \frac{-\mu}{Pr(\gamma-1)M^2 Re} \frac{\partial T}{\partial r}, \\ q_\theta &= \frac{-\mu}{Pr(\gamma-1)M^2 Re} \frac{1}{r} \frac{\partial T}{\partial \theta}. \end{aligned} \quad (2.4d)$$

where γ is the specific heat ratio. The non-dimensional dynamic viscosity is modelled using the power law:

$$\mu = T^n, \quad (2.5)$$

where $n = 0.76$. The non-dimensional parameters are

$$Re = \frac{\rho_{ref} u_{ref} L_{ref}}{\mu_{ref}}, \quad M = \frac{u_{ref}}{a_{ref}}, \quad Pr = \left(\frac{\nu}{D_t} \right)_{ref}, \quad (2.6)$$

where Re is the Reynolds number, M is the Mach number, Pr is the Prandtl number, a is the sound speed, ν is the kinematic viscosity, and D_t is the thermal diffusion coefficient.

In order to conduct the reacting flow simulations in this study, the number of governing equations was extended with the addition of governing equations for the reactive species. The non-dimensional species is introduced as

$$Y_i = \frac{Y_i^*}{Y_{i,ref}}, \quad (2.7)$$

where Y_i is the mass fraction of i th of total n species considered. The additional non-dimensionalized governing equations are written as:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_1}{\partial z} + \frac{\partial \mathbf{F}_2}{\partial r} + \frac{1}{r} \frac{\partial \mathbf{F}_3}{\partial \theta} = \frac{\partial \mathbf{G}_1}{\partial z} + \frac{\partial \mathbf{G}_2}{\partial r} + \frac{1}{r} \frac{\partial \mathbf{G}_3}{\partial \theta} - \frac{1}{r} \mathbf{H} + \mathbf{S}, \quad (2.8)$$

where

$$\begin{aligned}
\mathbf{Q} &= [\dots, \dots, \dots, \dots, \rho Y_1, \dots, \rho Y_n]^T, \\
\mathbf{F}_1 &= [\dots, \dots, \dots, \dots, \rho u_z Y_1, \dots, \rho u_z Y_n]^T, \\
\mathbf{F}_2 &= [\dots, \dots, \dots, \dots, \rho u_r Y_1, \dots, \rho u_r Y_n]^T, \\
\mathbf{F}_3 &= [\dots, \dots, \dots, \dots, \rho u_\theta Y_1, \dots, \rho u_\theta Y_n]^T, \\
\mathbf{G}_1 &= [\dots, \dots, \dots, \dots, J_{z,1}, \dots, J_{z,n}]^T, \\
\mathbf{G}_2 &= [\dots, \dots, \dots, \dots, J_{r,1}, \dots, J_{r,n}]^T, \\
\mathbf{G}_3 &= [\dots, \dots, \dots, \dots, J_{\theta,1}, \dots, J_{\theta,n}]^T, \\
\mathbf{H} &= [\dots, \dots, \dots, \dots, \rho u_r Y_1 - J_{r,1}, \dots, \rho u_r Y_n - J_{r,n}]^T, \\
\mathbf{S} &= [\dots, \dots, \dots, \dots, \dot{Q}, \dot{\Omega}_1, \dots, \dot{\Omega}_n]^T.
\end{aligned} \tag{2.9}$$

The first five equations remain the same as in Eq. 2.3 except for the addition of a heat release term $\dot{Q}$ in the energy equation (found in $\mathbf{S}$). In Equation 2.9, the reactant mass flux components $\mathbf{J}$ are defined as:

$$J_z = \frac{\mu}{RePrLe} \left(\frac{\partial Y_i}{\partial z} \right), \quad J_r = \frac{\mu}{RePrLe} \left(\frac{\partial Y_i}{\partial r} \right), \quad J_\theta = \frac{\mu}{RePrLe} \frac{1}{r} \left(\frac{\partial Y_i}{\partial \theta} \right). \tag{2.10}$$

In this study, the reaction mechanism is modelled using single-step chemistry, where one governing equation is to be solved for Y_R representing the mass fraction of the reactant mixture. Single-step chemistry is used for computational feasibility, though it is recognised that detailed chemistry may be required for certain details of the flame to be captured. Nevertheless, the use of single-step chemistry has been shown to provide a wealth of information in many studies on flame strain and curvature (Chakraborty and Cant, 2005; Chakraborty and Swaminathan, 2007a; Dunstan et al., 2012; Dopazo et al., 2015; Karami et al., 2016), flame geometry (Veynante et al., 2010), flame acoustics (Jiménez et al., 2015; Haghiri et al., 2018), and model development (Chakraborty and Swaminathan, 2007b; Klein et al., 2017). The reaction rate $\dot{\Omega}$ is defined by the following form consistent with the present non-dimensionalisation of the governing equation,

$$\dot{\Omega}_R = RePrLeDaSL^2 \rho Y_{R\exp} \left(-\frac{\beta(1-\Theta)}{1-\alpha(1-\Theta)} \right), \tag{2.11}$$

where $\Theta = (T - T_u)/(T_b - T_u)$ is the reduced temperature. The heat release rate $\dot{Q}$ is defined as:

$$\dot{Q} = \frac{\alpha}{1-\alpha} \frac{1}{(\gamma-1)M^2} \dot{\Omega}_R. \tag{2.12}$$

Additional non-dimensional parameters are now present in the equations:

$$Da = \frac{D_m B_o}{S_L^2} \exp\left(-\frac{\beta}{\alpha}\right), \quad Le = \left(\frac{D_t}{D_m}\right)_{ref}, \quad (2.13)$$

where Da is the Damköhler number, Le is the Lewis number, D_m is the mass diffusion coefficient, $S_L = S_L^*/u_{ref}$ is the non-dimensional laminar flame speed, α is the heat release parameter, and β is the Zeldovich parameter.

2.2.3 Numerical Schemes

HiPSTAR features numerous capabilities which can be chosen to suit the needs of different cases. The capabilities used in this study are as follows. The governing equations described in Section 2.2.2 are discretised in the x_1 and x_2 directions with a 4th-order standard finite differencing scheme with the Carpenter boundary stencils (Carpenter et al., 1999). A spectral method by Fourier decomposition is used in the x_3 direction.

The coefficients of the finite differencing scheme are based on equidistant grid spacing, so a coordinate mapping to η - ξ space is applied to the grid. This coordinate mapping is unnecessary in the x_3 direction as the distribution of Fourier modes is uniform, so the procedure is restricted to two-dimensions, resulting in a smaller number of metric terms. The mapping is based on the following transformations:

$$\frac{\partial}{\partial z} = \frac{1}{J} \left(\frac{\partial r}{\partial \eta} \frac{\partial}{\partial \xi} - \frac{\partial r}{\partial \xi} \frac{\partial}{\partial \eta} \right), \quad (2.14a)$$

$$\frac{\partial}{\partial r} = \frac{1}{J} \left(-\frac{\partial z}{\partial \eta} \frac{\partial}{\partial \xi} - \frac{\partial z}{\partial \xi} \frac{\partial}{\partial \eta} \right), \quad (2.14b)$$

where $J = \frac{\partial z}{\partial \xi} \frac{\partial r}{\partial \eta} - \frac{\partial z}{\partial \eta} \frac{\partial r}{\partial \xi}$ is the determinant.

Symmetric skew-splitting is applied to the convective terms of the governing equations to improve numerical stability (Kennedy and Gruber, 2008). An 11 point explicit filter with a weight factor of 0.2 is used after each time step to dampen spurious oscillations (Bogey et al., 2009).

Time marching is accomplished by a low-storage (two registers), explicit fourth-order, five-stage Runge-Kutta scheme (Kennedy et al., 2000). The low storage scheme is memory efficient, which is a desired feature for large-scale simulations, as RAM access can be a bottleneck for performance.

Another feature in HiPSTAR used in this study is multi-blocking, where the computational domain can be divided into individual blocks each with different sets of boundary

conditions. The values at block interfaces are calculated by the same halo exchange procedure as processor interfaces. The multiblock feature allows for efficient distribution of structured grid points, and parallelisation of boundary conditions.

2.2.4 Boundary Conditions

In this section, the boundary conditions implemented in HiPSTAR which are relevant to the current study are briefly discussed.

2.2.4.1 Turbulent inflow

The turbulent inflow is implemented by adding fluctuating quantities to prescribed mean profiles. These fluctuations are generated using the digital filter method (DF), which establishes a Gaussian two-point correlation function to random fluctuations. Designed to match ad hoc first and second order statistical moments and spectra, the method applies a filtering operation on a random number distribution to create correlated length scales, so that the generated fluctuations feature prescribed length scales. The digital filter method was originally proposed by Klein et al. (2003), with additional modifications proposed by others to speed up the technique by reducing the dimensionality of the filtering operation (Xie and Castro, 2008) and extension to compressible flows (Touber and Sandham, 2009).

The method consists of a few steps. First a set of random values is generated with a normal distribution (“white noise”) for each velocity component; in HiPSTAR, the Mersenne Twister generator is used for the random number generator (Matsumoto and Nishimura, 1998). At this point, adding this set of values to the prescribed mean values will provide homogeneous turbulence at the inlet. The distribution is filtered using the following operator, written here in one-dimension as:

$$\dot{u}_k = \sum_{j=-W}^W b_j r_{k+j}, \quad (2.15)$$

where $\dot{u}$ is the filtered velocity fluctuation at point k , r is the original random value, b_j are the filter coefficients, and $W = 2I_x/\Delta x$ is the filter size described by a prescribed integral length scale I_x and grid spacing Δx . The filtering operation results in the field now having the prescribed length scale.

The filter coefficients b_j are defined by solving the following two-point correlation function:

$$R(x_k + q\Delta x) = \frac{\overline{\dot{u}_k \dot{u}_{k+p}}}{\overline{\dot{u}_k \dot{u}_k}} = \frac{\sum_{j=-W+q}^W b_j b_{j-q}}{\sum_{j=-W}^W b_j^2} = \exp\left(-\frac{\pi q}{2n}\right), \quad (2.16)$$

where q is the number of grid points of uniform spacing Δx away from the reference point x_k and n is the number of points such that $n = I_x/\Delta x$. The exponential form on the right hand side of Equation 2.16 was proposed by Xie and Castro (2008) as an improvement over the Gaussian function originally used by Klein et al. (2003). The operation above is extended to two-dimensions by defining the coefficients as $b_{jk} = b_j b_k$. The fluctuations are then correlated in time by the following operator:

$$\check{u}_k = \dot{u}_k^{old} \exp\left(-\frac{\pi \Delta t}{2\tau}\right) + \dot{u}_k \sqrt{1 - \exp\left(-\frac{\pi \Delta t}{\tau}\right)}, \quad (2.17)$$

where $\dot{u}^{old}$ is the fluctuation at the previous time, Δt is the time step, and τ is the Lagrangian time scale. An additional approach by Veloudis et al. (2007) is used here which defines different sets of filter widths for the near-wall region and outer-region.

While the above formulation satisfies the two-point correlations, cross-correlation between the different velocity components is done by the transformation method of Lund et al. (1998), so that the fluctuations match with a prescribed stress tensor which represent the desired stress profiles. The 3D transformation is written as:

$$\begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} U \\ V \\ W \end{bmatrix} + \begin{bmatrix} \sqrt{R_{11}} & 0 & 0 \\ R_{21}/\sqrt{R_{11}} & \sqrt{R_{22} - R_{21}^2/R_{11}} & 0 \\ 0 & 0 & \sqrt{R_{33}} \end{bmatrix} \begin{bmatrix} \check{u} \\ \check{v} \\ \check{w} \end{bmatrix}, \quad (2.18)$$

where U, V, W are the prescribed mean velocity components and R_{ij} are the prescribed Reynolds-stress tensor components.

Compressibility effects were added by applying the strong Reynolds analogy to obtain the temperature fluctuations (Touber and Sandham, 2009):

$$\frac{T'}{\overline{T}} = -(\gamma - 1)M^2 U \frac{u'}{\overline{T}}, \quad (2.19)$$

and assuming a constant pressure across the boundary, the density fluctuations were obtained using:

$$\frac{\rho'}{\overline{\rho}} = -\frac{T'}{\overline{T}}. \quad (2.20)$$

2.2.4.2 Navier-Stokes Characteristic Boundary Conditions

In DNS of compressible flows, waves are generated that propagate towards the boundaries, where they can be reflected back into the domain. One solution is to apply a filter to the numerical scheme to remove higher wavenumbers from the solutions. However, using high filter strengths can result in inaccurate results due to numerical dissipation. To minimise the effect of this numerical viscosity, a solution is to treat the waves at the boundaries in order to avoid reflections. This is done by implementing non-reflecting or absorbing boundary conditions.

Navier-Stokes Characteristic Boundary Condition (NSCBC) was proposed by Poinso and Lele (1992), originally developed for DNS of turbulent non-reacting flows. The method is based on the analysis of characteristic waves crossing the boundary. It is assumed that waves associated with diffusive processes are negligible; in other words, only the hyperbolic part of the Navier-Stokes equations are considered (Euler equations). Outgoing waves (exiting the domain) are defined by the solution inside the domain and at the boundary; however, incoming waves are defined by the solution outside of the computational domain, and cannot be obtained directly. The NSCBC method addresses this by taking the local inviscid conditions (Euler) and adding viscous conditions by inferring that the wave amplitude variations are caused by viscous effects. This results in a set of equations called the Local One-Dimensional Inviscid (LODI) relations. The formulation of Kim and Lee (2000), which extends the approach to generalised coordinates, is the implementation used in HiPSTAR.

Referring back to Eq. 2.8, the equation is rewritten for the three general directions $x_{1,2,3}$ and grouping the RHS terms into a term $\mathbf{R}$:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_1}{\partial x_1} + \frac{\partial \mathbf{F}_2}{\partial x_2} + \frac{\partial \mathbf{F}_3}{\partial x_3} = \mathbf{R}. \quad (2.21)$$

The above equation is transformed into a characteristic form in the direction normal to the computational boundary (assume here as x_1 for example) by applying the Jacobi matrix $\mathbf{A}_k = \partial \mathbf{F}_k / \partial \mathbf{Q}$ to the derivative flux term and grouping the derivative flux terms in the parallel directions (x_2 and x_3) with $\mathbf{R}$ into $\mathbf{R}^*$:

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{A}_1 \frac{\partial \mathbf{Q}}{\partial x_1} = \mathbf{R}^*. \quad (2.22)$$

The Jacobi matrix is diagonalised by defining $\mathbf{A}_1 = \mathbf{P}_1 \mathbf{\Lambda}_1 \mathbf{P}_1^{-1}$, where $\mathbf{\Lambda}_1$ is a diagonal matrix and $\mathbf{P}$ is a transformation matrix, and the result is

$$\frac{\partial \mathbf{C}}{\partial t} + \mathbf{\Lambda}_1 \frac{\partial \mathbf{C}}{\partial x_1} = \mathbf{R}^{**}, \quad (2.23)$$

where $\delta \mathbf{C} = \mathbf{P}_1^{-1} \delta \mathbf{Q}$ and $\mathbf{R}^{**} = \mathbf{P}_1^{-1} \mathbf{R}^*$. The wave equation 2.23 can be cast to the LODI system by neglecting the source term $\mathbf{R}^{**}$ and defining the expression for the characteristic convection term as:

$$\mathbf{L} = \lambda \partial \mathbf{C} / \partial x_1, \quad (2.24)$$

where the signs of eigenvalues λ determine whether the wave is incoming or outgoing from the domain, and the eigenvectors $\mathbf{L}$ correspond to the rate of change of the wave amplitudes.

The physics of the waves entering the computational domain through the boundary are interpreted by modifying the appropriate components of $\mathbf{L}$. The outlet condition implemented here allows for a small level of reflection, while still preventing numerical oscillations. In the LODI equations, L_1 , L_2 , L_3 , L_4 , and L_6 are outgoing waves defined in the domain and L_5 is the incoming wave imposed by the relation,

$$L_5 = \frac{\sigma c}{L} (1 - M^2) (p - p_\infty), \quad (2.25)$$

where σ is a constant. When σ is zero, the amplitude of the incoming wave is forced to zero, and the boundary becomes perfectly non-reflecting. A non-zero value of σ is used to allow some oscillation to occur at the boundary. The value of $\sigma = 0.25$ has been typically used (Poinsot and Lele, 1992).

The above characteristic boundary condition was extended to a zonal characteristic boundary condition (Sandberg and Sandham, 2006) to gradually dampen fluctuations over a finite spatial distance. Whereas the NSCBC is applied locally at the domain boundary, the zonal characteristic boundary condition applies the treatment over a finite number of grid points before the domain boundary. This is done by introducing a smooth ramping function. For the outlet condition this is achieved by modifying Eq. 2.25 such that:

$$L_5 = \frac{1}{2} \frac{\sigma c}{L} (1 - M^2) (p - p_\infty) \left(1 + \cos \frac{\pi(x - x_{start})}{x_{out} - x_{start}} \right), \quad (2.26)$$

where x_{start} is the starting coordinate of the zonal boundary condition and x_{out} is the coordinate of the domain boundary.

Defining $\mathbf{L}^*$ as the eigenvectors updated with the relations in Eq. 2.26, the modified normal derivative flux is obtained with:

$$\frac{\partial \mathbf{F}_1'}{\partial x_1} = \frac{1}{\mathbf{A}_1} \mathbf{P}_1 \mathbf{L}^*. \quad (2.27)$$

Finally, the derivative flux term in the normal direction in Eq. 2.21 is replaced by the modified term:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}'_1}{\partial x_1} + \frac{\partial \mathbf{F}_2}{\partial x_2} + \frac{\partial \mathbf{F}_3}{\partial x_3} = \mathbf{R}. \quad (2.28)$$

2.2.4.3 Integrated Characteristic Boundary Conditions

The integrated characteristic boundary condition (Sandhu and Sandham, 1994) is used for characteristic inflow boundary conditions. The integrated characteristic boundary condition follows the procedure of the NSCBC in Section 2.2.4.2 up to the formulation of the modified normal flux derivatives. Instead of replacing the derivative flux term as in Eq. 2.28, the modified derivative flux is integrated in time and subtracted from the values for the inlet conservative variables $\mathbf{Q}_{\text{in}}$:

$$\mathbf{Q} = \mathbf{Q}_{\text{in}} - \int \frac{d\mathbf{F}'_1}{dx_1} dt. \quad (2.29)$$

The time integration is done by using the Runge-Kutta scheme described in Section 2.2.3.

2.2.4.4 Axis boundary condition

The singularity at $r = 0$ for non-axisymmetric flows results in two issues. The first is that a method is needed to calculate the derivatives in the radial direction with one-sided schemes but still retains the accuracy of the interior numerical scheme. The second is to treat terms which contain $\frac{1}{r}$ to avoid divergent behaviour. To address these issues at the axis, the axis treatment proposed by Sandberg (2011) is used. The treatment uses parity conditions derived for the scalars, velocity vectors and equations in order to determine symmetry conditions for each azimuthal Fourier mode of the variables. The derivation of the parity conditions for each variable and equation can be found in Sandberg (2011).

The symmetry conditions are used to construct finite differencing stencils near the axis. For an even function, the derivative is zero at the axis, while for odd function, the symmetry is used to calculate the derivative.

To deal with the singularity at the axis due to terms with $\frac{1}{r}$, the values at the axis are interpolated. Using the symmetry conditions, Sandberg (2011) proposed the following sixth-order accurate stencil:

$$\phi_1 = \frac{1}{35} (56\phi_2 - 28\phi_3 + 8\phi_4 - \phi_5), \quad (2.30)$$

where ϕ_1 is the point at the axis and $\phi_{2,3,4,5}$ are the adjacent points.

At the axis boundary, the zeroth azimuthal mode (mean mode) is calculated from the governing equations, except for u_r and u_θ which are set to zero. The first mode of u_r and u_θ can be non-zero. All other modes are set to zero at the axis.

2.2.4.5 Isothermal wall boundary conditions

Isothermal non-slip wall boundary conditions are used in this study. The velocity components are imposed as $u = v = w = 0$. Due to compressibility effects of the turbulent boundary layer, the wall temperature is higher than the freestream temperature. To account for this effect, the wall temperature T_w is set to the adiabatic temperature of the freestream by (Banks et al., 2000):

$$T_w = \left(1 + \frac{\gamma - 1}{2} M^2\right) T_{freestream}. \quad (2.31)$$

2.2.5 Validation Simulations

As part of the implementation of the reacting flow framework to HiPSTAR, a number of validation cases were performed. This means that results from the DNS algorithm should generate physically feasible results, and of comparable accuracy to results from analytical solutions, experiments, or other DNS algorithms. A series of relatively low-cost validation cases have been chosen. Each case aims to either isolate certain aspects of the implementation, to test certain features, or to increase the complexity from previous validation cases. Reference results were generated from the combustion code NTMIX (Cuenot et al., 1997).

2.2.5.1 1-Dimensional Stationary Laminar Premixed Flame

Simulations of one-dimensional laminar premixed flames were conducted. The simulation parameters are based on the test case reported in the NTMIX report by Massebeuf (2002). A sketch of the computational domain is shown in Figure 2.1. The lengths of the computational domain are 2 and 0.1 in the x and y directions, respectively. A uniform computational grid of 201 by 11 points in the x and y directions, respectively, resulting in a uniform grid spacing of 0.01 is used. The integrated characteristic boundary condition described in Section 2.2.4.3 is imposed at the inlet boundary ($x = 0$) with $u_x = 1$, $u_y = 0$, and $T = 1$. The outlet boundary condition ($x = 2$) is the NSCBC outlet described in Section 2.2.4.2. Periodic boundary conditions are imposed for the boundaries

at $y = 0$ and $y = 0.1$. The simulation was conducted with a timestep of $3e^{-5}$, resulting in a CFL condition of 0.612. A total of 100,000 timesteps were completed. The domain was decomposed into three subdomains in the x direction and computation was done with one core per subdomain.

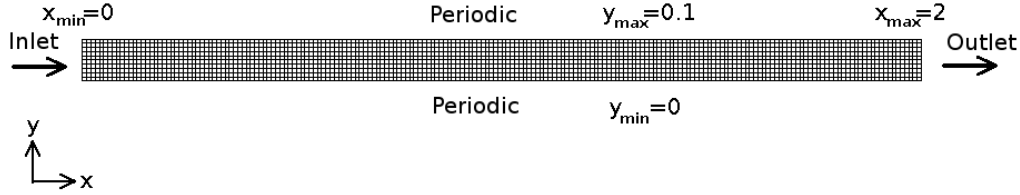


FIGURE 2.1: Computational grid and boundary conditions for the 1D laminar flame validation simulations.

Following the test cases of Massebeuf (2002), two simulations were conducted where $n = 0$ and $n = 0.76$ in the power law viscosity of Eq. 2.5. The parameters of the simulation are presented in Table 2.1.

Parameter	$n = 0$	$n = 0.76$
Re	20	31.8
Pr	0.75	0.75
Le	1.0	1.0
Da	129.62	129.62
S_L^*	0.01	0.01
α	0.75	0.75
β	8	8
γ	1.4	1.4
M	0.01	0.0159

TABLE 2.1: Parameters for the 1D laminar flame validation simulations.

The flow field was initialized with estimated profile for Y , u , ρ , and T :

$$Y(x) = \frac{1}{2} (1 - \tanh(40(x - 1))), \quad (2.32a)$$

$$T(x) = u_x(x) = \frac{1}{4} (10 + 6 \tanh(40(x - 1))), \quad (2.32b)$$

$$\rho(x) = \frac{\gamma p_\infty}{(\gamma - 1)T(x)}, \quad (2.32c)$$

$$v(x) = 0. \quad (2.32d)$$

Figure 2.2 shows a visualisation of the resulting Y field. The unburnt mixture corresponding to $Y = 1$ (red) enters from the left side of the domain, while fully burnt mixture corresponding to $Y = 0$ (blue) exits the domain through the right side. A

flame front, or reaction zone, separates the unburnt and burnt mixtures, marked by the gradient between the two extremes (white). The consumption of the species causes a propagation of the flame front towards the unburnt mixture; however, in this case, the rate of fresh mixture entering the domain is set to balance the propagation speed of the flame front.

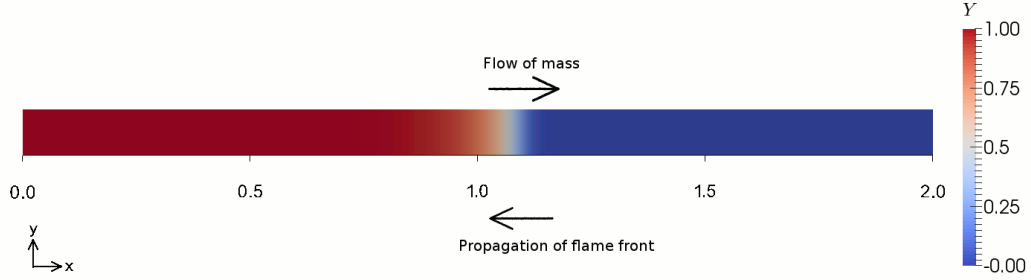


FIGURE 2.2: Visualization of Y for the 1D laminar flame validation simulation. The directions of mass flow and flame front propagation are marked.

The steady state profiles of T , Y , and u along the x direction for both $n = 0$ and $n = 0.76$ are shown in Figure 2.3. For both simulations, the results obtained from the HiPSTAR implementation agrees with the reference results obtained from NTMIX.

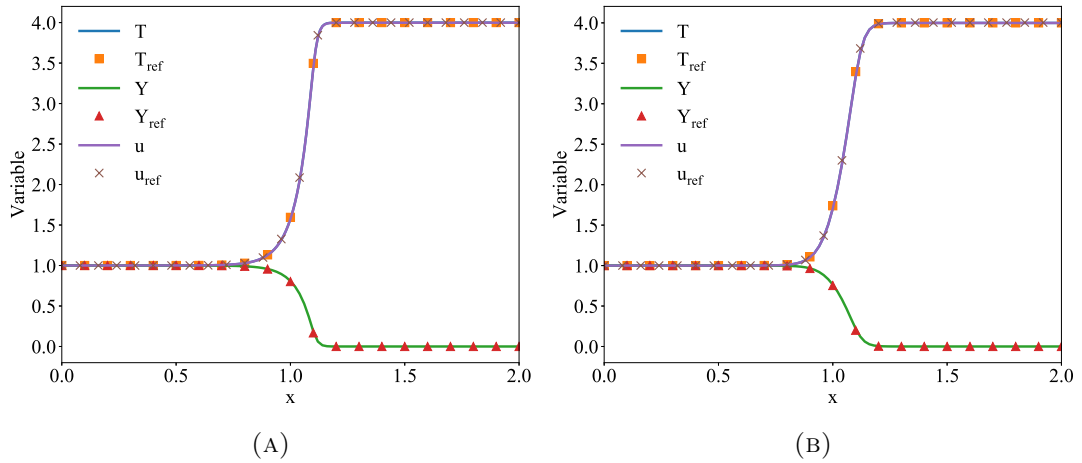


FIGURE 2.3: Steady state profiles of T , Y , and u for the 1D flame validation simulations with (A) $n = 0$ (constant viscosity) and (B) $n = 0.76$ (variable viscosity). Results from simulation with NTMIX are used as reference data (denoted by “ref”).

Figure 2.4 shows the pressure profile. The resulting p for burnt gas is 7142.86 and unburnt gas is 7145.85, leading to a pressure ratio of $\frac{p_b}{p_u} = 0.99958$. A theoretical expression for the pressure ratio is given in (Massebeuf, 2002) as

$$\frac{p_b}{p_u} \approx 1 - \gamma S_L^2 \frac{\alpha}{1 - \alpha}, \quad (2.33)$$

which results in a theoretical pressure ratio of 0.99958. The simulated and theoretical values of the pressure ratio are within 10^{-5} precision.

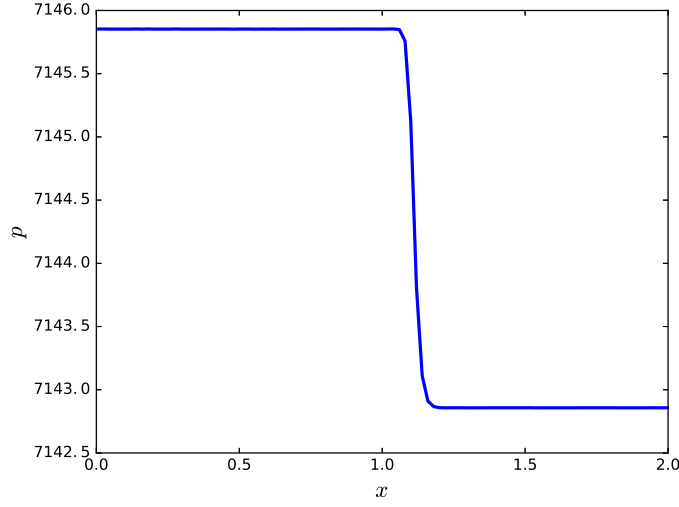


FIGURE 2.4: Pressure results for constant viscosity 1D flame validation simulation.

2.2.5.2 2-Dimensional Laminar Premixed Flame

Simulations of two dimensional laminar premixed flames were conducted. The simulation parameters were based on the simulation of Poinso et al. (1992). This setup includes gradients and non-periodic boundary conditions in both x and y directions. Two simulations are presented in this section: the first simulation is a planar flame solved with the Cartesian form of the governing equations and the second is an axis-symmetric flame solved with the cylindrical form of the governing equations.

The set-up of the computational domain is shown in Figure 2.5. The dimensions of the computational domain are 4.5 and 1 in the x and y directions, respectively, the same dimensions as the computational setup in Poinso et al. (1992). The domain was discretised uniformly into 300 by 100 cells, resulting in grid cells of size 0.015 by 0.01.

Table 2.2 summarizes the parameters of the simulations.

The flames were initialised by imposing one-dimensional profiles of Y and T in the y direction, centred at $y/L = 0.5$, and constant values for velocity and pressure:

$$Y(y) = \frac{1}{2} (1 - \tanh(15(y - 0.5))), \quad (2.34a)$$

$$T(y) = \frac{1}{4} (10 + 6 \tanh(15(y - 0.5))), \quad (2.34b)$$

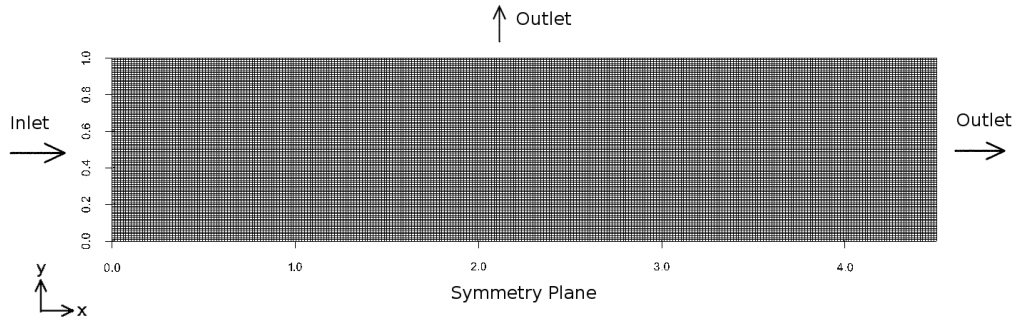


FIGURE 2.5: Computational grid and boundary conditions for the 2D laminar flame validation simulations

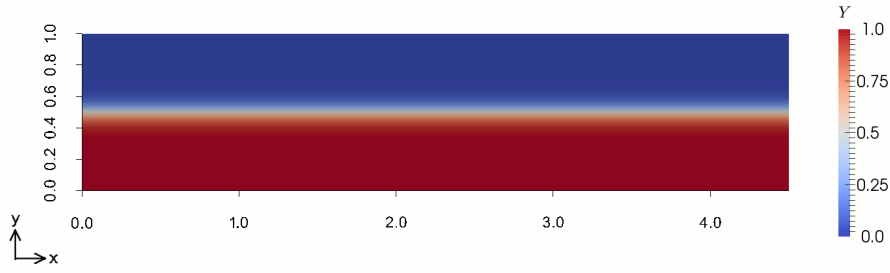
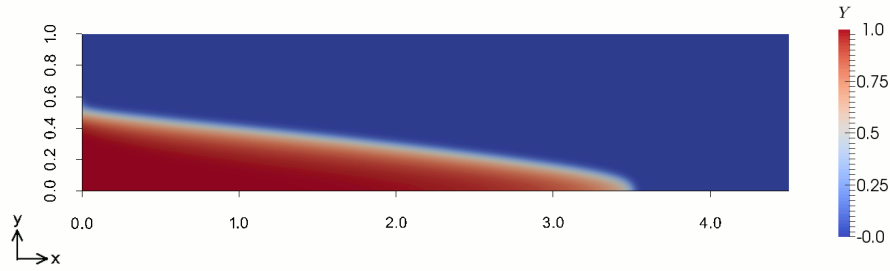
Parameter	Value
M	0.08
Re	160
Pr	0.75
Le	1.0
Da	129.62
S_L^*	0.01
α	0.75
β	8
γ	1.4

TABLE 2.2: Parameters for the 2D laminar flame validation simulations.

$$u_x = 1; \quad u_y = 0; \quad p = p_\infty = \frac{1}{\gamma M^2}, \quad (2.34c)$$

while ρ was initialised by Eq 2.4a. The initial condition for Y is shown in Figure 2.6. The integrated characteristic boundary condition was used at the the inlet boundary ($x = 0$) with imposed values shown in Eq. 2.34. The outlet boundaries at $x = 4.5$ and $y = 1$ are NSCBC outlet boundary conditions. The lower $y = 0$ boundary was a symmetry boundary in the case of the planar flame, while for the case of the cylindrical flame, the boundary was the axis boundary described in Section 2.2.4.4. The time step employed for the simulation was $\Delta t = 2e^{-4}$, resulting in a CFL condition of 0.43, and a total of 100,000 timesteps were completed.

Figure 2.7 shows the steady state 2D planar flame after 100,000 timesteps visualized by Y and the flow field visualised by u . The flame front propagates towards the axis after the initial timestep shown in Figure 2.6. Steady state is reached when the local velocity component normal to the flame front balances the propagation speed of the flame front. The increase in temperature across the flame front causes acceleration of the local flow. The velocity is highest close to the tip of the flame, corresponding to the location of the highest curvature on the flame surface.

(A) $t = 0$ FIGURE 2.6: Initial conditions of Y for the 2D laminar flame validation simulations.

(A)

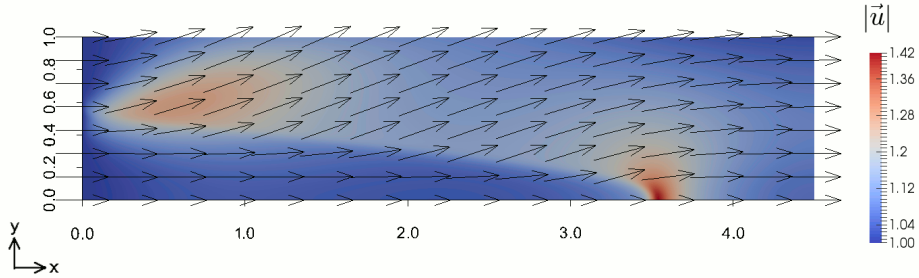
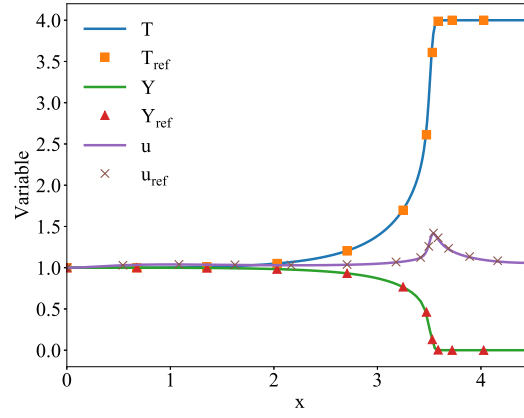
(B) $t = 10$ FIGURE 2.7: Visualization of (A) Y and (B) u for the 2D laminar planar flame validation simulation.

Figure 2.8 shows the profiles of u , T , and Y plotted along the centerline ($y = 0$), comparing the results of HiPSTAR and NTMIX. The flame length is the location of the flame front at the centerline (symmetry boundary) located at the maximum T and Y gradients, just upstream of the region of maximum velocity, which is approximately 3.5. The maximum velocity is approximately 1.42. It is shown that the results obtained from HiPSTAR agrees with the reference results obtained from NTMIX.

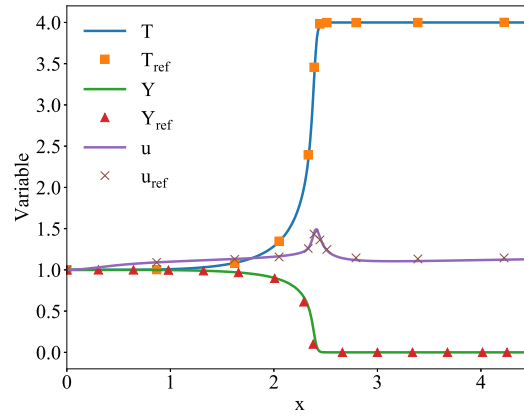
The comparison of the HiPSTAR and NTMIX centerline ($y = 0$) profiles for the 2D axi-symmetric flame is shown in Figure 2.9. The axi-symmetric flame has a shorter flame length (≈ 2.3) compared to the flame length of the planar flame (≈ 3.5), a result



(A)

FIGURE 2.8: Steady state profiles of T , Y , and u for the 2D planar flame validation simulation. Results from simulation with NTMIX are used as reference data (denoted by “ref”).

of lower reactant mass flow rate due to the smaller area of the inflow in the cylindrical domain. Once again, the results from HiPSTAR show a good agreement with the reference NTMIX results, which validates the implementation of the cylindrical form of the governing equations.



(A)

FIGURE 2.9: Steady state profiles of T , Y , and u for the 2D axisymmetric flame validation simulation. Results from simulation with NTMIX are used as reference data (denoted by “ref”).

2.2.5.3 3-Dimensional Laminar Premixed Flame

The 2D axisymmetric laminar flame simulation in Section 2.2.5.2 is adapted to a 3D laminar flame simulation by modifying the inflow velocity profile to include azimuthal

perturbations. The inflow streamwise velocity profile is imposed by:

$$\begin{aligned} u_z(r, \theta, t) &= u_0(r) \left(1 + a \sin \left(\frac{2\pi St \cdot t}{M} \right) \sin(m\theta) \right), \\ u_0(r) &= \frac{1}{2} \left(1 - \tanh \left[2.5 \left(r - \frac{1}{r} \right) \right] \right), \end{aligned} \quad (2.35)$$

where a is the perturbation amplitude, m is the number of modes in the forcing function, L_{ref} is the reference length defined here as the jet radius R , c_u is the sound speed of the unburnt reactant, and St is the Strouhal number, representing the normalized frequency,

$$St = \frac{f L_{ref}}{c_u}. \quad (2.36)$$

Thus the introduction of variation in the azimuthal direction results in u_θ that is no longer zero everywhere. The inlet boundary conditions for the other variables are:

$$Y(r) = \frac{1}{2} \left(1 - \tanh \left[2.5 \left(r - \frac{1}{r} \right) \right] \right), \quad (2.37a)$$

$$T(r) = \frac{1}{4} \left(10 + 6 \tanh \left[2.5 \left(r - \frac{1}{r} \right) \right] \right), \quad (2.37b)$$

$$u_r = 0; \quad u_\theta = 0; \quad p = p_\infty = \frac{1}{\gamma M^2}. \quad (2.37c)$$

The dimensions of the computational domain shown in Figure 2.5 is extended to 9 and 3 in the x and r directions, and 2π in the θ direction. The domain is discretised into 490 by 400 cells in the x and r directions, respectively. Cells are uniform for $x \leq 4.5$ and $r \leq 1$, with cell size of 0.0125 by 0.005, so that a sufficiently fine resolution is present in the flame. Algebraic grid stretching was applied for $x > 4.5$ and $r > 1$ to lighten the computational load, with local grid stretching of no more than 2% between adjacent cells. 32 Fourier modes are used for the azimuthal direction, which corresponds to 66 collocation points in physical space. The flame parameters are summarized in Table 2.2.

The time-step used for the simulation was $\Delta t = 4e^{-5}$, resulting in a CFL condition of approximately 0.68. One period of forcing corresponds to 102,400 time-steps. The simulation was first run without inflow forcing ($a = 0$) so that the solution for a flame was a steady axisymmetric flame, after which the amplitude of the inflow forcing was increased with $a = 0.25$, $m = 2$, and Strouhal number $St = 0.0195$ resulting in a forcing period $t_f = 4.096$.

Figure 2.10 shows an instantaneous snapshot of the flame visualised by a temperature iso-surface of $T = 2.5$. The flame front is observed to exhibit some wrinkling caused by

the periodic forcing at the inflow. The highest values of velocity appear to be in regions with the highest curvature in the flame surface.

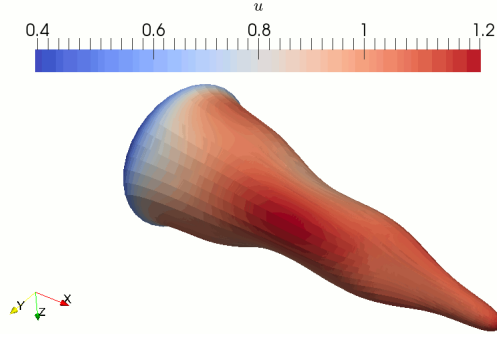
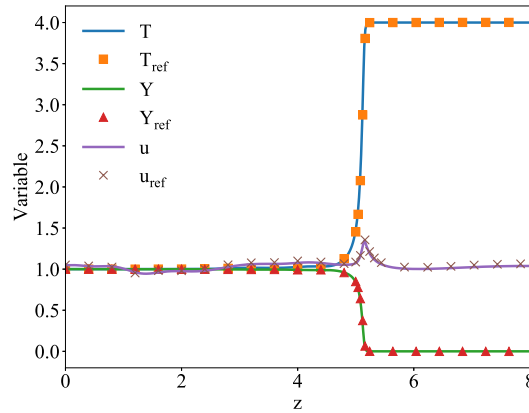


FIGURE 2.10: Instantaneous temperature iso-surface of $T = 2.5$ for the 3D laminar flame validation simulation, colored by u values.

The comparison of the HiPSTAR and NTMIX instantaneous profiles of the 3D laminar flame is shown as a function of the streamwise direction at $r = 0$ in Figure 2.11. The profiles along the radial direction are also shown for two streamwise locations, $z = 2.5$ and $z = 5$, in Figure 2.12. The results from HiPSTAR show good agreement with the reference NTMIX results, which validates the implementation of the cylindrical form of the governing equations.



(A)

FIGURE 2.11: Instantaneous streamwise profiles of T and u for the 3D laminar flame validation simulation at $r = 0$. Results from simulation with NTMIX are used as reference data (denoted by “ref”).

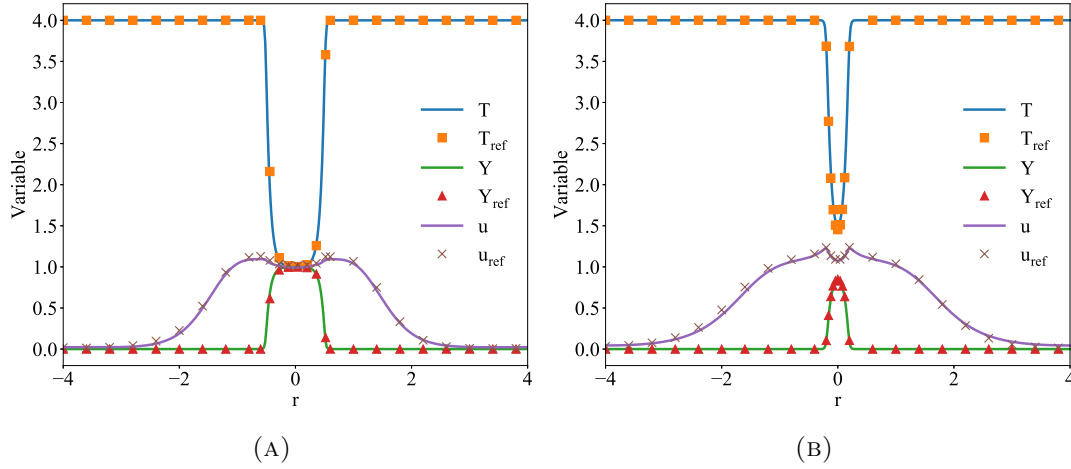


FIGURE 2.12: Instantaneous radial profiles of T and u for the 3D laminar flame validation simulation at (A) $z = 2.5$ and (B) $z = 5$. Results from simulation with NTMIX are used as reference data (denoted by “ref”).

2.3 DNS Setup

2.3.1 Flame configuration

Three DNS of statistically stationary methane-air premixed round jet flames were conducted in this study using HiPSTAR:

- a low Ka flame with an upstream pipe denoted by “Flame-WP”/“Flame-low” (Figure 2.13a)
- a low Ka flame without an upstream pipe denoted by “Flame-NP” (Figure 2.13b)
- a high Ka flame with an upstream pipe denoted by “Flame-high” (Figure 2.13a)

In the simulations, a turbulent stream of unburnt reactants ($Y_R = 1$) was injected into a surrounding of hot burnt mixture ($Y_R = 0$) from a low velocity coflow.

The flame and flow parameters are summarised in Table 2.3. The jet Reynolds number based on the inlet diameter and the Mach number are constant for the three flames. In order to study the effect of inflow conditions, the parameters for Flame-WP and Flame-NP in Table 2.3 are the same, and the difference is in the computational domains as observed in Figure 2.13. To study the effect of flame Karlovitz number, the unburnt mixture temperature is varied between Flame-low and Flame-high, resulting in different laminar flame speeds and laminar flame thicknesses.

The reaction rate was modelled using single-step irreversible Arrhenius chemistry given in Eq. 2.11. The laminar flame speed, laminar flame thickness, and adiabatic flame

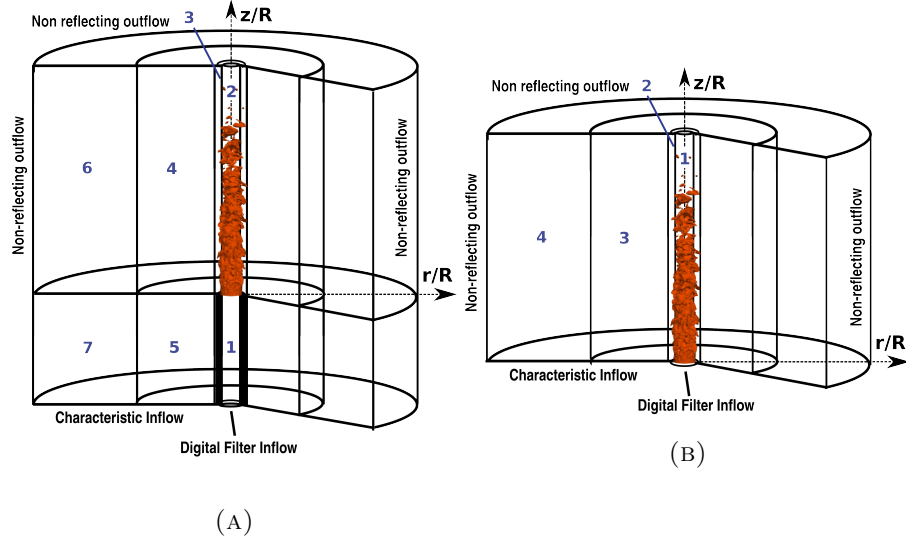


FIGURE 2.13: Layout of computational domain a) including upstream pipe (“Flame-WP”) and b) without upstream pipe (“Flame-NP”).

Parameter	Flame-WP/Flame-low	Flame-high	Flame-NP
Equivalence ratio (Φ)	1.0	1.0	1.0
Jet Reynolds number (Re_D)	10,000	10,000	10,000
Inlet Mach number (M)	0.35	0.35	0.35
Laminar flame speed (S_L/U_b)	0.012	0.003	0.012
Heat release parameter (α)	0.675	0.8645	0.675
Unburnt temperature (T_u)	800K	300K	800K
Burnt temperature (T_b)	2460K	2460K	2460K
Zel’dovich parameter (β)	7.9	12.1	7.9
Prandtl number (Pr)	0.72	0.72	0.72
Laminar thermal flame thickness (δ_{th}/D)	0.038	0.245	0.038
Zel’dovich flame thickness (δ_z/D)	0.0167	0.0463	0.0167
Ka_{in}	4.2	90	4.2
Kolmogorov length scale	0.009	0.009	0.009

TABLE 2.3: Flame parameters.

temperature are calculated by simulating an unstrained laminar flame with GRI-MECH 3.0 (Smith et al., 1999) mechanism using Cantera (Goodwin et al., 2018). The 1D laminar flame profiles are shown in Figure 2.14, which is used for initial and boundary conditions described below.

2.3.2 Computational Domain and Grid

The computational domain of Flame-WP/Flame-low and Flame-high shown in Figure 2.13a consists of seven blocks: block 1 represents the pipe, blocks 5 and 7 the upstream

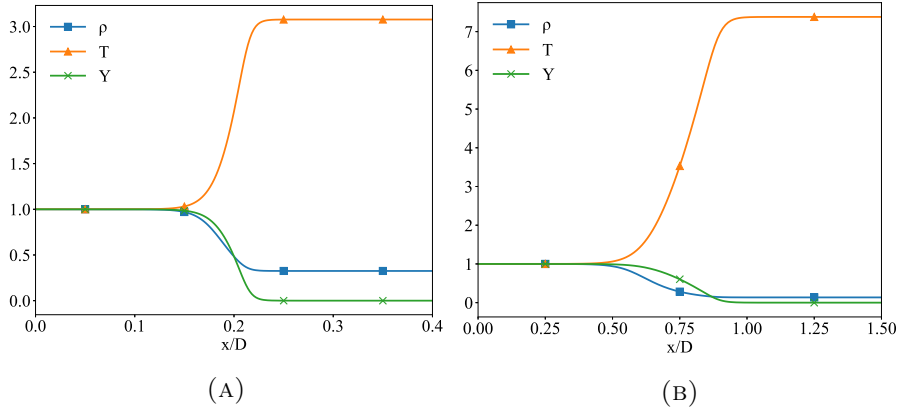


FIGURE 2.14: Laminar flame profiles for (A) Flame-WP/Flame-low and Flame-NP, and (B) Flame-high.

coflow, and blocks 2, 3, 4, and 6 the flame region downstream of the pipe exit. The domain for Flame-NP shown in Figure 2.13b is similar to Flame-WP except with blocks 1, 5, and 7 of Figure 2.13a removed. In both domains, the origin ($z = 0$ and $r = 0$) is defined at the axis of the pipe exit in Figure 2.13a and at the jet inflow in Figure 2.13b. The use of a multiblock domain is cost effective and well suited for this geometry.

Table 2.4 presents for each block the streamwise dimensions L_z , radial dimensions L_r , streamwise grid points N_z , radial grid points N_r , azimuthal Fourier modes k , and the azimuthal collocation points N_θ . The grid is smallest at the radial location of the pipe wall, so that the resolution at $r/R = 1$ corresponds to approximately 20 points across the laminar flame thickness for Flame-low. Polynomial stretching is applied with increasing radial and streamwise distance. In the azimuthal direction, the spacing in physical coordinates corresponds to at least 6 collocation points per laminar flame thickness. The grid spacing in the flame region is smaller than the estimated Kolmogorov length scale shown in Table 2.3.

2.3.3 Boundary conditions

The turbulent inflow boundary condition in block 1 of Figure 2.13 was imposed by superposing turbulent fluctuations onto a mean velocity profile. The mean velocity profile and Reynolds stress tensor were obtained by performing a precursor periodic, 8 diameter axial length pipe simulation at the Reynolds number and Mach number reported in Table 2.3, and with an imposed pressure gradient of $dp/dz = -0.029$ for a constant mass flux. The turbulent fluctuations imposed onto the mean profile were generated using the digital filter method described in Section 2.2.4.1. The prescribed integral length scales are $I_z/D = 1$, $I_r/D = 0.2$, and $I_\theta/D = 0.3$ (Sandberg and Tester, 2016). Figure 2.15 shows a comparison of the prescribed profiles and the statistics of the

A)	Block	L_z	L_r	N_z	N_r	k	N_θ
	1	50.0	1.0	560	75	192	386
	2	60.0	1.0	2000	75	192	386
	3	60.0	0.1	2000	25	192	386
	4	60.0	7.0	2000	200	192	386
	5	50.0	7.0	480	200	32	66
	6	60.0	37.0	2000	300	8	18
	7	50.0	37.0	480	300	8	18

B)	Block	L_z	L_r	N_z	N_r	k	N_θ
	1	50.0	1.0	560	75	128	258
	2	100.0	1.0	2400	75	128	258
	3	100.0	0.1	2400	25	128	258
	4	100.0	17.0	2400	290	128	258
	5	50.0	17.0	480	290	32	66
	6	100.0	27.0	2400	240	8	18
	7	50.0	27.0	480	240	8	18

C)	Block	L_z	L_r	N_z	N_r	k	N_θ
	1	60.0	1.0	2000	75	192	386
	2	60.0	0.1	2000	25	192	386
	3	60.0	7.0	2000	200	192	386
	4	60.0	37.0	2000	300	8	18

TABLE 2.4: Lengths, grid points, and Fourier modes (k)/collocation points (n_{zp}) for each block in the computational domain as depicted in figure 2.13 for A) Flame-WP/Flame-low, B) Flame-high and C) Flame-NP. All dimensions are normalized with the pipe radius R .

inlet generated by the digital filter boundary condition, with good agreement observed between the two sets of profiles.

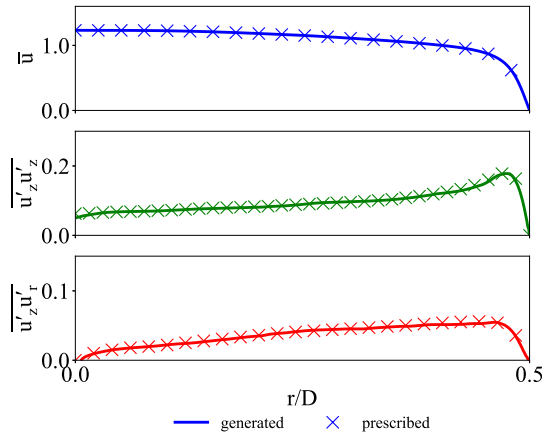


FIGURE 2.15: Comparison of prescribed and generated profiles by the digital filter inlet.

A Neumann boundary for pressure was imposed to account for pressure gradient in the pipe flow. Density was calculated from Eq. 2.4a, while the mass flow rate ρU was fixed at

the inlet by scaling the velocity profile of Figure 2.15 with the calculated instantaneous ρ . Accounting for compressibility effects of the pipe flow, the mass flow rate was fixed at the inlet to the desired value, while the density ρ was free to change.

The coflow inlet boundary condition for blocks 5 and 7 in Figure 2.13a, and blocks 3 and 4 in Figure 2.13b were imposed using the integrated characteristic inlet boundary condition with a Blasius boundary layer velocity profile with a freestream velocity of 1% of the jet bulk velocity and burnt product $Y_R = 0$ with temperature $T = \frac{1}{1-\alpha}$. Characteristic boundary conditions described in Section 2.2.4.2 were used at the outermost radial boundary and at the furthest downstream boundary. The zonal boundary developed by Sandberg and Sandham (2006) was applied over 50 points from $z/D = 25$ to $z/D = 30$ in Flame-WP/Flame-low and Flame-NP, and from $z/D = 45$ to $z/D = 50$ in Flame-high to dampen the velocity fluctuations and therefore minimize unphysical reflections.

The reactants and coflow streams are separated by a wall with a thickness of 5% the pipe diameter. The flame is anchored at the nozzle lip by imposing the temperature profile obtained from the 1D simulation results shown in Figure 2.14. Isothermal walls are also imposed on the inner and outer pipe walls with $T = 1$ and $T = \frac{1}{1-\alpha}$ respectively. At the axis, the boundary treatment based on parity conditions described in Section 2.2.4.4 was used.

2.4 Flow Analysis Tool (FAT)

The Flow Analysis Tool (FAT) (Bechlars, 2015) was developed as a companion Fortran program to HiPSTAR for post-processing HiPSTAR output data format. Specifically, instantaneous variables from HiPSTAR are written into “subspaces”, which are subsets of the flow field. The code is paralised by MPI so that the reading and processing of the data is subdivided to multiple processors and post-processing routines are written in a modular structure so that new features can be easily added, or existing features can be extended. The features used in this study include the calculation of instantaneous derived quantities (i.e. velocity gradient invariants), time and spatially averaged statistics, probability density functions, and conditional averages. Explicit filtering operations were also performed with this tool. For this study, FAT was extended to include post-processing for quantities of interest to reacting flows. This includes quantities such as flame surface density, flame normal vectors, flame curvature, reaction rate, and flame strain rates.

2.4.1 Explicit spatial filtering

Explicit filtering is used on HiPSTAR output data to obtain filtered quantities. The filtering operation in the three dimensions is defined as,

$$\bar{\phi}(\mathbf{x}) = \frac{\iiint_{-\infty}^{\infty} \phi(\mathbf{x}') G(\mathbf{x}, \mathbf{x}') d\mathbf{x}'}{\iiint_{-\infty}^{\infty} G(\mathbf{x}, \mathbf{x}') d\mathbf{x}'}, \quad (2.38)$$

where ϕ is the unfiltered quantity, $\bar{\phi}$ is the filtered quantity, $G(x, x')$ is the kernel operation. The Gaussian kernel is defined as,

$$G(\mathbf{x}, \mathbf{x}') = e^{-\frac{|\mathbf{x}-\mathbf{x}'|^2}{2\sigma^2}}. \quad (2.39)$$

where the standard deviation σ is defined based on the filter size Δ :

$$\sigma = \frac{\Delta}{\sqrt{8 \ln(2)}}. \quad (2.40)$$

To reduce the cost of the filtering operation, the integral operation of Eq. 2.38 is truncated as

$$\bar{\phi}(\mathbf{x}) = \frac{\iiint_{-s\sigma}^{s\sigma} \phi(\mathbf{x}') G(\mathbf{x}, \mathbf{x}') d\mathbf{x}'}{\iiint_{-s\sigma}^{s\sigma} G(\mathbf{x}, \mathbf{x}') d\mathbf{x}'}, \quad (2.41)$$

such that the truncation error is,

$$erf\left(\frac{s}{\sqrt{2}}\right). \quad (2.42)$$

The truncation error for different values of s is given in Table 2.5.

s	truncation error
1	0.682689492137086
1.5	0.866385597462284
2	0.954499736103642
2.5	0.987580669348448
3.0	0.997300203936740

TABLE 2.5: Truncation error for filtering.

2.5 Machine Learning (Eve)

2.5.1 Brief overview of the algorithm

The GEP toolset, referred to as Eve (Weatheritt, 2015), is a set of serial Python libraries for performing the GEP approach used in the works described in Section 1.2.5.2. The

work-flow of using Eve to conduct the GEP-based symbolic regression is illustrated in Figure 2.16. First, a set of input is defined. This includes the definition of the symbols to be used, i.e. $+$, $-$, $\exp$, x , y , and the reading of the training data associated with the symbols, i.e. x , y . The probabilities of the genetic operations are defined, as well as the number of generations, population size, tournament size, number of genes per individual, genotype length, and convergence criteria. An initial population of individuals is then generated. The fitness of every individual is calculated using the input training data. The convergence is then checked to see if any fitness is below the defined tolerance. If the convergence criteria are met, the best solution is taken to be the output of the process. If convergence is not met, a selection (survival of the fittest) is done through the tournament selection process to pick out surviving individuals that are carried to the new generation. Genetic operators are then applied to create the new population. With the new population generated, the process loops back to begin the computation of the fitness again. A more in-depth description of this algorithm is given in the following section.

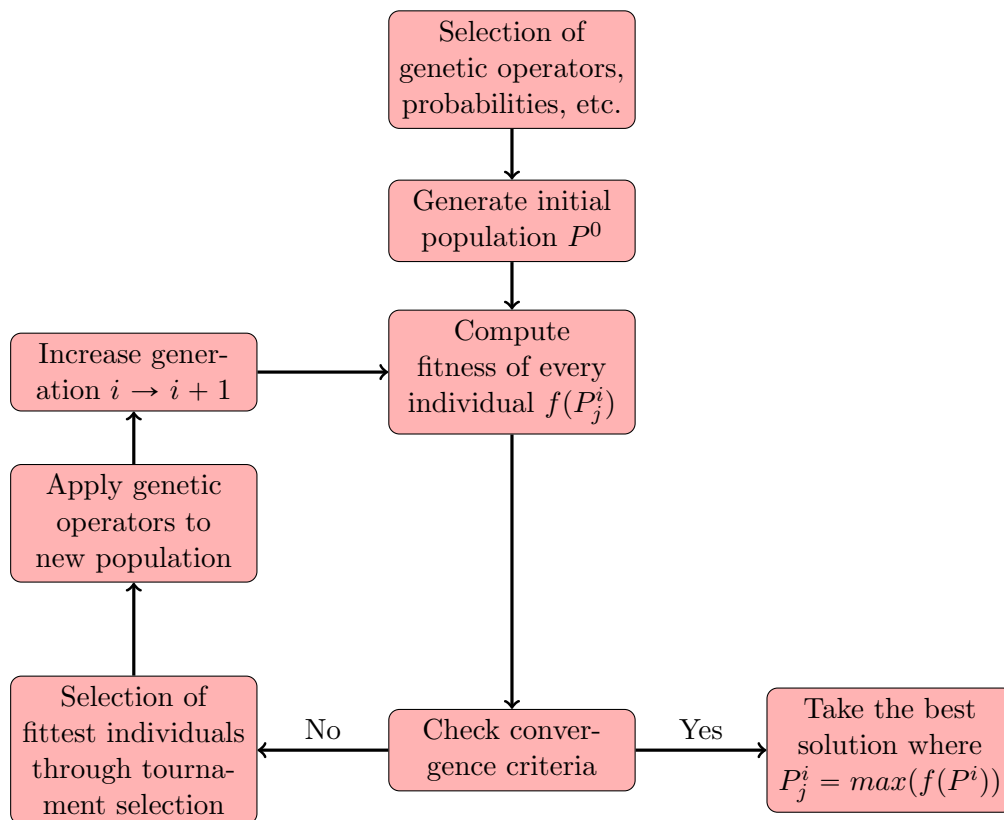


FIGURE 2.16: Work-flow of Eve algorithm.

2.5.2 Method Description

Three branches of EA are described in this section: Genetic Algorithms (GA), Genetic Programs (GP), and Gene Expression Programming (GEP). The GA and GP approaches are only briefly introduced here as certain concepts from each are used to form the basis of GEP, but more details can be found in the works of Holland (1962); Cramer (1985) for the interested readers. The main difference between the three algorithms is in the way that the individuals are represented. Individuals, which are the candidate solutions of a given problem, contain information which are representative of the problem. For example, individuals can be made of a set of directions (left, right, up, down, ...) for navigating a maze, or mathematical symbols for solving a function (+, -, *, /, x, y, ...). There are two representations for describing these individuals: the genotype and the phenotype.

Genotypes and Phenotypes

To understand the advantages of GEP over the two predecessors, the genotype–phenotype distinction as observed in genetics must be made. In biological terms, the genotypes are hereditary information, or the “code”, while phenotypes are the physical traits, such as blue eyes. The evolution of the genotypes is predicted by Mendelian genetics, i.e. mutation, while the evolution of phenotypes is governed by natural selection where individuals with unfavourable traits die out (Norton, 1928). Between these two processes is the mapping of genotypes to phenotypes and vice-versa.

The GA approach follows the Mendelian description, in other words, the individuals take forms similar to the structure of chromosomes, genes, and alleles. The individuals are represented by fixed length strings. In GP, the individuals are represented by a non-linear tree structure (Parse tree). Using the example of symbolic regression, where each element of the individual is represented by a symbol (i.e. +, -, *, /, x, y), examples of the two approaches of defining the individual are illustrated in Figure 2.17.

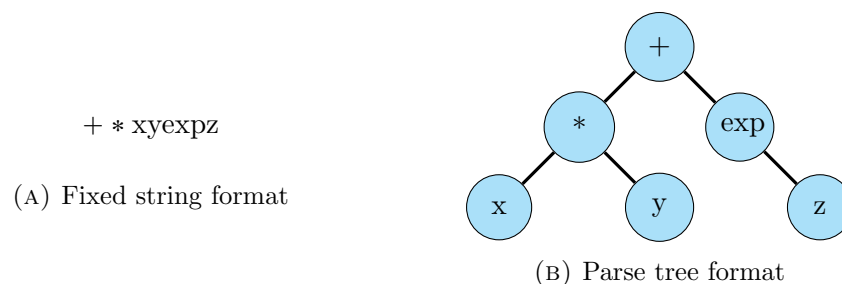


FIGURE 2.17: Individuals for symbolic regression.

While the simplicity of the string structure in GA makes them easy to manipulate, it is obvious that one of the constraints of GA is the fixed length of the individuals. This limits the approach to suit only problems where the solution has a predefined length and fixed number of parameters. Regression problems where the functional form is not known is then ill suited for this approach, as limiting the length of the solution limits the diversity of solutions.

The nature of the Parse tree in GP makes it suited for symbolic regression, as symbols have a certain degree of freedom assigned to them, measured by their arity. For example, a “+” has an arity of two, meaning that it can take on two arguments (branches of the tree). This enables meaningful functional forms to be created. However, the more structured form introduces additional constraints on the genetic operations to avoid producing invalid trees, therefore reducing the evolutionary efficiency of the approach. GP can also result in bloated individuals, where they grow larger through repeated genetic crossover. Bloated individuals become harder to interpret and increase storage and computing time.

One of the major disadvantages common to both methods is understood by referring to the genotype–phenotype distinction. In the two methods both the genotype and the phenotype are represented by the same string (in the case of GA) or the same tree (in the case of GP). This means that an individual lives with all of its genetic information, both desired and undesired information. As all of its information is passed on to the next generation (with some variation), good genetic material may be disposed due to the presence of a few bad portions in the inherited individuals. Another consequence of having the same genotype and phenotype is that genetic material will never be dormant. The advantage of having dormant genes is that they can be protected from being lost, until new beneficial combinations can be found when the bad traits die out.

GEP was proposed by Ferreira (2001) as an extension of GA and GP, which tries to resolve the disadvantages found in GA and GP. The approach combines the manipulability of strings in GA with the functional complexity of parse trees in GP. To be more specific, the genotype in GEP is a linear fixed-length string, while the phenotype is a non-linear expression tree. This approach is closer to the evolution of genotypes and phenotype in biological genetics. Natural selection occurs with the phenotype as it is the functional form of the genotype, while processes associated with Mendelian genetics occurs at the genotype.

The basis which allows for the distinction between the genotype and phenotype in GEP is the introduction of Open Reading Frames (ORFs), a concept found in molecular genetics for gene prediction. The ORF is a portion of a genotype from which the phenotype is constructed, in other words, only a portion of the genotype is observable. Figure 2.18

shows an example of the genotype and its corresponding phenotype using this definition. In this example, the string “+*xyexpz” is realized in the phenotype, while the string “-cosx*yx” is repressed. Similar to genetics, these dormant genes are passed down to the children, and can become active again through mutation (known as atavism). The addition of the ORF allows the phenotype (expression tree) to vary in size despite the fixed length of the genotype by allowing the ORF to vary in size. The length of the genotype is then no longer the exact length of the phenotype, but an upper limit on the size of the phenotype. In GEP, the start position of the ORF is the beginning of the genotype string (root). The phenotype is formed by reading the genotype recursively, such that the phenotype is formed from the top, and branches from the left to the right, moving to the next highest branch once a terminal branch (arity=1) is reached. The functional form of the individual in Figure 2.18 is $(x * y) + \exp(z)$.

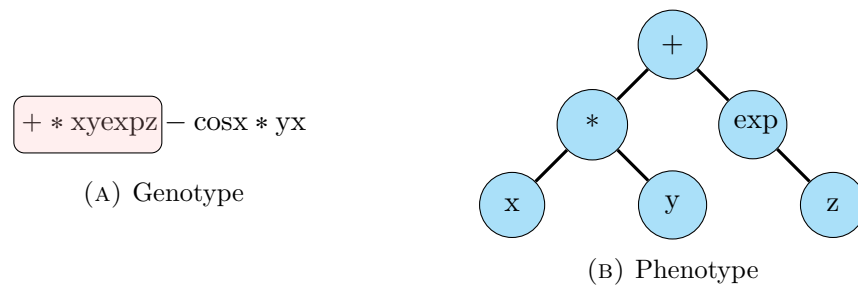


FIGURE 2.18: Individual in GEP. The red frame is the ORF.

One possible issue with the basic definition of the genotype above is that a syntactically correct expression may not always occur as the expression might not be terminated by the end of the genotype. In other words, an increase in the number of higher arity elements, such as by genetic mutation, may mean that there is not enough low arity elements to fill all the arguments. To counter this issue, the concept of head and tail of the gene is introduced. The head is the front elements of a gene and can contain elements from any of the chosen symbols. The tail is the later part of a gene where elements are selected only from the pool of terminal symbols (arity=1). For example, in a gene given as $+ * xyz|yyxxyz$, the $|$ symbol denotes the split between the head and tail of the gene. The gene contains $h = 5$ element in its head and $t = 6$ elements in its tail. It can be seen that the tail only consists of terminal symbols, guaranteeing that there are always enough terminals to close the expression.

Another concept allowed by the GEP method is multigenics, where each individual consists of multiple genes. The genes are connected by linking functions. Figure 2.19 shows an example of a multigenic individual, where the linking function denoted by $<>$ is $*$, resulting the full functional form of $((x * y) + \exp(z)) * ((x / (x - y)) * z)$. There are two main uses for multigenics. The first is for the optimisation problems where there may

be multiple outputs. The other use is to increase the non-linearity between genotype and phenotype, as each gene will be subject to the genetic operators.

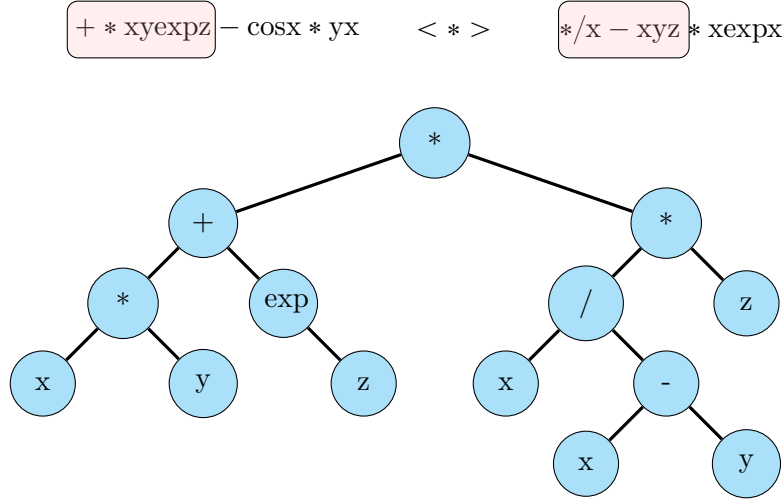


FIGURE 2.19: Multigenic individual

The nature of individuals defined in GEP allows for additional genetic operations which are not possible, or not useful, in GA and GP. The genetic operations used in GEP will be explained later in this section.

Fitness and survival of fittest

Individuals from generation P^i are selected for the next generation P^{i+1} by gauging their fitness. A fitness function f is defined which measures an individual's chances of survival. For example, fitness functions can be the absolute error of individual P_j^i

$$f(P_j^i) = \frac{1}{n} \sum_{k=1}^n |\Phi_k - E_k|, \quad (2.43)$$

or the relative error

$$f(P_j^i) = \frac{1}{n} \sum_{k=1}^n \frac{|\Phi_k - E_k|}{|E_k|}. \quad (2.44)$$

where Φ is the calculated value using P_j^i and E is the expected/target value (the training data) for each of the n number of data points. A solution is found when a desired fitness F and the maximum fitness of the population, $\max(f(P^i))$, are within a defined tolerance ϵ . The choice of the fitness function is problem dependent, as it may affect convergence to a good solution.

Two common methods for the selection of individuals are the roulette wheel and the tournament selection. The Roulette wheel selection is analogous to spinning a roulette wheel to select N number of individuals to survive to the next generation $i + 1$. Each

individual P_j^i in the generation are represented by a slice of the wheel. The size of the slice assigned to each individual is based on its fitness; individuals with better fitness are given larger slices, so that their probability of survival is higher compared to those with worse fitness. The major disadvantage of this selection method is the tendency to select the same few individuals with better fitness repeated, resulting in a fast convergence toward suboptimal solutions.

The tournament selection method involves the competition of individuals in tournaments to select the fittest individual, illustrated in Figure 2.20. Each of the N number of tournaments contain a set number of competitors, given by the tournament size s . At generation i , each tournament randomly selects s number of individuals to compete in its tournament. The fittest individual from each tournament is selected to survive, so that the winners make up the N individuals in the next generation $i + 1$. The addition of tournament size adds an extra degree of control compared to the Roulette wheel selection. Large tournament sizes give higher chances of each tournament containing a strong individual, while smaller sizes make surviving easier. Therefore, varying s and N will tune the variation for a given problem.

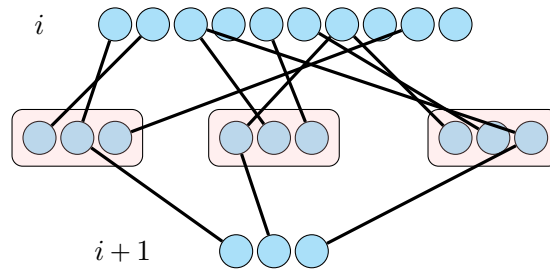


FIGURE 2.20: Tournament selection. Individuals from generation i selected for $N = 3$ tournaments (red) of size $s = 3$. Best individual from each tournament survives to generation $i + 1$.

One potential issue is that there is a chance that the best individuals may not be selected to participate in a tournament, since the selection of participants is random. To avoid this, the concept of elitist selection is used. In elitism, the best solution is carried forward into P^{i+1} , bypassing the tournament selection process.

Genetic Operators

Genetic operators are used to provide variation after replication of genes (reproduction) for the next generation. In GA and GP, the main genetic operators used are mutation and crossover. In GEP, mutation and crossover are also available operators, while additional operators of transposition and inversion are also possible due to the more sophisticated genotype/phenotype definition. A brief description of each is given here.

In mutation, a gene selected for the genetic operation is replaced with another gene. For example the following is a mutation operator on a gene:

$$+ * \underline{xy} \exp z \quad \longrightarrow \quad + * \underline{xz} \exp z$$

where the fourth element is changed from y to z . The mutation operator can be quite destructive to the gene.

The crossover involves the swapping of genetic information between two genes, such as in the following example:

$$\begin{array}{ccc} + * \underline{xy} - \underline{yexpz} & \longrightarrow & + * \underline{xyx} + \underline{xy} \\ * - z + \underline{x + xy} & & * - z + \underline{-yexpz} \end{array} .$$

This is an example of a one-point crossover, where one point is selected on each gene (position 6 in first gene and position 8 in second gene), and the string of element after those points are swapped between the two genes. A two-point crossover would swap the strings between two selected points on each gene; for example:

$$\begin{array}{ccc} + * \underline{xy} - \underline{yexpz} & \longrightarrow & + * \underline{+x + yexpz} \\ * - z + \underline{x + xy} & & * - z \underline{xy} - \underline{xy} \end{array} .$$

Transposition is the copying of a portion of a gene to another gene. The following example shows the transposition operator:

$$\begin{array}{ccc} + * \underline{xy} - \underline{yexpz} \cos xy & \longrightarrow & + * \underline{xy} - \underline{yexpz} - \cos xy \\ * - \underline{zy} + x + xy \exp x & & * - \underline{yexpzx} + xy \exp x \end{array}$$

where the 5th to 8th elements of the first gene are copied, and replaces the 2th to 5th elements of the second gene. Note the portion of the second gene that was replaced is the same length as the portion copied from the first gene in order to keep the length of the genotype fixed.

The last genetic operator described here is inversion. The premise is to take a portion of the gene and inverting the string. A simple example of inversion operator is:

$$+ * \underline{xy} \exp z \quad \longrightarrow \quad + * \underline{expyx} * z .$$

Inversion can result in large variations as the importance of elements is greatly changed by modifying the order. It is usually recommended to keep the occurrence of inversion low to avoid to excessive amounts of variation.

It is usually good in a GEP algorithm to allow the probability of occurrence of each genetic operator type to be specified. This would allow more control over the degree of genetic variation for better convergence to a good solution.

2.5.3 Interfacing with FAT

Most of the previous studies using Eve described in Section 1.2.5.2 have been conducted using relatively small to medium sized training data. For a large dataset, the serial nature of Eve results in long run times. To scale up the computational performance of the framework, the most computation and memory intensive component of the work-flow, which is the calculation of the individuals' fitness $f(P_j^i)$, is externalised to an efficient parallelised code. FAT is the perfect candidate code to undertake this task, as the post-processing code is MPI parallelised and can directly read HiPSTAR format output as the training data. Additionally, as seen later in Chapter 5, the explicit filtering framework in FAT is used for the preparation of the training data. Therefore, an interface between FAT and Eve is implemented in this study.

The basis of this implementation is that Eve will output the genotype of the individuals at each new generation. Eve will then wait for FAT to read the genotype, calculate the fitness, and output the fitness. Next, Eve will collect the fitness, and perform the rest of the tasks such as selection of the fittest individuals and applying genetic operators for the new generation. Modifying the work-flow in Figure 2.16, the new work-flow for the Eve-FAT framework is illustrated in Figure 2.21.

2.6 Summary

This chapter presented the numerical methods and the configurations of the turbulent premixed jet flame DNS conducted in this study. The governing equations and boundary conditions used in HiPSTAR were discussed, including the implementation of reacting flow capabilities to the solver. Various validation simulations of laminar premixed flames were conducted and the comparison with results obtained from a different solver, NT-MIX (Cuenot et al., 1997), showed that the results obtained with HiPSTAR are in good agreement with the reference results. The computational setup of the DNS cases were presented. The postprocessing algorithm (FAT) and the GEP algorithm (Eve) were briefly described. In order to improve the computational performance of the Eve, parallelisation was implemented by interfacing the algorithm with FAT so that the fitness of candidate solutions are computed with multiple processors using FAT.

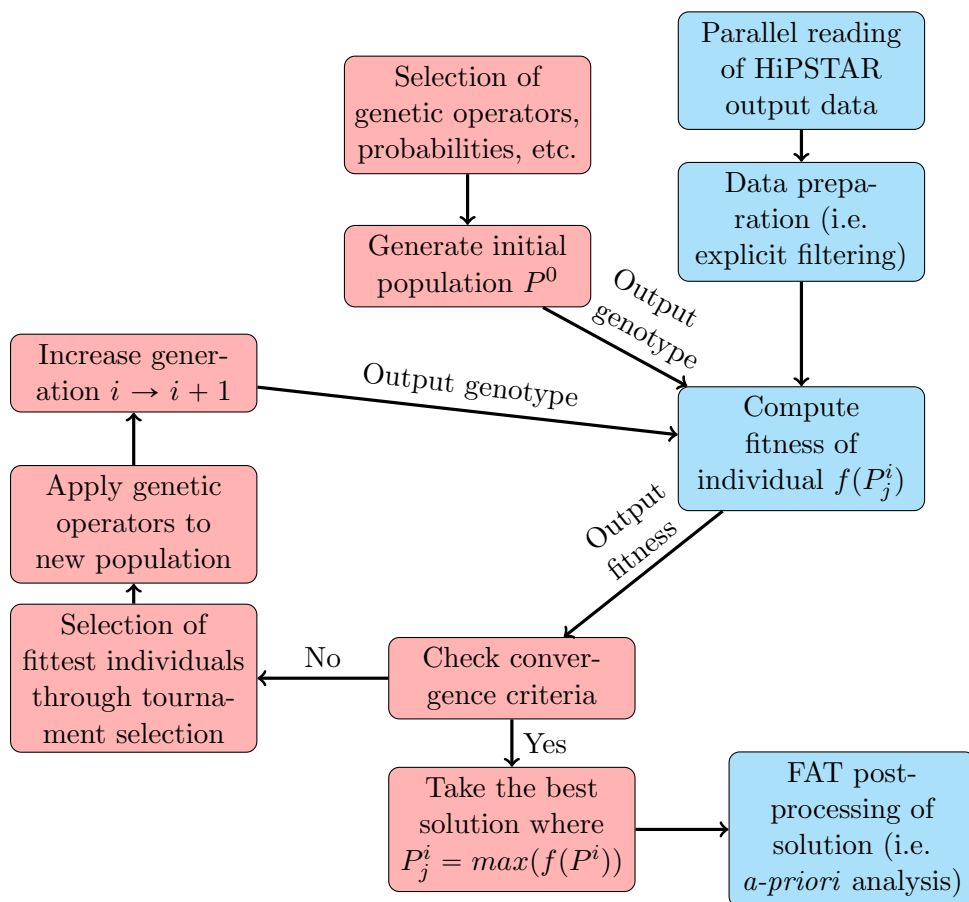


FIGURE 2.21: Work-flow of Eve-FAT framework. Red nodes are performed by Eve and blue nodes are performed by FAT.

Chapter 3

Effect of inflow turbulence generation methods

3.1 Introduction

The restrictive cost of DNS coupled with additional costs from considering chemistry have likely discouraged simulations which include resolving conditions upstream of the jet exit, though the experimental and numerical studies discussed in Section 1.2.3 show that this is a topic worth investigating.

In this chapter, two DNS cases of turbulent premixed round jet flames with different inflow turbulence generation methods are analysed. One simulation consists of an upstream pipe and coflow region to provide the flame with a fully-developed turbulent inflow (Flame-WP), while the other simulation uses a digital filter synthetic turbulence inflow for the flame (Flame-NP). As described in Section 2.3, the two simulations have the same flame parameters, differing only in the inflow boundary condition method.

Global evolution of the flame and the jet flow are compared for the two simulations. Local statistics at the flame front are also analysed, including the orientations of the flame front and turbulence strain, and variation of the flame thickness across the flame brush.

3.2 Turbulent inflow

In this section, the turbulent flow associated with the two inflow boundary conditions are analysed by comparing the pipe flow of Flame-WP with the synthetically generated flow

of Flame-NP. Figure 3.1 shows an instantaneous velocity fluctuation, $u' = u - \bar{u}$, snapshot on a cross-section on the z - r plane, where $\bar{u}$ is the Reynolds averaged velocity. The snapshot shows the flow in the vicinity of the pipe exit ($z/D = -5$ to $z/D = 0$), where $z/D = 0$ indicates the pipe exit plane and negative streamwise locations indicate distance upstream of the pipe exit plane. The flow pattern features patches of positive and negative u' , reminiscent of typical visualizations of pipe flow (Wu and Moin, 2008). These patches, especially in the near wall regions appear to be elongated in the streamwise direction, suggesting coherence in the flow structure.

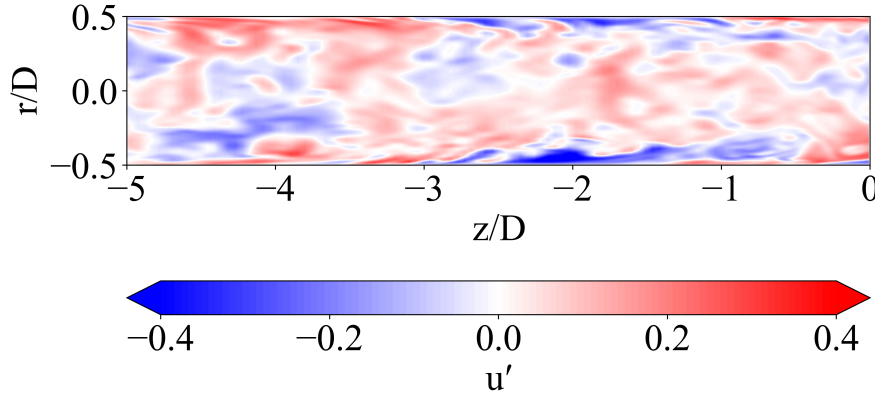


FIGURE 3.1: Instantaneous velocity fluctuation u' in the pipe on the z - r plane.

The statistics of the turbulent pipe flow in Flame-WP are examined to access the quality of the inflow boundary conditions. The temporally and azimuthally averaged streamwise velocity, shear stress, and root-mean-squares of streamwise and radial velocity in wall coordinates are shown in Figure 3.2, for streamwise locations $z/D = -5$, -1 , and 0 . The results are compared with the incompressible experimental reference data of Den Toonder and Nieuwstadt (1997) and numerical data of El Khoury et al. (2013). The good agreement of the turbulence statistics with the reference pipe flow data demonstrates that the upstream conditions for the flame inlet are well-defined in Flame-WP.

To verify that the digital filter boundary condition is able to replicate the lower order statistics of the pipe flow based on prescribed values, Figure 3.3 shows a comparison of the prescribed profiles and the statistics of the inlet generated by the digital filter boundary condition. The profiles show good agreement between the generated and the prescribed values.

Finally, the flow at $z/D = 0$ is compared between Flame-WP and Flame-NP. Figure 3.4 shows a comparison of the temporally and azimuthally averaged streamwise velocity and turbulent kinetic energy at $z/D = 0$ between Flame-WP (presented by the solid lines) and Flame-NP (presented by the dashed lines). The Flame-WP results correspond to the conditions at the pipe exit plane, while the Flame-NP results correspond to

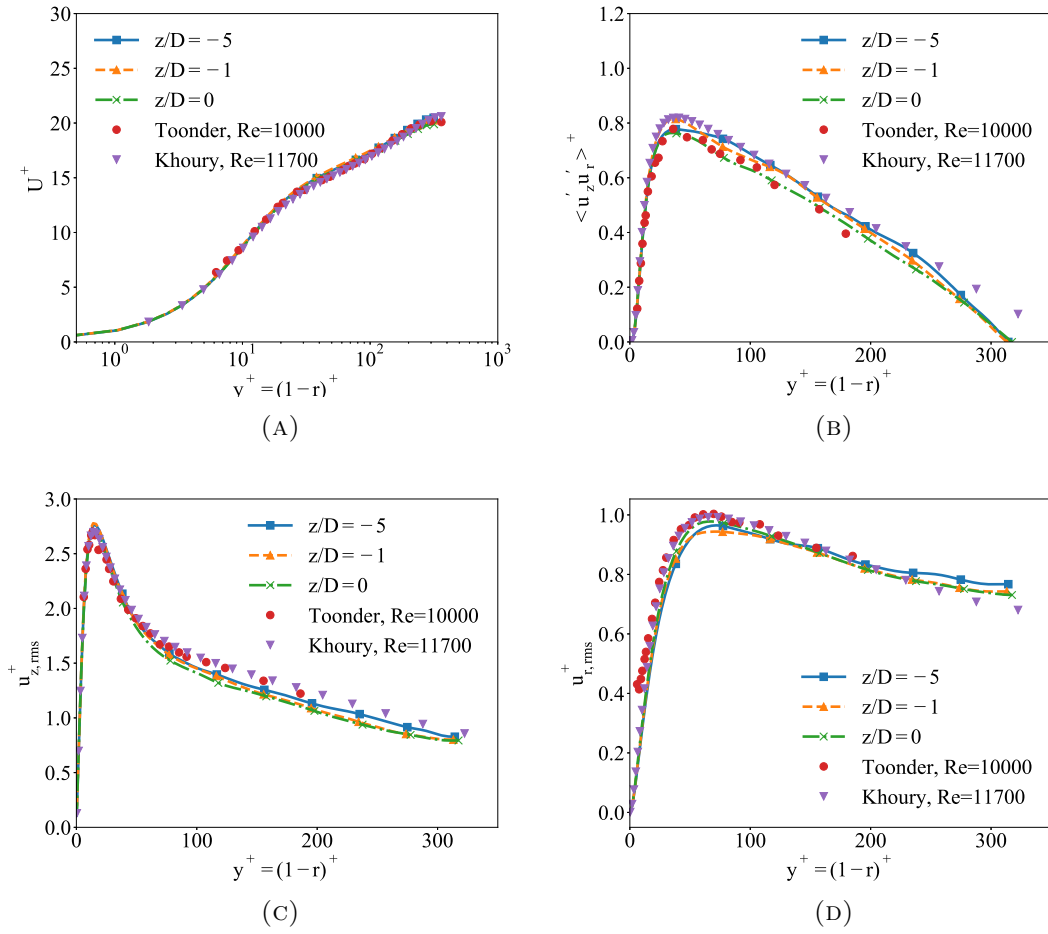


FIGURE 3.2: (A) Mean axial velocity U^+ , (B) shear stress, (C) RMS of streamwise velocity, (D) RMS of radial velocity in the pipe. Reference data from Den Toonder and Nieuwstadt (1997) and El Khoury et al. (2013).

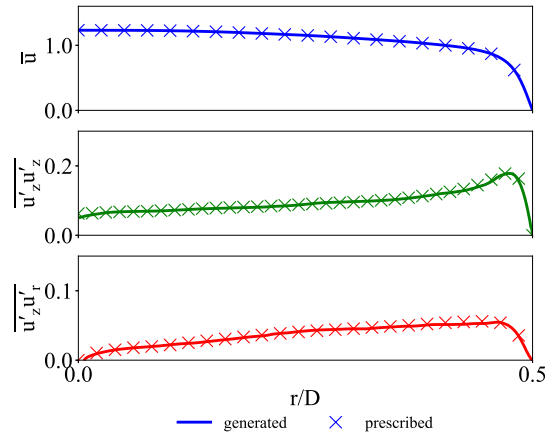


FIGURE 3.3: Comparison of prescribed and generated profiles by the digital filter inlet.

the inlet conditions generated by the digital filter boundary and characteristic coflow boundary. The profiles for the reactants stream ($r/D \leq 1$) of the two cases are in very

close agreement. The inflow generated by the digital filter inflow method in Flame-NP resulted in first and second order mean statistics that are in good agreement with the statistics of the pipe exit in Flame-WP, which is important to provide a rigorous comparison of the two cases.

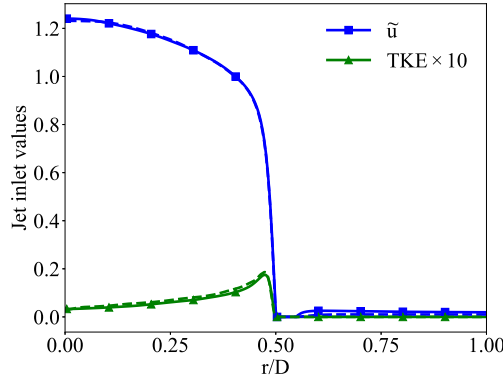


FIGURE 3.4: Favre averaged streamwise velocity $\tilde{u}$, and turbulent kinetic energy at $z/D = 0$ for Flame-WP (solid line) and Flame-NP (dashed line).

3.3 Global flame structure and flow field

To quantify the effect of the two inflow turbulence generation methods on flame characteristics, the global flow field and structure of the jet flame is examined. Both flames are visualized at an instant in time in Figure 3.5, presented by red iso-surfaces of $Y_R = 0.134$ corresponding to the location of maximum reaction rate. Vortical structures are visualized with blue iso-surfaces of $\lambda_{ci} = 1.5$. The quantity λ_{ci} , referred to as the local swirling strength of the vortex (Zhou et al., 1999), is the imaginary component of the complex conjugate eigenvalue following the decomposition of the velocity gradient tensor,

$$\nabla u = [\bar{\nu}_r \bar{\nu}_r \bar{\nu}_r] \begin{bmatrix} \lambda_r & 0 & 0 \\ 0 & \lambda_{cr} & \lambda_{ci} \\ 0 & -\lambda_{ci} & \lambda_{cr} \end{bmatrix} [\nu_r \nu_r \nu_r], \quad (3.1)$$

where λ_r and ν_r are the real eigenvalue and its corresponding eigenvector, and $\lambda_{cr} \pm \lambda_{ci}i$ and $\nu_{cr} \pm \nu_{ci}i$ are the complex conjugate eigenvalues and their corresponding eigenvectors. The local streamlines are expressed in the $(\nu_r, \nu_{cr}, \nu_{ci})$ coordinates, where stretching and compressing of local flow is along the ν_r axis, and swirling is on $\nu_{cr}-\nu_{ci}$ plane. The strength of the swirling is quantified by λ_{ci} . The surface of the flames becomes progressively more wrinkled in Figure 3.5. In the flame tip region, pockets of unburnt reactants are separated from the flame. The unburnt reactants appear to extend further downstream in Flame-NP, indicating a longer flame compared to Flame-WP. The jet

shear layer coincides with the flame front in the upstream flame regions, and the horse-shoe structures are found along the surface of the flame. Sparse and irregular elongated structures appear outside of the flame at downstream locations, and appear to exhibit no consistent pattern in their orientation. Similar structures outside the flame were observed by Duwig and Dunn (2013).

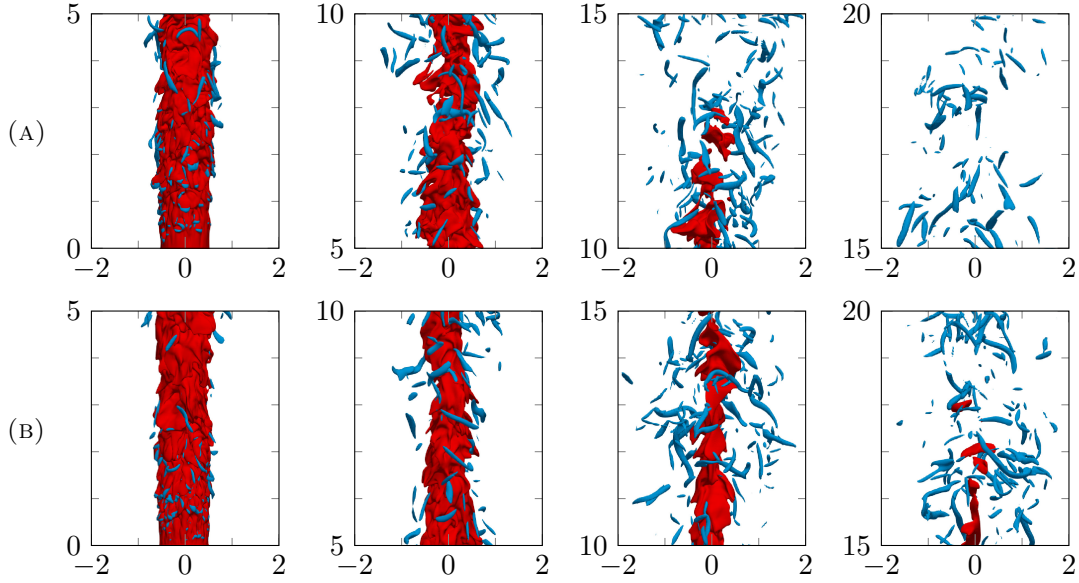


FIGURE 3.5: Iso-surfaces of $\lambda_{ci} = 1.5$ (blue) and $Y_R = 0.134$ (red) for (A) Flame-WP and (B) Flame-NP.

Figure 3.6 shows an instantaneous cross section of the flame coloured by λ_{ci} with a red iso-contour of $Y_R = 0.134$. The high viscosity in the burnt region is expected to dampen the structures in the jet core and inhibit the development of the coherent structures (Savas and Gollahalli, 1986). There is an observable difference in the density of the vortical structures inside the flame between Figures 3.6a and 3.6b. A range of structures with different sizes are observable throughout most of Flame-WP. In contrast, a large number of structures in Flame-NP appear to be concentrated near the inflow. Additionally, Flame-NP shows a decrease in the number of structures towards the jet centerline.

The vortical structures in the region of the pipe exit are more closely examined in Figure 3.7 with iso-surfaces of $\lambda_{ci} = 2$ coloured by Y_R . As can be seen, the pipe exhibits coherent vortical structures which are oriented in the streamwise direction and are seen to convect into the jet core. By $z/D \approx 2$, long streamwise structures seen at the pipe exit are not observed as smaller structures appear. In both flames, azimuthally oriented vortical structures can be observed on the outside of the jet core forming from the shear layer of the jet. Most of these structures show a variation in Y_R across their length, which indicates that these structure also lie across the flame front. In contrast to Flame-NP,

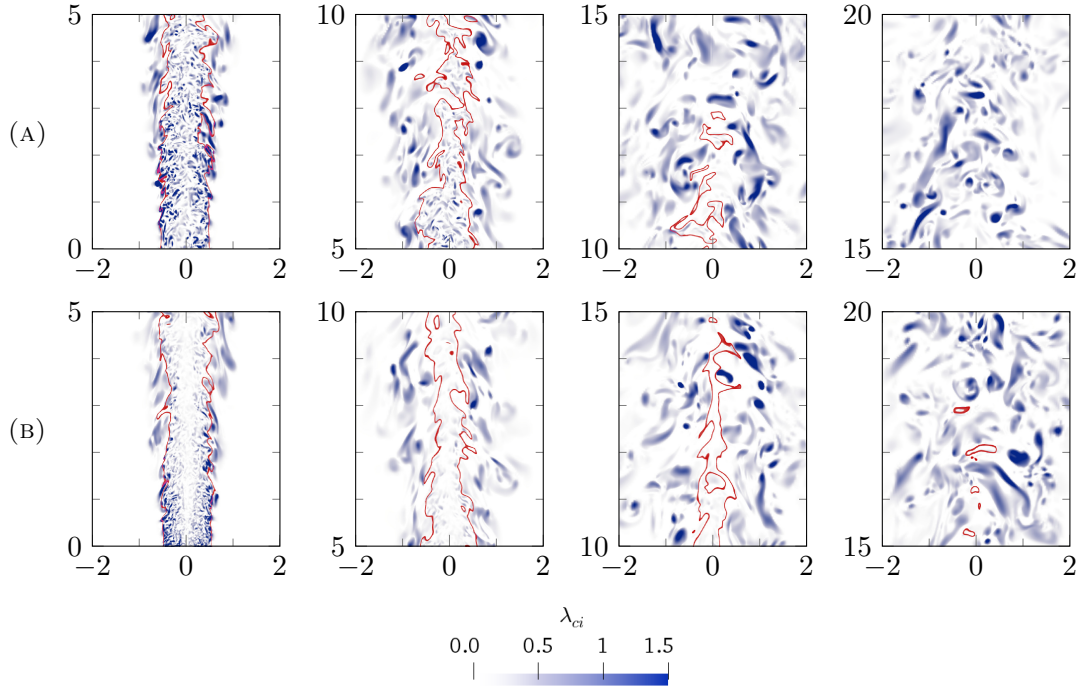


FIGURE 3.6: Cross-section on $z - r$ plane coloured by λ_{ci} with an isocontour of $Y_R = 0.134$ (red) for (A) Flame-WP and (B) Flame-NP.

the structures at the base of Flame-NP appear to be denser and more “noise”-like. The breakdown of structures occur earlier compared to Flame-WP, as the sparse occurrence of $\lambda_{ci} = 2$ iso-surfaces by $z/D \approx 1$ indicate lower vortex strengths in Flame-NP.

In order to quantify the vortical structures development observed in Figures 3.5 to 3.7, the average spatial orientations of structures are estimated by the variable Γ defined as (Jones and Sandberg, 2012),

$$\Gamma = \frac{\overline{p_z p_z} - \overline{p_\theta p_\theta}}{\overline{p_z p_z} + \overline{p_\theta p_\theta}}, \quad (3.2)$$

where $p_z = \partial p / \partial z$ and $p_\theta = \partial p / \partial \theta$ are the streamwise and spanwise partial derivatives of pressure respectively, and the bar denotes time and azimuthally averaged quantities. $\Gamma = 1$ indicates that streamwise gradients are dominant and structures are orientated in the spanwise direction while $\Gamma = -1$ indicates that spanwise gradients are dominant and structures are orientated in the streamwise direction. Figure 3.8 shows the contour plot of Γ for both flames. Radial profiles of Γ at various streamwise locations are also shown. Regions of turbulence intensity $u'/U < 1\%$ corresponding to the laminar coflow are filtered out. The radial profile at two diameters upstream of the pipe exit at $z/D = -2$ shows that Γ is negative across the radius of the pipe, which is consistent with the dominance of streamwise oriented structures observed in Figure 3.7. The most negative values of Γ are observed in the near wall regions of the pipe, up to $\Gamma \approx -0.57$ approximately $0.05D$ from the pipe wall. Downstream of the pipe exit plane, three distinct regions can be identified. A region inside the flame can be seen to consist of mostly positive values

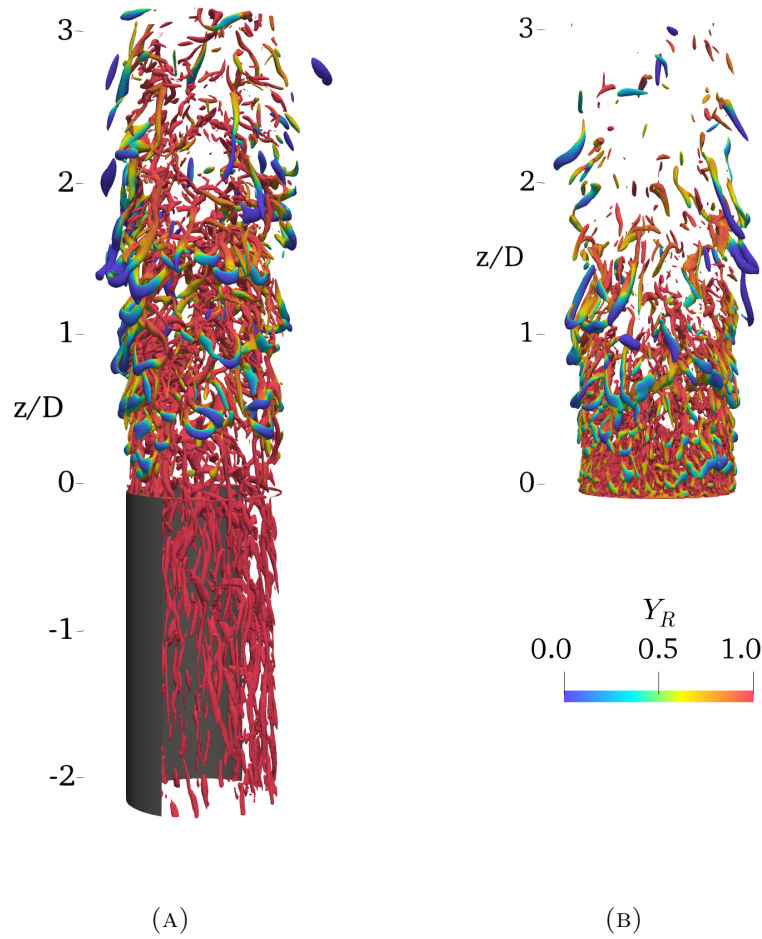


FIGURE 3.7: Iso-surfaces of $\lambda_{ci} = 2$ coloured by Y_R in the region of the pipe exit for (A) Flame-WP and (B) Flame-NP.

of Γ , indicating a preference towards azimuthally oriented structures. The magnitude of Γ in this region is higher in Flame-NP in comparison to Flame-WP. Towards the flame tip, some areas within this region show $\Gamma < 0$, particularly close to the axis for Flame-NP. It is likely that narrowing of the flame and separation of pockets of reactants at these downstream locations, as well as the lower levels of turbulence in Flame-NP, as seen in Figure 3.6, causes the difference in behaviour compared to upstream locations of the flame. A second region at the edge of the jet beside the low velocity coflow show the highest values of Γ , as expected due to dominance of azimuthal oriented large eddies from Kelvin-Helmholtz instability in the shear layer (Yule, 1978). Between the flame and the shear layer region, a third region is observed consisting mainly of slightly negative Γ values ($\Gamma < -0.1$) with intermittent patches of small positive Γ . Both streamwise and azimuthal vortex structures are observable in this region, though there is a preference towards streamwise orientated structures. This is consistent with the observations in Figure 3.5 where irregular elongated structures appear outside the flame, some of which exhibit a strong alignment in the streamwise direction.

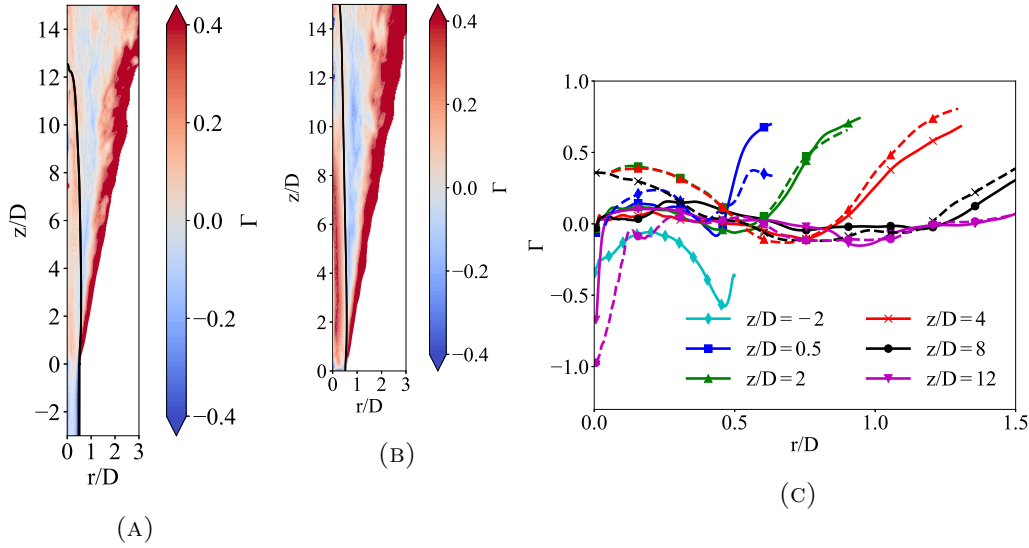


FIGURE 3.8: Contours of Γ for (A) Flame-WP and (B) Flame-NP, and (C) radial profiles of Γ at various streamwise locations for Flame-WP (solid line) and Flame-NP (dashed line). Regions with turbulence intensity $< 1\%$ are filtered out.

The flame and flow statistics are now examined to quantify the evolution of the jet and flame and to discuss the causes of the difference observed in the qualitative analysis. The growth of the flame is quantified by the mean reactant mass fraction in Figure 3.9, where Figure 3.9a shows the isosurfaces of $\widetilde{Y}_R = 0.134$ and Figure 3.9b shows the radial profiles at specific streamwise locations. In Figure 3.9a, it is observed Flame-WP is shorter than Flame-NP. Figure 3.9b shows that the profiles $\widetilde{Y}_R$ are in good agreement between the two cases at the first two specified streamwise locations close to the pipe exit. At $z/D = 4$, the difference between the $\widetilde{Y}_R$ radial profiles is observable, where Flame-WP shows a wider $\widetilde{Y}_R$ profile. Flame-WP clearly exhibits higher rate of decay of reactant mass fraction with streamwise distance, as the centerline value of $\widetilde{Y}_R$ in Flame-WP at $z/D = 8$ and $z/D = 12$ are lower compared to Flame-NP, consistent with the observation of shorter flame length in Flame-WP. The difference in the flame length is further explored by examining the flow field statistics.

The evolution of the turbulent jet is examined in Figure 3.10. Figure 3.10a shows the jet half-width $r_{1/2}$ as a function of streamwise distance, where $r_{1/2}$ is defined as the radial distance from the central axis where the local mean streamwise velocity is equal to half of the local mean centerline streamwise velocity. Flame-WP is observed to have a higher spreading rate than Flame-NP, as the difference in $r_{1/2}$ increases with streamwise distance. In Figure 3.10b, the mean axial velocity profiles as a function of radius are in good agreement between the two cases up to $z/D = 2$. With increasing streamwise location, the $\widetilde{u}$ profiles of Flame-WP become wider compared with those in Flame-NP. Most importantly, the jet exhibits higher momentum in Flame-NP at downstream locations in the core region. At $z/D = 12$, the centerline velocity is $\approx 10\%$ higher in

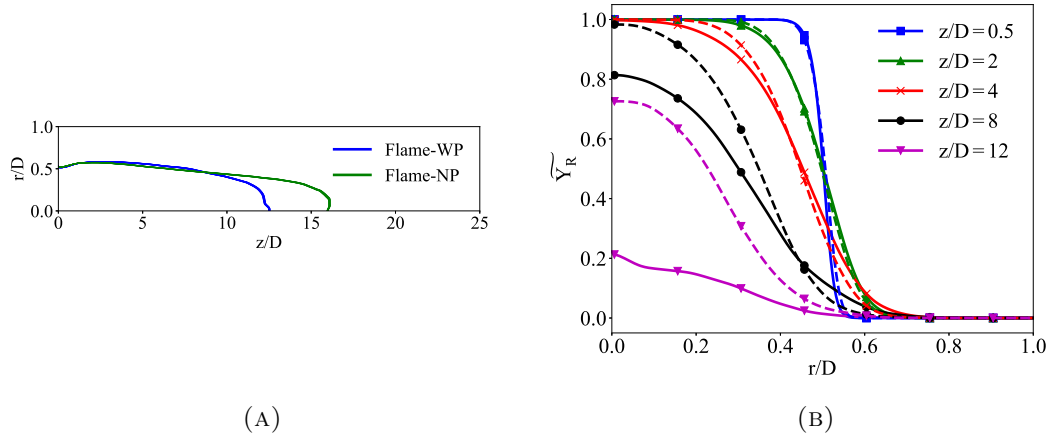


FIGURE 3.9: (A) Isocontour of Favre averaged reactant mass fraction $\widetilde{Y}_R = 0.134$ and (B) radial profiles $\widetilde{Y}_R$ at various streamwise locations for Flame-WP (solid line) and Flame-NP (dashed line).

Flame-NP in comparison with Flame-WP. The higher streamwise momentum in the jet core of Flame-NP results in a longer flame observed, since the reactants are convected further downstream before they are consumed.

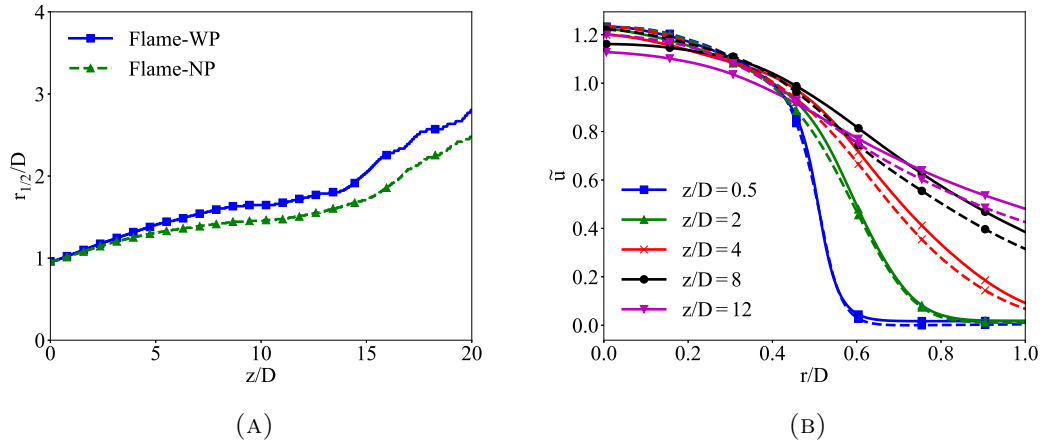


FIGURE 3.10: (A) Jet half-width as a function of streamwise distance and (B) radial profiles of $\tilde{u}$ at various streamwise locations for Flame-WP (solid line) and Flame-NP (dashed line).

The evolution of the turbulence kinetic energy (TKE), given by $\frac{1}{2}\overline{u'_i u'_i}$, is examined in Figure 3.11. In Flame-NP, the TKE is observed to rapidly decay in the core of the jet immediately downstream of the inflow boundary. In contrast, the TKE in the jet core of Flame-WP does not experience any significant decay near the pipe exit. The decrease of TKE in Flame-NP is due to the rapid breakdown of turbulent structures after they enter the computational domain. This has been observed to occur when the length scales of the structures generated in the digital filter inflow are not large enough to sustain the

structures. Overestimation of the prescribed length scales may result in lessen the degree of breakdown in the turbulence structures (Touber and Sandham, 2009), which may result in a faster recovery of TKE in the adaptation distance associated with synthetic turbulence inflow boundary conditions (Keating et al., 2004; Dhamankar et al., 2014). The decrease in TKE here led to the higher streamwise momentum in the jet core of Flame-NP and subsequently a longer flame length as unburnt reactants are carried further downstream before the chemical reactions can consume them. At $z/D = 12$, the centerline TKE in Flame-NP has recovered to approximately 50% of the Flame-WP value. In a non-reacting jet, shear layer instability drives the transition to turbulence after a drop in fluctuations shortly downstream of the inlet (Glaze and Frankel, 2003). In a turbulent premixed flame, the high viscosity in the burnt region appears to prevent such influence, and turbulent fluctuations do not recover until towards the end of the flame. The lower level of turbulence in Flame-NP is observed at all locations, as the near inflow effects clearly propagate downstream.

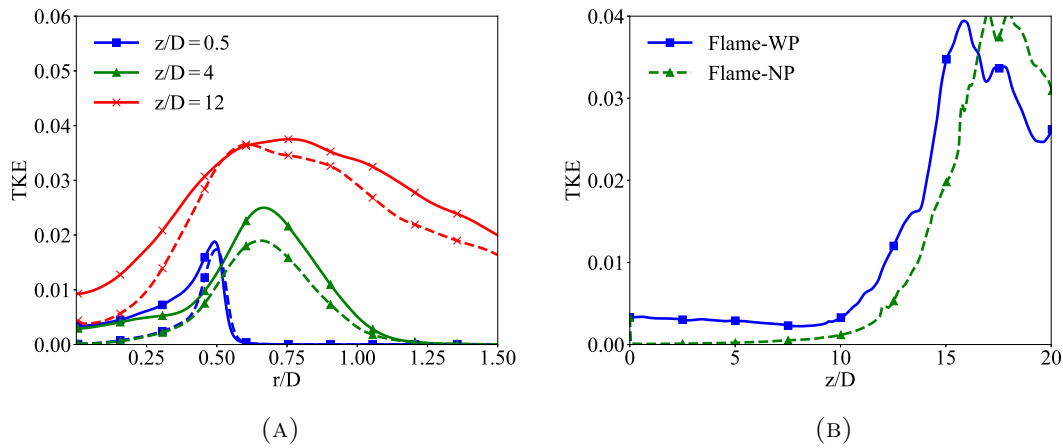


FIGURE 3.11: (A) Radial profiles turbulent kinetic energy at various streamwise locations and (B) centerline turbulent kinetic energy as a function of streamwise distance for Flame-WP (solid line) and Flame-NP (dashed line).

Figure 3.12a shows the spectra of the streamwise velocity fluctuations at the pipe exit/inflow ($z/D = 0$) for two radial locations for both cases. The spectra of the streamwise velocity fluctuations in the time domain were obtained first. Taylor's frozen field hypothesis were used to relate them to the streamwise wavenumber $k_z = f/U_b$, where f is the frequency and $U_b = 1$ is the non-dimensionalized bulk velocity, and then k_z was normalized by the laminar thermal flame thickness δ_{th} . The wave number associated with the flame thickness, $k_z/\delta_{th} = 1$, can be interpreted as the cut-off scale for TFI (Fragner et al., 2015). A portion of the spectrum in Flame-WP exhibits the $-5/3$ slope consistent with literature of pipe flows (Guala et al., 2006), which approximately indicates the inertial range. The inertial range is then followed by the dissipation range

starting at about $k_z/\delta_{th} = 0.3$. The energy containing scale in Flame-WP are mostly larger than the laminar flame thickness ($k_z/\delta_{th} < 1$), and the energy is found to decay over approximately 10 orders of magnitude from large to small scales. In contrast, the Flame-NP spectrum appears to show the inertial range up to higher wavenumbers, and decays about 3 orders of magnitude. The results show both inflow boundary conditions are similar up to $k_z/\delta_{th} = 0.3$, however, the synthetic turbulence inflow of Flame-NP contains more small scale structures in comparison to the inflow of Flame-WP, such that the spectrum follows the $-5/3$ slope for all length scales. This is expected to result in a higher dissipation of turbulence downstream of the inflow boundary as there is more energy contained in the smaller scales.

Figure 3.12b shows the streamwise velocity spectra at three streamwise locations at the radial positions where $\widetilde{Y}_R = 0.134$ for both flames. In comparison to the spectra at the inlet, the spectra conditioned on $\widetilde{Y}_R = 0.134$ show a noticeably narrower inertial range estimated by the $-5/3$ slope as energy is shifted to the lower wave numbers due to an increase in viscosity across the flame (Gökalp et al., 1988). At $z/D = 0.5$, Flame-NP features structures with a higher level of energy across all length scales. At $z/D = 2$, the two spectra are similar up to $k_z/\delta_{th} = 1$, and Flame-NP exhibits structures with a higher energy than those in Flame-WP for $k_z/\delta_{th} > 1$. Interestingly, at $z/D = 8$, both flames show similar spectra for all length scales suggesting that the differences between the two inflow boundary conditions have a negligible impact at the downstream locations.

3.4 Flame local statistics

The analysis of the global flow field and flame structure in the prior section have led to the observation of some differences between the two flames with different inflow boundary conditions. In this section, statistics local to the flame front are examined to analyse the TFI in these two sets of results. Firstly, the orientations and alignments of vectors related to turbulence and flame geometry are discussed. The flame front orientation can be quantified by the flame normal vector defined as,

$$\mathbf{n} = \nabla Y_R / |\nabla Y_R|, \quad (3.3)$$

such that the vector points towards the fresh reactants. In the works of Veynante et al. (2010) and Wang et al. (2016), an in-plane angle and an out-of-plane angle are defined to quantify the orientation of the vectors on the axis planes. The in-plane angle and out-of-plane angle of $\mathbf{n}$ are defined respectively as,

$$\alpha = \arctan 2(n_x, n_r), \quad (3.4)$$

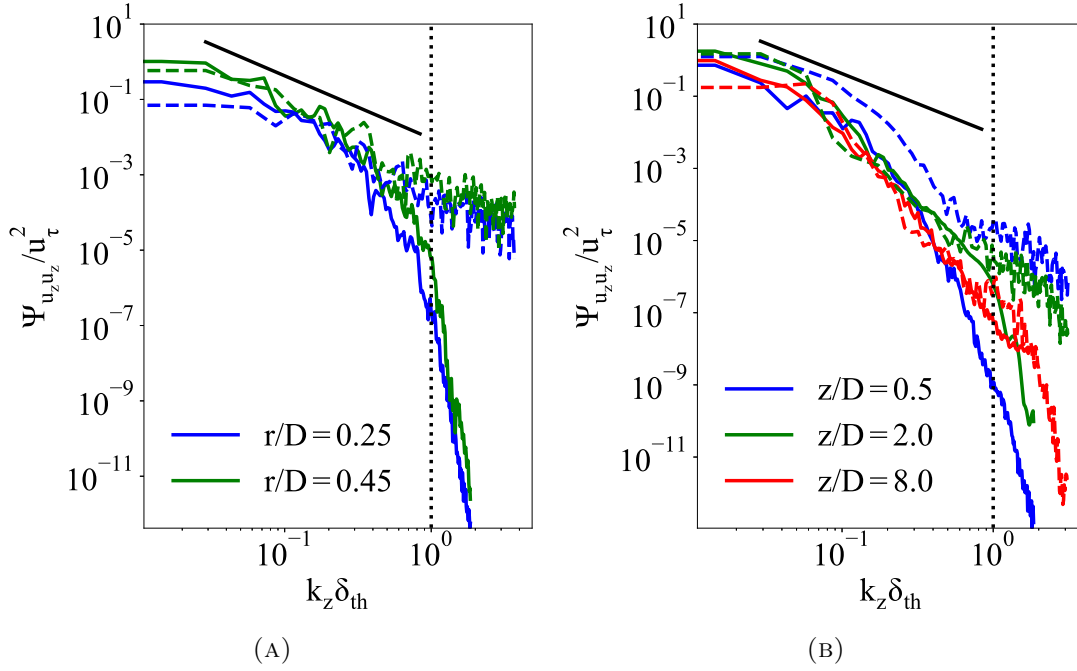


FIGURE 3.12: Spectra of streamwise velocity fluctuations for Flame-WP (solid line) and Flame-NP (dashed line) at (a) the inflow ($z/D=0$) at two radial positions and (b) three different streamwise locations with radial positions corresponding to $\widetilde{Y}_R = 0.134$. Black solid line indicates the $-5/3$ slope.

and

$$\beta = \arccos(n_\theta). \quad (3.5)$$

Schematics of the angles are shown in Figure 3.13. The variable α provides the angle between the positive radial axis and the project of $\mathbf{n}$ on the $z-r$ plane, such that $\alpha = 0$ would indicate complete misalignment with the streamwise axis. The variable β provides the angle between the azimuthal axis and $\mathbf{n}$, so that $\beta = 0$ indicates alignment in the positive azimuthal direction.

Figure 3.14 shows the PDFs of α and β conditioned on the instantaneous value of $Y_R = 0.134$ at various axial locations for both flames. The isotropic distributions (Veynante et al., 2010; Wang et al., 2016; Hawkes et al., 2011) are shown with the dotted lines. At $z/D = 0.5$, the most probable value of α is 180° , indicating the preferred orientation of the flame normal vector is towards the center axis. The narrow distribution of the PDF close to this angle suggests that the flame is similar to a laminar cylindrical flame in this region. However, a small difference can be observed between Flame-WP and Flame-NP. The α PDF of Flame-NP exhibits a lower peak and a slightly wider spread compared to Flame-WP. For both flames, the distribution becomes more spread out with increasing streamwise distance from the flame base, showing that the distributions tend towards an isotropic distribution. At downstream locations, a secondary peak is also observed around 45° , consistent with the observations of Wang et al. (2016). This

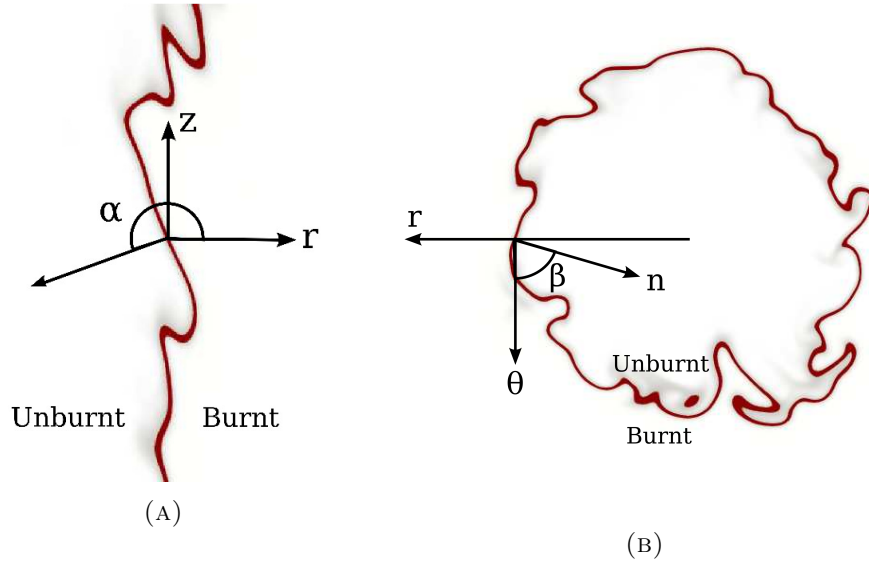


FIGURE 3.13: Schematics of (A) in-plane angle α and (B) out-of-plane angle β .

is attributed to the orientation of the flow strain rate to be shown later. At downstream locations, the PDF distribution in Flame-WP is closer to isotropic compared to Flame-NP. This is expected as Flame-WP experiences a higher level of turbulence and therefore the distribution tends towards isotropy more quickly. The PDFs of β in Figure 3.14b show distributions centred around 90° . For locations downstream of $z/D = 0.5$, the distributions are close to isotropic, and show that angles other than the preferred 90° are observed with frequent probability. The main difference between the two flames is observed at $z/D = 0.5$ where the PDF exhibits a much stronger preference to $\beta = 90^\circ$ for Flame-WP.

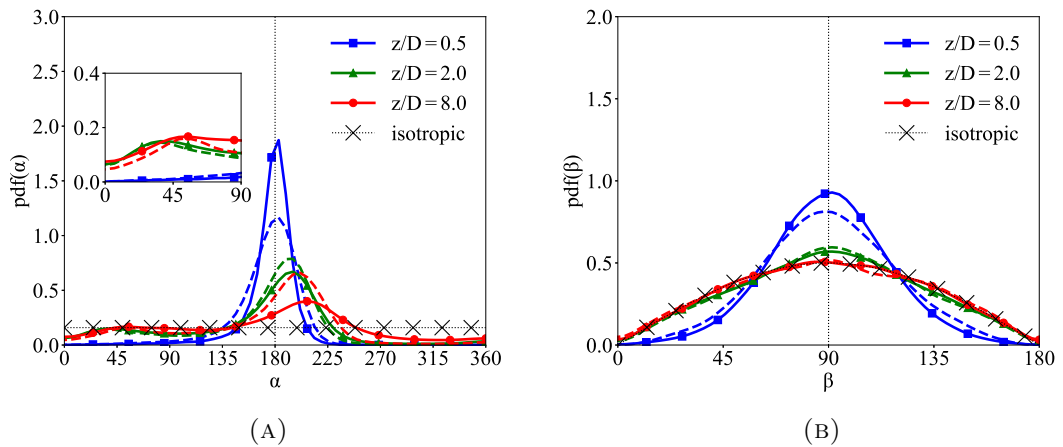


FIGURE 3.14: PDFs of flame normal vector (A) in-plane angles α and (B) out-of-plane angles β for Flame-WP (solid line) and Flame-NP (dashed line).

The orientation of the strain rate tensor is now examined. The characteristic equation of the symmetric strain rate tensor $\mathbf{S}_{ij} = 1/2(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ is

$$\lambda^3 + P_S \lambda^2 + Q_S \lambda + R_S = 0, \quad (3.6)$$

where P_S , Q_S , and R_S are the invariants of $\mathbf{S}_{ij}$ defined by:

$$P_S = -\mathbf{S}_{ij} \quad (3.7)$$

$$Q_S = \frac{1}{2} (P_S^2 - \mathbf{S}_{ij} \mathbf{S}_{ji}), \quad (3.8)$$

$$R_S = -\frac{1}{3} (-P_S^3 + 3P_S Q_S - \mathbf{S}_{ij} \mathbf{S}_{jk} \mathbf{S}_{ki}), \quad (3.9)$$

where $\mathbf{W}_{ij} = 1/2(\partial u_i/\partial x_j - \partial u_j/\partial x_i)$ is the skew-symmetric rotation rate tensor. $\lambda = [\lambda_1, \lambda_2, \lambda_3]$ are the eigenvalues, and the eigenvectors of λ_1 , λ_2 , and λ_3 are $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ respectively, and they denote the directions of the principal strains of the fluid elements. To isolate the effect of strain rate due to the bulk flow, Zhou and Frank (2019) removed its contribution by calculating the strain rate tensor with the fluctuating velocity field such that $\mathbf{S}_{ij} = 1/2(\partial u'_i/\partial x_j + \partial u'_j/\partial x_i)$. The orientation of strain rate tensor eigenvectors for both definitions of S_{ij} are investigated below.

Similar to Eqs. 3.4 and 3.5, the in-plane and out-of-plane angles of the strain rate tensor eigenvectors are defined as,

$$\mu_i = \arctan 2(\mathbf{e}_{ix}, \mathbf{e}_{ir}), \quad (3.10)$$

and

$$\sigma_i = \arccos(\mathbf{e}_{i\theta}), \quad (3.11)$$

where $\mathbf{e}_i$ for $i = 1, 2, 3$ are the extensive, intermediate, compressive strain rate tensor eigenvectors, respectively. The PDFs of μ_i conditioned on $Y_R = 0.134$ are shown in Figure 3.15 along with the isotropic distributions using both definitions of the strain rate tensor. The PDFs calculated from the strain rate based on the full velocity field show that the preferred angles of the extensive eigenvector μ_1 at $z/D = 0.5$ and $z/D = 2$ are 135° and 315° , and by extension the preferred angles of the compressive eigenvector μ_3 , which is orthogonal to e_1 , are 45° and 225° . It can be seen that there is a high probability of the preferred angles at $z/D = 0.5$ whereas the PDFs tend towards an isotropic distribution with increasing streamwise location. At $z/D = 8$, the PDFs of Flame-WP show that the preference of μ_1 and μ_2 decreases, indicating an increased alignment of e_1 with the z axis (and e_3 with the r axis). At the same location, the PDFs of Flame-NP still show the same preferred angles as at the upstream locations. The distribution of μ_2 at $z/D = 0.5$ is closer to isotropic in comparison with μ_1 and μ_3 ,

and shows a preference towards $0^\circ/180^\circ$. Similar to μ_1 and μ_3 , the PDF of μ_3 spreads out with increasing streamwise locations.

The PDFs calculated with strain rates based on the velocity fluctuations show that both μ_1 and μ_3 exhibit the four preferential angles of 45° , 135° , 225° and 315° . Comparison of the PDFs of μ_1 and μ_3 between the two flames show very little difference, even for $z/D = 8$ where differences were observed when the strain rate tensor was calculated based on the full velocity vector. However, the PDFs of μ_2 are similar using either methods of calculating the strain rate.

The PDFs of the out-of-plane angles σ_i are shown in Figure 3.16. The preferred angle of σ_1 and σ_3 is 90° , indicating that the compressive and extensive strains preferentially lie on the $z-r$ plane, while the orthogonal σ_2 exhibits a preference towards $0^\circ/180^\circ$. When the strain rates are calculated from the full velocity field, the PDFs tend towards the isotropic profile with increasing streamwise distance. These observations are consistent with the observations of Wang et al. (2016). In contrast to this trend, the PDFs of σ_i calculated with strain rates based on the fluctuating velocity field show strong probability to their preferred angles for all streamwise locations. Similar to the observations for μ_i PDFs, the two flames do not show significant differences for the PDFs of σ_i .

To further explain the observations above, the correlation between turbulence and flame orientation is examined in Figure 3.17 by PDFs of the product between the flame normal vector and strain rate eigenvectors, $|\mathbf{n} \cdot \mathbf{e}_i|$, conditioned on $Y_R = 0.134$. A value of $|\mathbf{n} \cdot \mathbf{e}_i| = 1$ indicates alignment between the two vectors, while $|\mathbf{n} \cdot \mathbf{e}_i| = 0$ indicates misalignment. Past studies have shown that the alignment of the flame normal with the extensive or compressive eigenvector is dependent on factors such as the presence of strong heat release and the level of turbulence intensity. For flames with $Ka < 1$ where the effects of heat release is more prominent, the flame normal vector tends to align with the extensive strain rate (Swaminathan and Grout, 2006; Chakraborty et al., 2009). On the other hand, for flames with $Ka > 1$ where turbulence strain rates dominate over the effects of heat release, studies have observed that there is a preferential alignment of the flame normal vector to the compressive strain rate eigenvector (Chakraborty and Cant, 2007; Hartung et al., 2008; Kim and Pitsch, 2007; Nilsson et al., 2018).

The PDFs calculated with the strain rates based on the full velocity field show that at all streamwise locations, the intermediate eigenvector $\mathbf{e}_2$ is misaligned with $\mathbf{n}$. Consistent with the observations in the PDFs of α , β , μ_i , and σ_i , the PDFs show strong deviation from the isotropic distribution at $z/D = 0.5$, but they tend towards an isotropic distribution with increasing streamwise distance. At $z/D = 0.5$, the PDFs of $|\mathbf{n} \cdot \mathbf{e}_1|$ and $|\mathbf{n} \cdot \mathbf{e}_3|$ show higher peaks for Flame-WP compared to Flame-NP. Wang et al. (2016) observed that in the upstream region, the PDFs of $|\mathbf{n} \cdot \mathbf{e}_1|$ and $|\mathbf{n} \cdot \mathbf{e}_3|$ are similar and

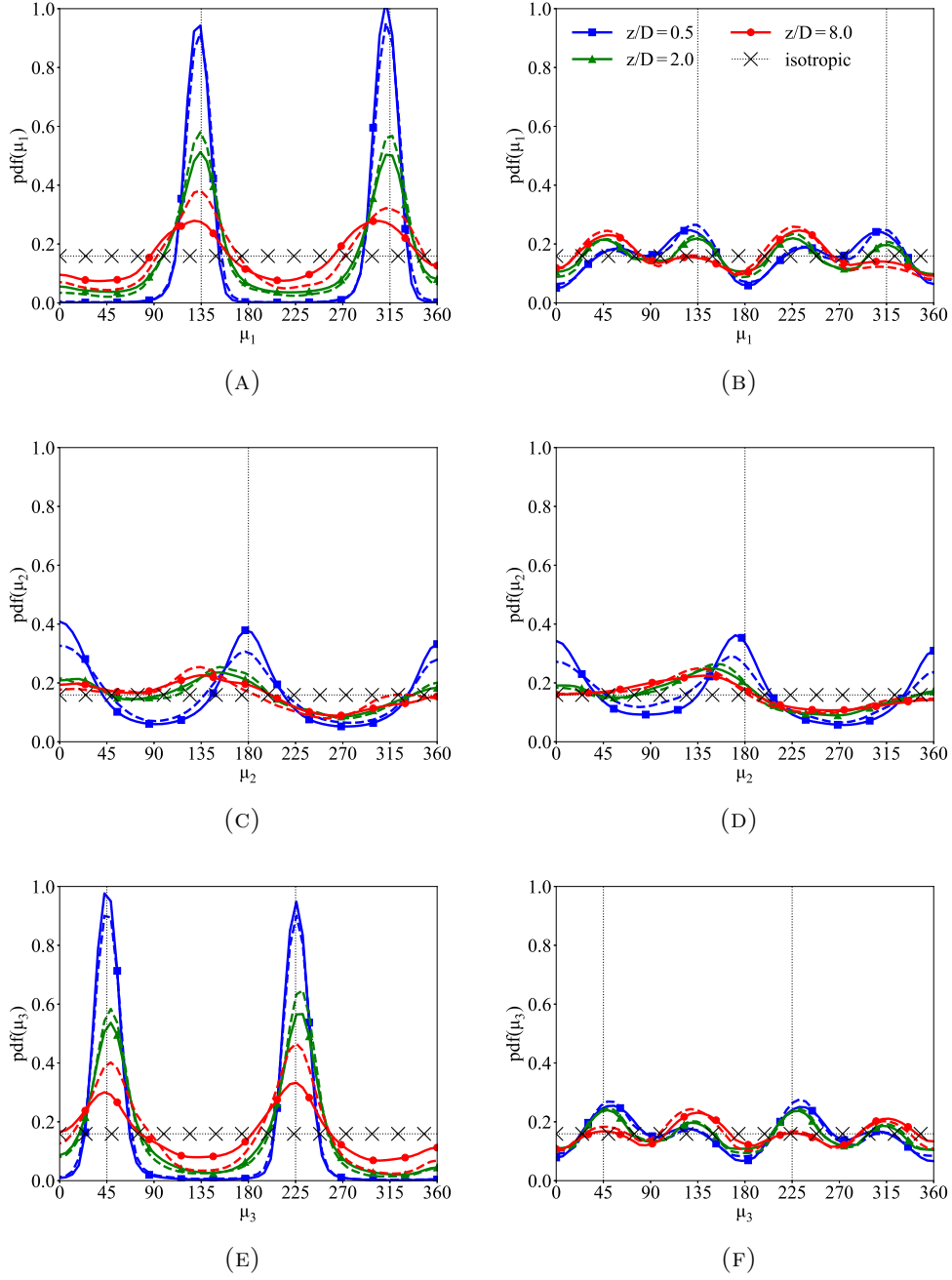


FIGURE 3.15: PDFs of in-plane angles μ_i of (a,c,e) strain rate tensor based on full velocity field and (b,d,f) strain rate tensor based on fluctuating velocity field for Flame-WP (solid line) and Flame-NP (dashed line).

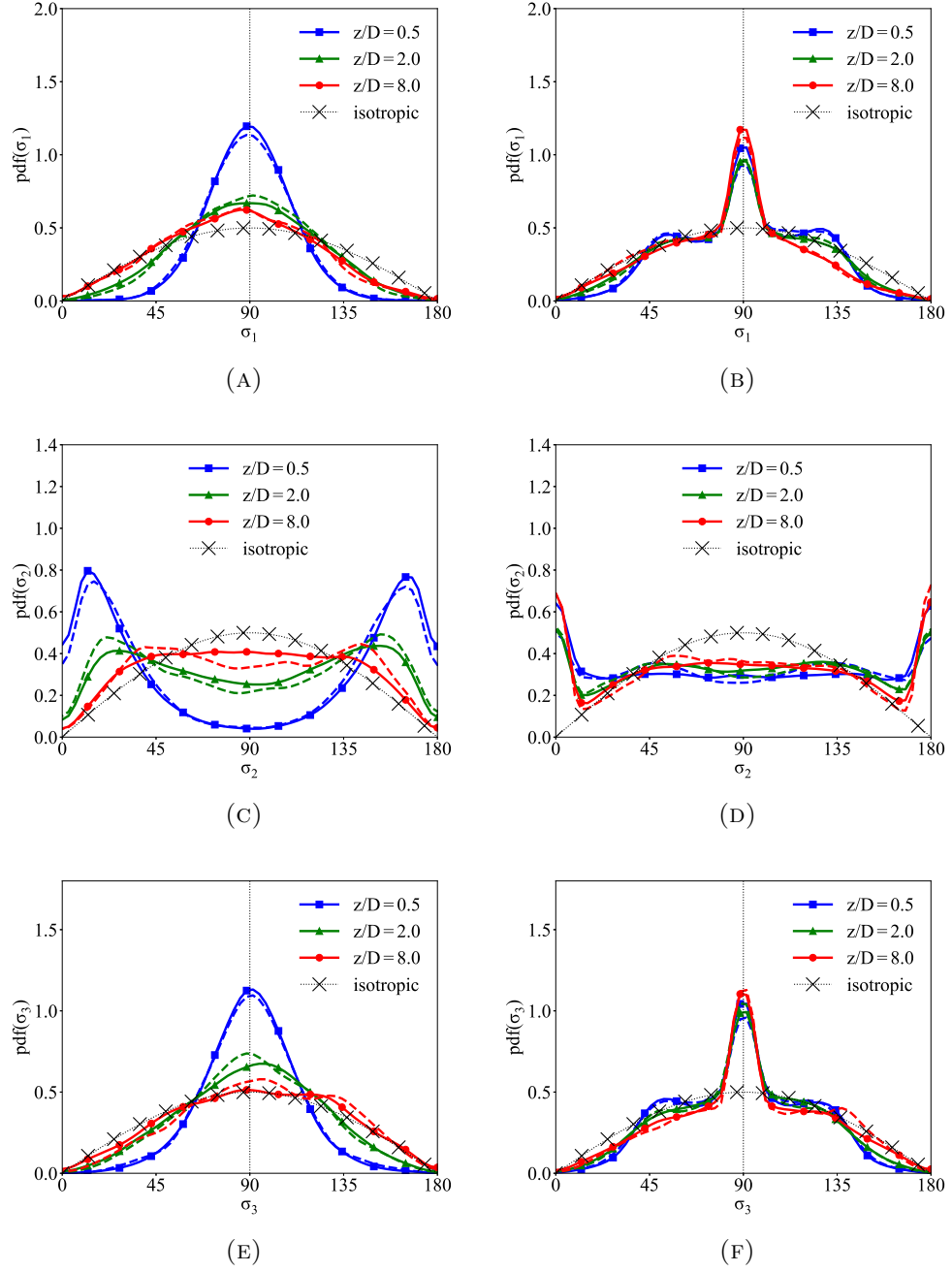


FIGURE 3.16: PDFs of out-of-plane angles σ_i of (a,c,e) strain rate tensor based on full velocity field and (b,d,f) strain rate tensor based on fluctuating velocity field for Flame-WP (solid line) and Flame-NP (dashed line).

both peak at approximately 45° . In comparison, the PDFs for the current flames show a small difference in the location of the peaks, particularly for Flame-WP, indicating that the flame normal has a slightly higher probability to be aligned with the compressive strain rate. With increasing streamwise distance, the probability of alignment of $\mathbf{n}$ with both $\mathbf{e}_1$ and $\mathbf{e}_3$ increases, though the probability of alignment with $\mathbf{e}_3$ is still greater than the alignment with $\mathbf{e}_1$, consistent with the observations for flames with $Ka > 1$ (Wang et al., 2016; Kim and Pitsch, 2007; Hartung et al., 2008).

In Figure 3.17b, the PDFs of alignment calculated with strain rates based on velocity fluctuations are observed to be closer to isotropic distributions. This difference is especially noticeable for upstream locations where the PDFs based on the previous strain rate calculations are far from isotropic. One observation between the calculations with the two strain rate definitions is that at $z/D = 8$, $|\mathbf{n} \cdot \mathbf{e}_1|$ shows a higher alignment than $|\mathbf{n} \cdot \mathbf{e}_3|$, which is opposite of Figure 3.17a, showing that the bulk strain rate has an overall compressive effect which acts to suppress the extensive strain rate induced by heat release, which has also been observed by Zhou and Frank (2019). Another observation is that despite the isolation of bulk strain rate effects, the upstream locations still show preference towards a 45° alignment. This implies that at upstream locations, the mean geometry of the flame and the mean geometry of the underlying turbulence field are the dictating factors for the vector orientations, likely due to a finite response time between the inflow turbulence and the flame front. With streamwise distance, the turbulence and flame becomes increasingly coupled and the typical alignment characteristics are observed. A third observation can be made by examining the differences between the two flames. In comparison to Figure 3.17a, the differences between the PDFs of the two flames are reduced. This is consistent with the smaller differences in μ_1 and μ_3 between the two flames in Figure 3.15 by removing bulk strain rate effects. Based on the two previous observations, further comments on the effect of inflow turbulence on TFI can be made by referring back to the spectra in Figure 12. At the upstream location, the differences between the spectra at scales larger than δ_{th} does not appear to affect the alignment in Figure 3.17b, likely due to the dominant effect of mean geometry where the scales related to the mean geometry are larger than the inertial range. At the downstream location, differences in the energy spectrum at the downstream locations are only observed for scales smaller than the scales associated with δ_{th} , so that no significant difference is observed in the alignment in Figure 3.17b. These observations suggest that the different inflow turbulence methods are mainly seen to affect the bulk strain rates from the differences in the global flame and flow characteristics examined in Section 3.3, but does not have a significant effect local TFI at the smaller scales.

To examine the influence of turbulence on the inner flame structure, the mean second

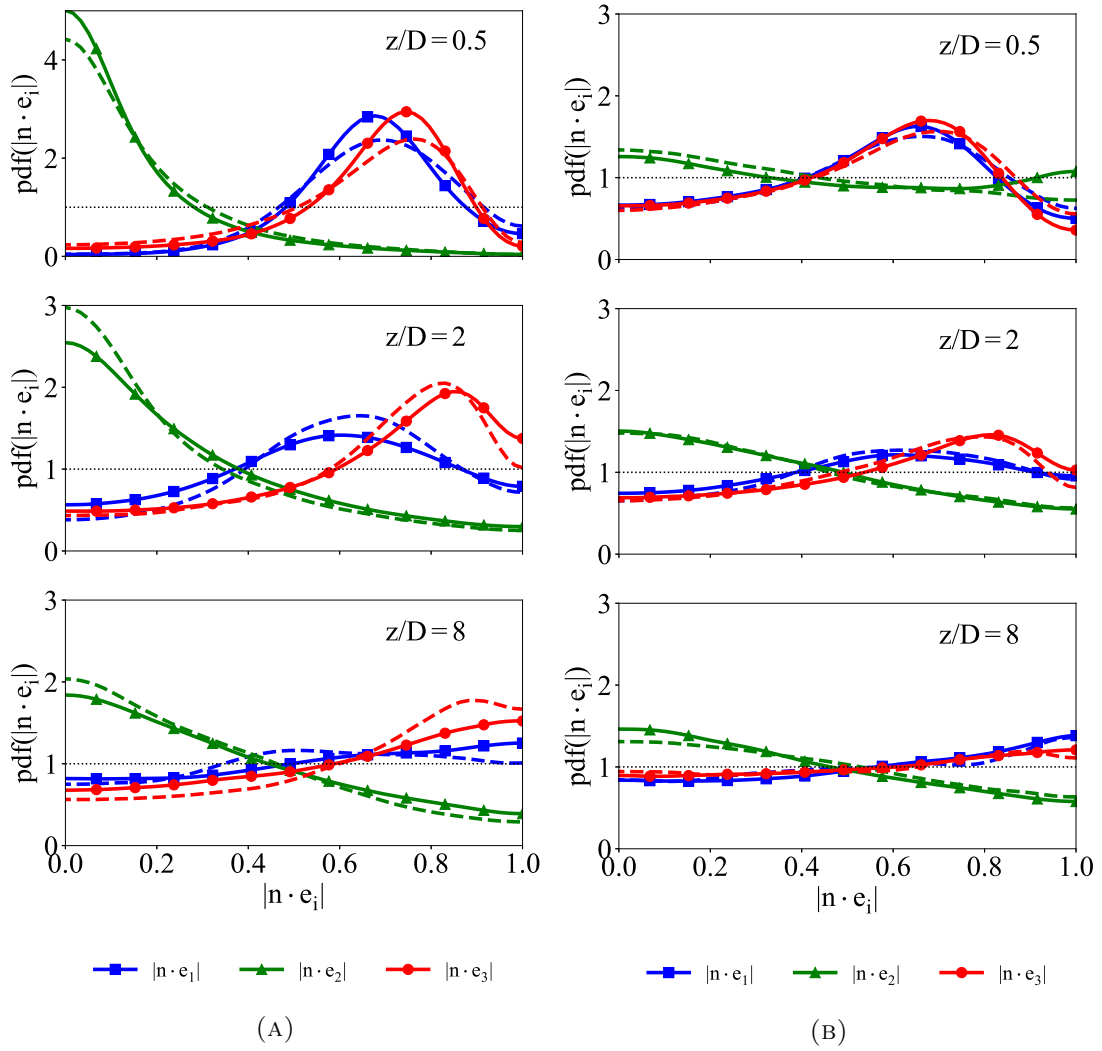


FIGURE 3.17: PDFs of alignment (a) between the flame normal vector and strain rate tensor based on full velocity field, and (b) between the flame normal vector and strain rate tensor based on fluctuating velocity field for Flame-WP (solid line) and Flame-NP (dashed line).

invariant of the velocity gradient tensor, Q , and the mean reactant mass fraction gradient, $|\nabla Y_R|$, are plotted against Y_R at various streamwise locations in Figures 3.18 and 3.19, respectively. The invariant Q is defined as,

$$Q = \frac{1}{2} (W_{ij}W_{ij} - S_{ij}S_{ij}), \quad (3.12)$$

where W_{ij} is the rotation rate tensor. For $Q > 0$, the rotation rate is greater than the strain rate corresponding to the presence of coherent fine-scale turbulent eddies, while $Q < 0$ indicates the dominance of TKE dissipation (Tanahashi et al., 2000). In Figure 3.18, the reaction region around $Y_R = 0.134$ shows $Q < 0$ at all streamwise locations as TKE dissipation due to the high viscosity is significant for lower Y_R . Peak values of $Q > 1$ are observed at the upstream locations of $z/D = 0.5$ and $z/D = 2$ for higher

Y_R , suggesting a greater presence of fine-scale eddies in the preheat zone compared with $z/D \geq 4$ where Q is small. At $z/D = 0.5$, the peak Q in Flame-NP is approximately two times of Flame-WP.

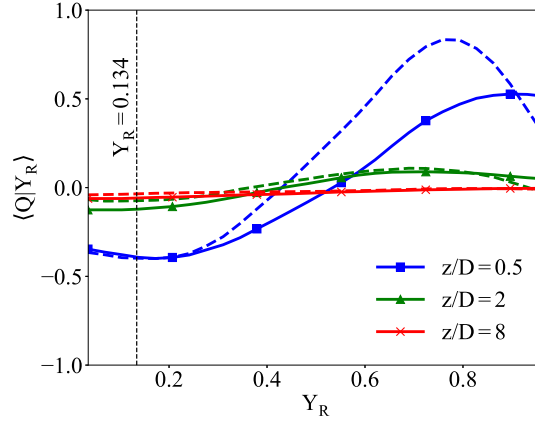


FIGURE 3.18: Second invariant of velocity gradient tensor based on the fluctuating velocity field as a function of reactant mass fraction for Flame-WP (solid line) and Flame-NP (dashed line).

In Figure 3.19, the mean mass fraction gradient, which is inversely proportional to the flame thickness, is used to quantify the response of the flame front structure to turbulence. The quantity $|\nabla Y_R|$ has also been referred to as the Surface Density Function (SDF) in the literature (Kollmann and Chen, 1998; Chakraborty and Cant, 2005). The $|\nabla Y_R|$ profile for a one-dimensional unstrained laminar flame is also presented in the same figure with a dash-dotted line. At $z/D = 0.5$ and $z/D = 2$, $|\nabla Y_R|$ is higher relative to the values for the one-dimensional unstrained laminar flame throughout the preheat region, indicating that the flame front is thinner in these regions. This can be attributed to the higher values of Q as observed in Figure 3.18. Tanahashi et al. (2000) found that flame elements in regions of $Q > 0$ are thinner than the laminar flame thickness due to tangential straining from the presence of coherent fine-scale turbulent eddies. The values of $|\nabla Y_R|$ are closer to the profile of the laminar flame at downstream locations. At $z/D > 4$, the preheat region exhibits slightly lower mean mass fraction gradient, which were also observed in the simulation of a planar jet flame by Sankaran et al. (2007). In the burnt region, deviation from the laminar profile is less compared to the preheat region, attributed to TKE dissipation from the higher viscosity of the reaction and burnt regions.

The flame local statistics show that the direction of principle strain influences the orientation of the flame front, especially at downstream locations as isotropy increases. Therefore, the decay rate of turbulence in the jet is shown to affect flame orientation downstream. In comparison, this did not appear to cause significant difference in the inner flame structure as the flames show close predictions for flame thickness regardless

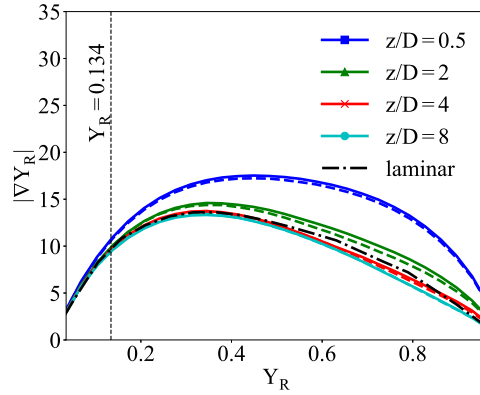


FIGURE 3.19: Scalar gradient as a function of reactant mass fraction for Flame-WP (solid line) and Flame-NP (dashed line).

of differences in the observed turbulence level. The minor influence of turbulence on the flame structure at downstream locations is expected for these low Karlovitz number flames.

3.5 Conclusions

Direct numerical simulations of turbulent premixed round jet flames in the low Karlovitz number regime were analysed in this chapter to determine the effect of inflow turbulence generated with two different methods on the flame characteristics.

The mean statistics at the pipe exit and the digital filter boundary were in close agreement with each other and with reference pipe data. However, instantaneous fluctuations showed significant differences in flow structures. This led to differences in statistics observed shortly downstream of the pipe exit plane. In the flame with the digital filter inflow boundary, the turbulent kinetic energy was underpredicted shortly downstream of the inflow boundary, caused by relaminarization of the flow. The underprediction of turbulent kinetic energy led to a lower decay rate of streamwise momentum in the jet core, which resulted in a longer flame length in comparison to the flame with the fully developed inflow. The adaptation length required by the synthetic turbulence inflow boundary condition played a major role in the prediction of flame growth.

The analysis of the local statistics related to the flame orientation, strain rate and the alignment showed some quantitative differences between the two flames. However, when the statistics are calculated with strain rate based on the fluctuating velocity field instead of the full velocity field, a smaller difference between the two flames was observed. This suggests that the main effect of the different inflow turbulence condition is on the global

flame and flow characteristics which influence the bulk strain rate, while local TFI are not greatly affected. This is consistent with observations in low Karlovitz number flames, the flow turbulence was found to influence the flame front orientation, but not the inner structure of the flame.

Chapter 4

Karlovitz number effects on premixed flames with fully developed pipe flow inlet

4.1 Introduction

This chapter presents a DNS study of two turbulent premixed jet flames with different inlet Karlovitz numbers (Flame-low at $Ka = 4.2$ and Flame-high at $Ka = 90$). The Karlovitz number is varied by changing the temperature of the reactants, which subsequently results in different laminar flame speeds. As shown in Chapter 3, the inclusion of the upstream pipe flow leads to a more accurate representation of the external flow. The global structure of the turbulent jets and flames are first investigated. The differences between the two flames are quantified. Next, the behaviour of turbulence across the local flame front is investigated. Lastly, the scalar gradient $|\nabla Y_R|$, an important quantity in the concept of Flame Surface Density, is investigated, by examining parameters such as flame strain rate, flame curvature and dilatation.

4.2 Global flow field and flame structure

Both flames are visualised in Figure 4.1 at an instant in time by iso-surfaces of $Y_R = 0.134$, which corresponds to the location of maximum reaction rate, and cross sections of the Y_R contours in a $z - r$ plane. Some differences can be observed between the two flames. To visualise the entirety of the flame, the streamwise extent plotted in Figure 4.1 for Flame-low is $z/D = 14$, while the extent for Flame-high is $z/D = 45$. It is

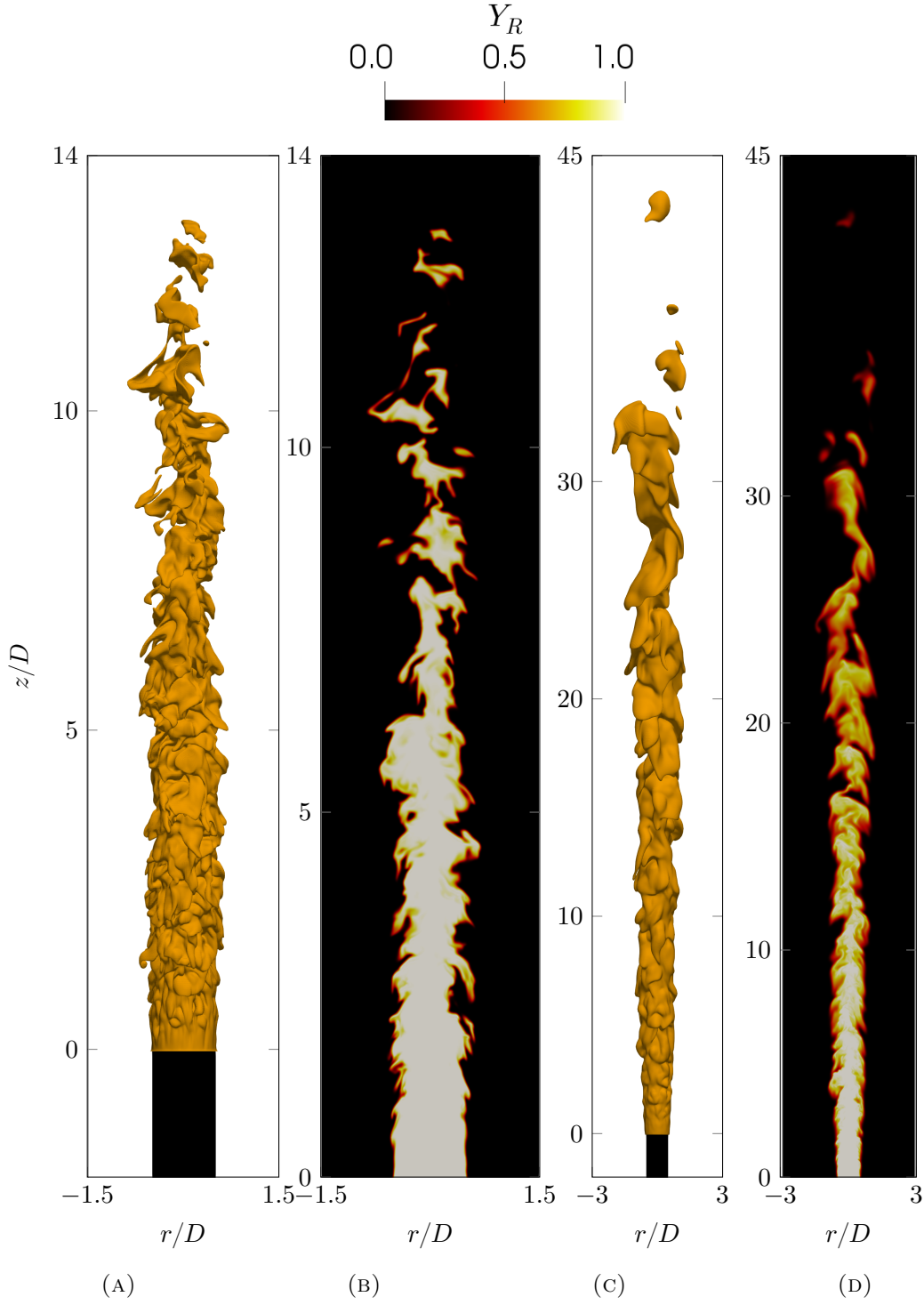


FIGURE 4.1: Iso-surface of $Y_R = 0.134$ and $z - r$ plane contours of Y_R for (A,B) Flame-low and (C,D) Flame-high.

clear that the length of Flame-high is much greater than the length of Flame-low. This is due to the lower S_L in Flame-high, such that the unburnt reactants are convected further downstream before they are consumed by the chemical reactions. While both flames exhibit wrinkling of the flame surface as expected in typical turbulent flames, the

iso-surface of Flame-low appears to show more small-scale wrinkling compared to the iso-surface of Flame-high where large-scale wrinkling appear to be more dominant. Both flames show pockets of unburnt reactants separating from the main flame, especially towards the tip of the flame. Flame-high also appears to display greater radial spreading downstream of the nozzle exit compared to Flame-low.

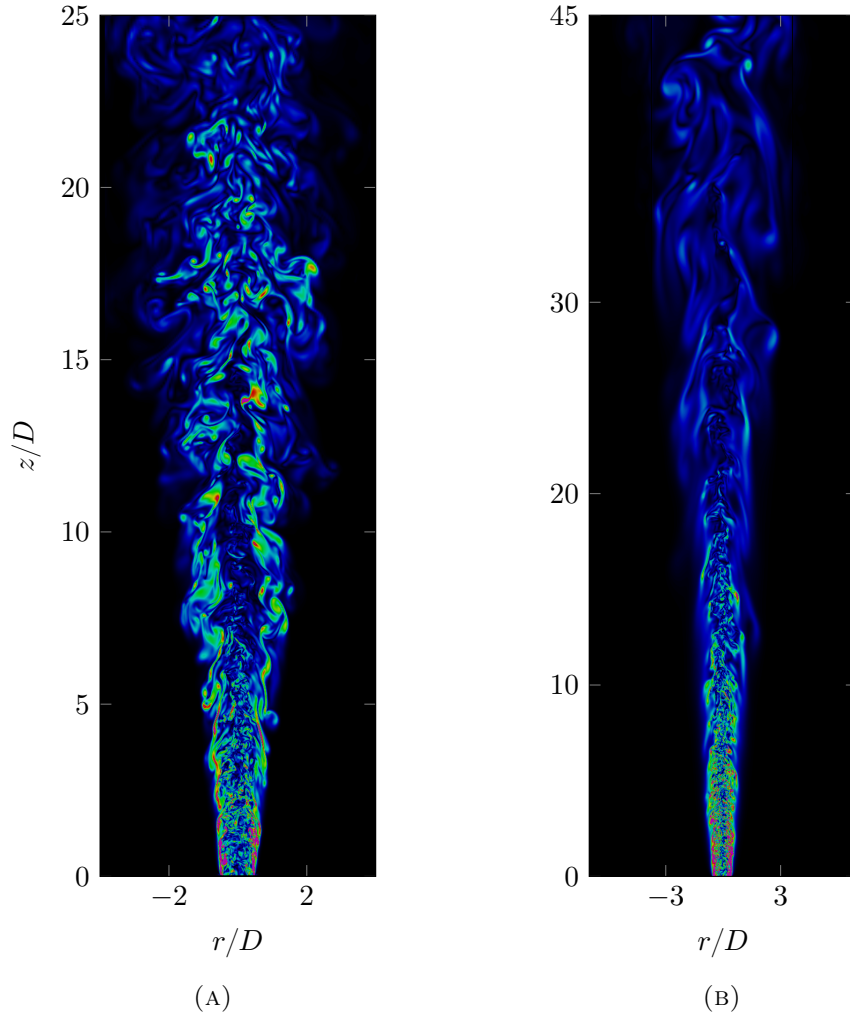
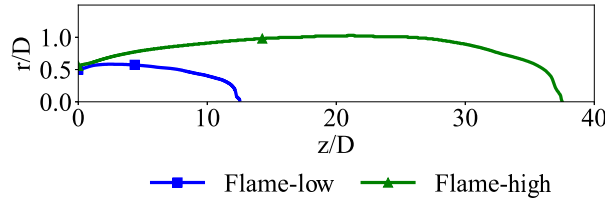


FIGURE 4.2: $z - r$ plane contour of vorticity for (A) Flame-low and (B) Flame-high.

The turbulent flow field is visualised in Figure 4.2 by an instantaneous vorticity magnitude on a $z - r$ plane. In both flames, high vorticity regions are observed close to the nozzle exit due to the jet shear layer development. The high viscosity of the burnt products dampens the turbulent structures. In Flame-high, the vorticity in the downstream region is lower in magnitude and exhibits structure stretched out in the streamwise direction. A decrease in the vorticity magnitude and larger stretched structures have been observed in the literature, such as in the DNS of Wang et al. (2018).

To quantify the earlier observations, the mean statistics are examined. The mean flame is quantified by the density-weighted time and azimuthally averaged reactant mass fraction

$\widetilde{Y}_R$ in Figure 4.3 showing iso-lines of $\widetilde{Y}_R = 0.134$. The flame lengths are quantified using the $\widetilde{Y}_R = 0.134$ iso-line and are equal to $12.5D$ and $37D$ for Flame-low and Flame-high, respectively, showing that the mean flame of Flame-high is approximately 3 times longer than Flame-low. As well, it can be observed that while the mean flame of Flame-low does not exhibit substantial radial spreading, the radial extent of mean flame of Flame-high is twice the pipe radius.



(A)

FIGURE 4.3: (A) Isolines of Favre averaged reactant mass fraction $\widetilde{Y}_R = 0.134$ (solid line) and $\widetilde{Y}_R = 0.85$ (dashed line).

The mean streamwise evolution of the turbulent jets is examined in Figure 4.4. The jet half widths $r_{1/2}$ as a function of the streamwise distance are shown in Figure 4.4a and the radial profiles of the density-weighted time and azimuthally averaged velocity $\tilde{u}$ at various streamwise locations are shown in Figure 4.4b. The $r_{1/2}$ of Flame-low is initially lower than Flame-high up to approximately $z/D = 12.5$, where an increase in the growth rate is observed. The growth rate of Flame-high appears fairly constant up to $z/D \approx 37$. This seems to suggest that the growth rate of the turbulent jet is mostly constant up to the mean flame lengths, after which an increase in the growth rate is observed. The radial profiles show that up to $z/D = 12$, $\tilde{u}$ along the z axis is in close agreement between the two jets. Away from the centerline, the radial spread of the profiles are increasingly different, due to the difference in the evolution of the flame.

The difference in the spreading rate of the jet in Figure 4.4 can be attributed to differences in the turbulent kinetic energy (TKE). The centerline TKE as a function of z/D and radial profiles of the TKE at various streamwise locations are shown in Figure 4.5. The centerline TKE for both flames show a relatively little change for approximately 70% of their respectively mean flame lengths. Further downstream from these locations, the TKE is observed to greatly increase. The increase in the centerline TKE can be attributed to interaction with intermittent flame structures and is representative of changes in the velocity field due to temperature changes across the flame. The radial

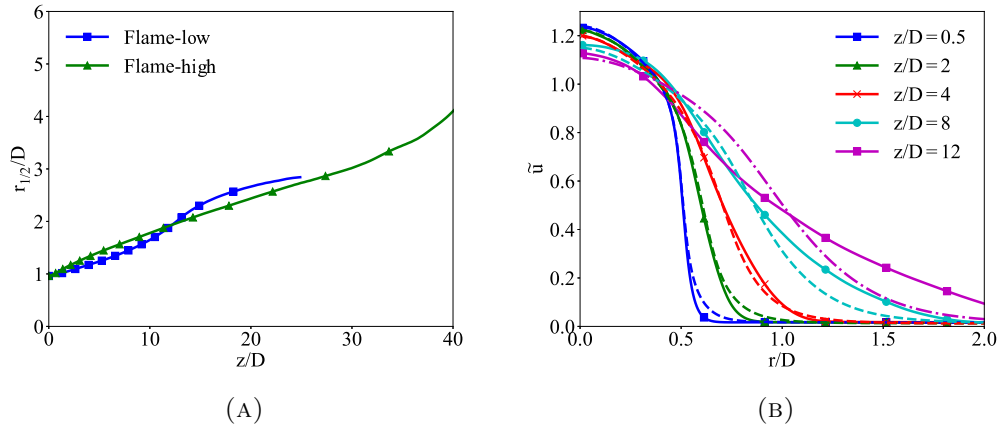


FIGURE 4.4: (A) Jet half-width as a function of streamwise distance and (B) radial profiles of $\tilde{u}$ at various streamwise locations for Flame-low (solid line) and Flame-high (dashed line).

profiles show that as the shear layer develops, the peak of the profiles are shifted outwards to higher r/D . The peak TKE in Flame-low increases with streamwise distance, while the profiles in Flame-high do not exhibit the same increase. The likely cause is the difference in the flame development relative to the shear layer development. In Flame-low, the mean flame front quickly converges towards the central axis, while the flame brush of Flame-high shows a greater spreading such that the shear layer is likely to be affected by the flame for a large distance.

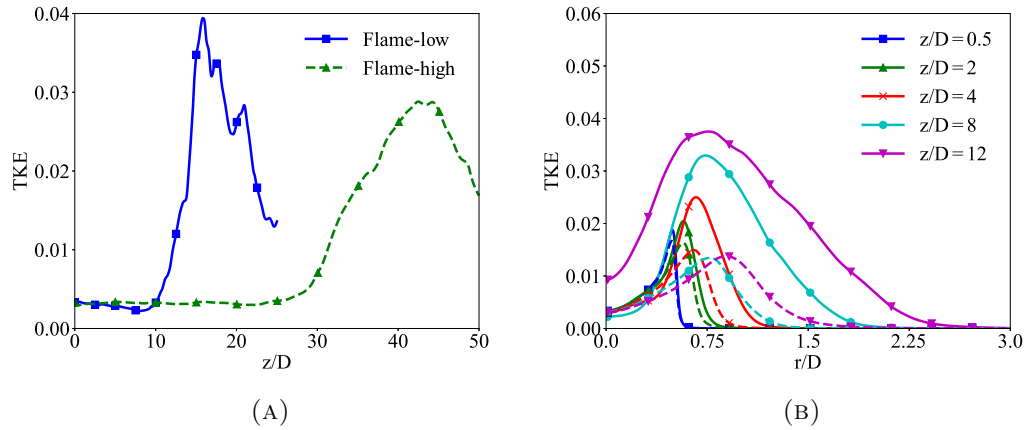


FIGURE 4.5: (A) Centerline turbulent kinetic energy as a function of streamwise distance and (B) Radial profiles of turbulent kinetic energy at various streamwise locations for Flame-low (solid line) and Flame-high (dashed line).

TFI is especially complex in spatially developing flows, such as jets, where a wider range of turbulence scales are observed, as the local Karlovitz number can vary orders of magnitude with spatial variation (Duwig and Dunn, 2013). The Karlovitz number determines whether the turbulence kinetic energy is produced by turbulence-induced

strain, or by combustion-induced velocity-pressure gradients (Macart et al., 2018). The streamwise evolution of the local Karlovitz number along the flame is shown in Figure 4.6, where values are taken from locations corresponding to $\tilde{Y}_R = 0.134$. The definition of the local Karlovitz number Ka^* used is the modified formula accounting for the change in viscosity across the flame (Hawkes et al., 2012):

$$Ka^* = \left(\frac{S_L \delta_{th}}{\tilde{\nu}} \right)^{\frac{1}{2}} \left(\frac{u'}{S_L} \right)^{\frac{3}{2}} \left(\frac{l_t}{\delta_{th}} \right)^{-\frac{1}{2}}. \quad (4.1)$$

The values are also shown on the premixed flame regime diagram, where the flames are found to mostly lie in the thin reaction zone regime (TRZ). The Ka^* values calculated at the center of the nozzle exit are approximately 8 and 95 for Flame-low and Flame-high, respectively. The streamwise locations close to the nozzle exit exhibit much higher Ka^* values at the flame compared to the inlet location, which can be attributed to the increase in turbulent fluctuations from the jet shear layer. With increasing streamwise distance, Ka^* decreases as the turbulence decays and the integral length scales increase.

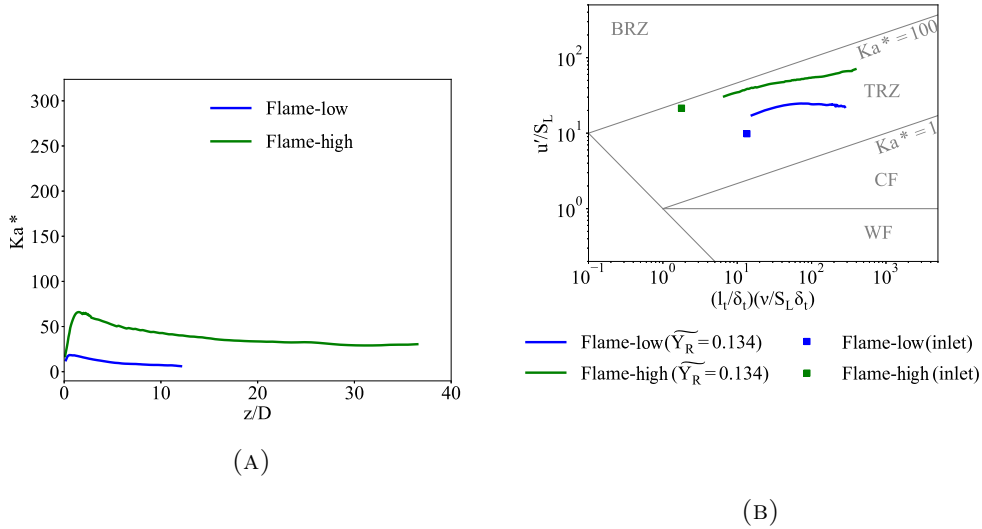


FIGURE 4.6: (A) Streamwise evolution of Ka^* at $Y_R = 0.134$, and (B) shown on the regime diagram

4.3 Flow structure behaviour across the flame front

The characterization of turbulent structures and how they interact with the flame is useful in understanding the physical mechanisms involved in TFI. The vortical structures, visualised by the local swirling strength λ_{ci} , are presented in Figure 4.7 for Flame-low and Flame-high at two streamwise locations. The iso-surfaces are coloured by Y_R to show the location of the structures relative to the flame, where red indicates the fresh reactants $Y_R = 1$ and blue indicates the burnt products $Y_R = 0$. Close to the nozzle

exit, both flames show streamwise oriented structures in the reactants stream. These structures begin to decrease in size to form smaller structures in the reactants stream, along with larger azimuthally oriented structures due to the jet shear layer. In Flame-low, many of these iso-surfaces are found to lie partially in the outside the flame, while these structures are found to lie within the flame brush in Flame-high due to the wider flame. At the $z/D \approx 4$ location for Flame-low, a stark difference is observed between the structures in the reactants and products. The magnitude of λ_{ci} is lowered to capture the vortex structures, showing that the swirling strength of the structures is lower in comparison to the upstream location. Red iso-surfaces are small and randomly oriented. In the flame brush, large structures with no apparent orientation are observed. Further away from the flame, large structures are again observed, though many appear to orient in the streamwise direction. This has been observed previously in Figure 3.5 and in the simulation of turbulent premixed flames by Duwig and Dunn (2013). The λ_{ci} iso-surfaces at $z/D \approx 12$ for Flame-high show that the vortex structures visualised by $\lambda_{ci} = 0.2$ are not visible for unburnt reactants, meaning that the vortical structures in this region are weak. Similar to Flame-low, structures in the flame brush have no consistent orientation and shape, while structures towards $Y_R = 0$ are large, elongated and tend towards a streamwise orientation.

Enstrophy production $\omega_i S_{ij} \omega_j$ plays a role in vortex stretching. The mean $\omega_i S_{ij} \omega_j$ conditioned on Y_R is shown in Figure 4.8. For Flame-low, enstrophy production is relatively similar in magnitude across the flame brush at each streamwise location. At $z/L_f = 0.04$, a large variation in mean $\omega_i S_{ij} \omega_j$ is observed across Y_R values, where $\omega_i S_{ij} \omega_j$ is high in magnitude on the reactants side and low on the products side. At $z/L_f = 0.65$, enstrophy production is low for both flames compared to the upstream location.

Enstrophy production can be written in the form:

$$\omega_i S_{ij} \omega_j = \omega^2 \left(\lambda_1 |\omega \cdot \mathbf{e}_1|^2 + \lambda_2 |\omega \cdot \mathbf{e}_2|^2 + \lambda_3 |\omega \cdot \mathbf{e}_3|^2 \right). \quad (4.2)$$

From this equation, enstrophy production is related to the alignment between the principal strain axes $\mathbf{e}_i$ and vorticity ω . Figure 4.9 shows $|\omega \cdot \mathbf{e}_i|$ at various streamwise locations for $Y_R = 0.134$ and $Y_R = 0.85$. At all streamwise locations, the vorticity vector is preferentially aligned with the immediate strain rate eigenvector, which is consistent with the observations in the literature (Ashurst et al., 1987; Ganapathisubramani et al., 2008; Hamlington et al., 2008; Wang et al., 2016). At $z/L_f = 0.04$, the probability of alignment with the extensive strain rate eigenvector $|\omega \cdot \mathbf{e}_1|$ is observed to increase in the preheat zone. With increasing streamwise location, the increase alignment with $\mathbf{e}_1$ is observed for both flames, consistent with the observations of Wang et al. (2016), while $|\omega \cdot \mathbf{e}_2|$ is still the most preferred. It is observed that with increasing streamwise distance

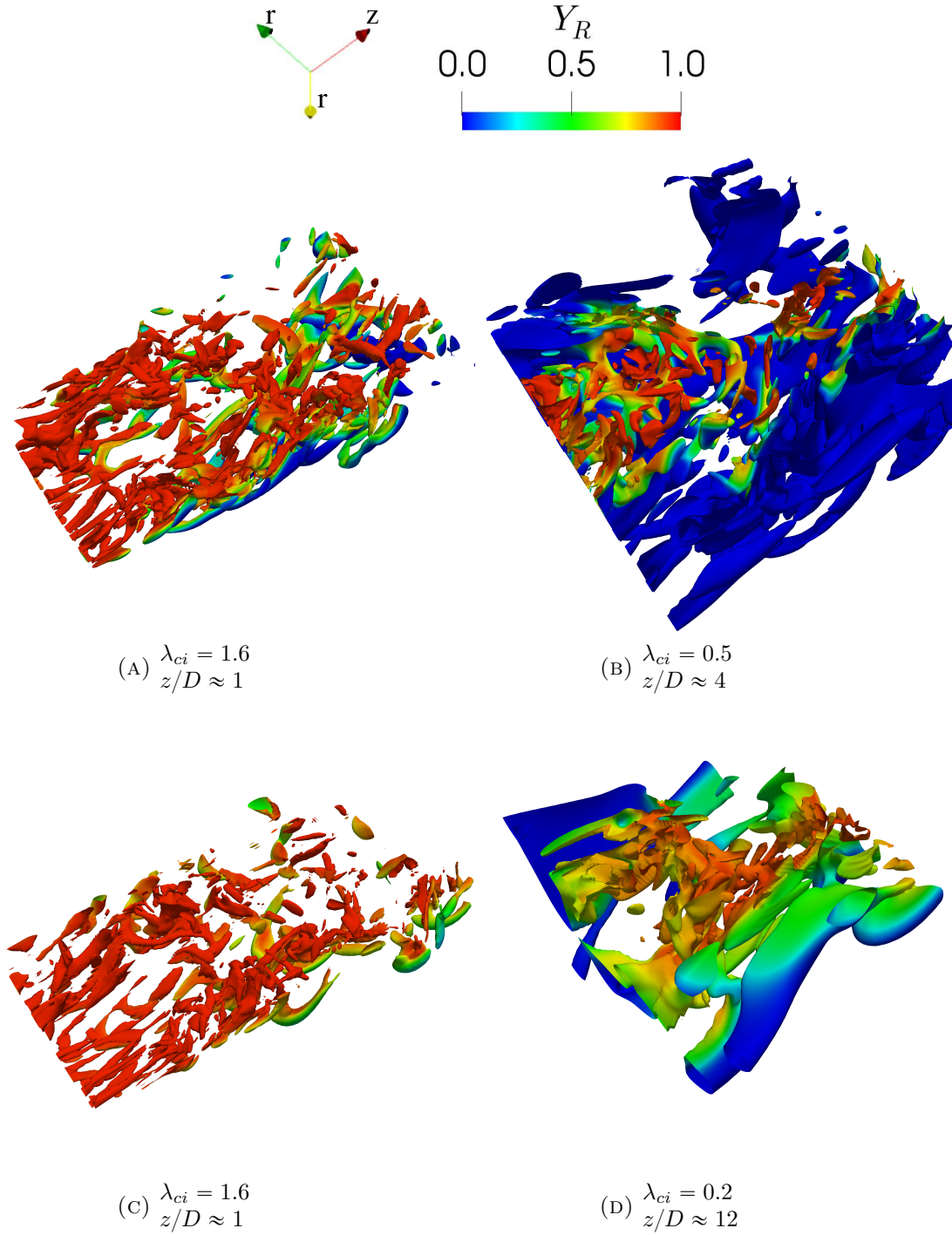


FIGURE 4.7: Iso-surfaces of λ_{ci} coloured by Y_R for (A,B) Flame-low and (C,D) Flame-high.

relative to the mean flame length, Flame-low shows greater variation in the strength of the preferential alignment of $|\omega \cdot \mathbf{e}_2|$ for both values of Y_R compared to Flame-high. The decreasing magnitude of $\text{PDF}(|\omega \cdot \mathbf{e}_2|)$ with streamwise distance shows flow towards an increase in compressibility effect of heat release on turbulence. Flame-high shows less

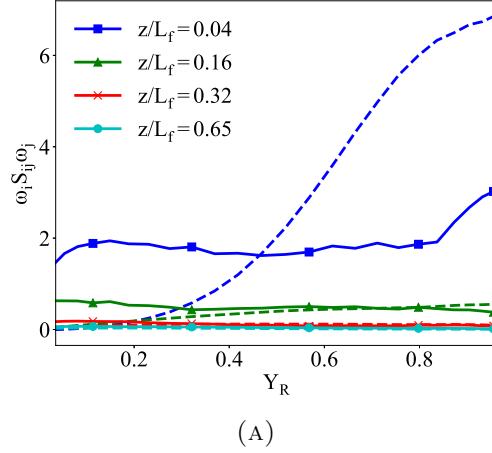


FIGURE 4.8: Conditional mean of enstrophy production $\omega_i S_{ij} \omega_j$ with Y_R for Flame-low (solid line) and Flame-high (dashed line).

variation in the magnitude of $\text{PDF}(|\omega \cdot \mathbf{e}_2|)$ with streamwise distance, though the decrease in magnitude is greater in the preheat zone than in the reaction zone. Close to the nozzle, both flames show strongest preferential alignment of $|\omega \cdot \mathbf{e}_2|$ similar to incompressible flows.

The alignment between the flame normal and vorticity vectors is shown in Figure 4.10. Consistent with the observations in Figures 4.9 and 4.17, where preferred alignment of the ω with $\mathbf{e}_2$ and alignment of $\mathbf{n}$ with $\mathbf{e}_3$ is observed, the vorticity vector shows a strong misalignment with the flame normal. The misalignment decreases with increasing streamwise location.

4.4 Surface density function

The local flame structure is analysed in this section. In particular, the scalar gradient $|\nabla c|$, also called the surface density function (SDF), and the factors influencing this quantity are examined. This quantity is closely related to the flame surface density Σ , so it is an important parameter for modelling. The flame structures at three different streamwise locations are visualised by $|\nabla c|$ in Figure 4.11. The first location is close to the nozzle exit ($z/D = 1$ to $z/D = 2$), while the second and third locations correspond to approximately 35% and 70% of each flame's L_f , respectively. At all three locations, the flame front of Flame-low is visibly thinner in comparison to Flame-high, due to the higher S_L in Flame-low. As such, the magnitudes of the gradient are higher in Flame-low. Flame-high shows clear broadening of the flame brush with increasing streamwise distance, while this effect is not as clear for Flame-low. In general, both flames exhibit local variations in flame thickness. For example, there appears to be a tendency for regions of higher curvature to show lower gradients magnitudes. The reasoning behind

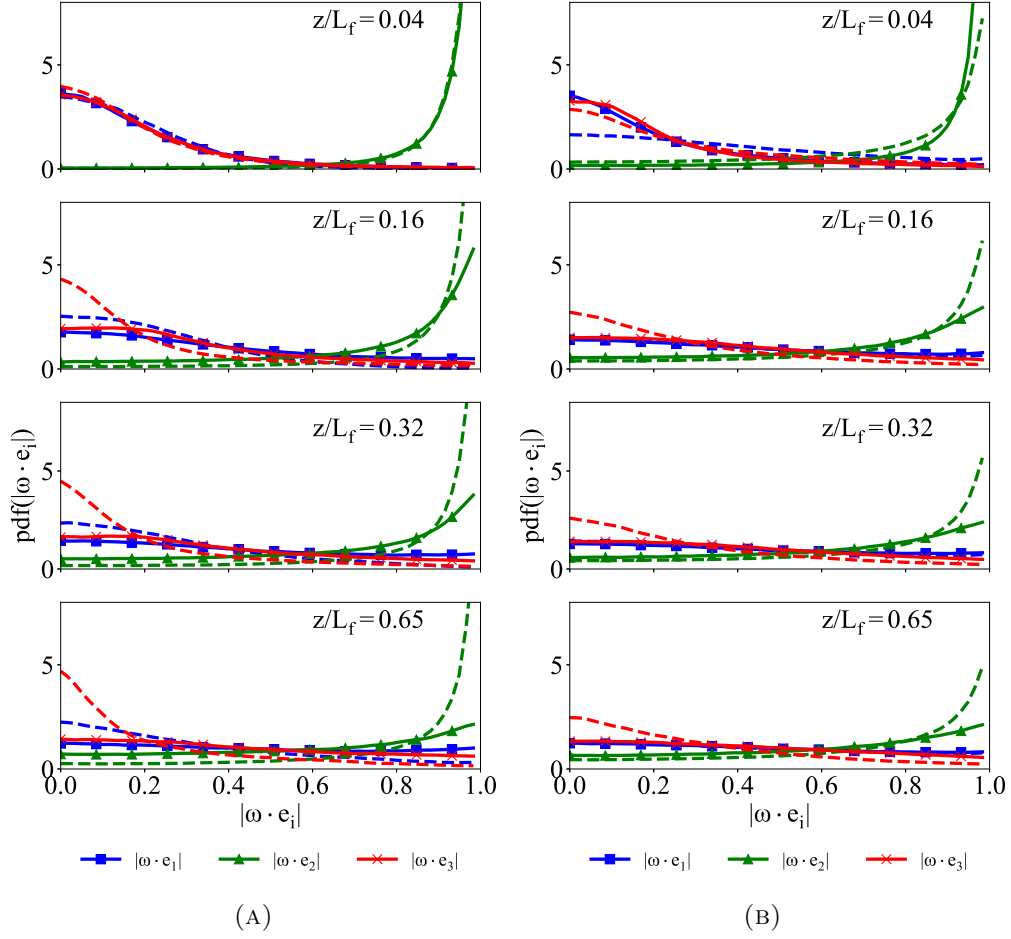


FIGURE 4.9: Alignment of vorticity and strain rate eigenvectors at (A) $Y_R = 0.134$ and (B) $Y_R = 0.85$ for Flame-low (solid line) and Flame-high (dashed line).

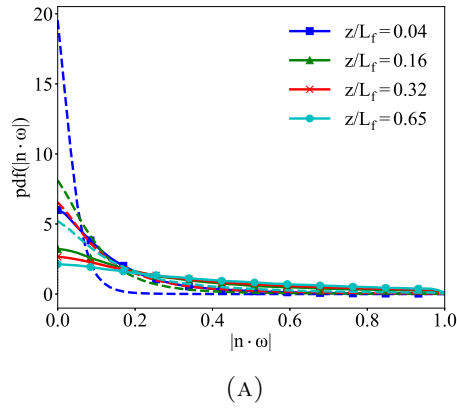


FIGURE 4.10: Alignment of flame normal and vorticity vectors for $Y_R = 0.134$ for Flame-low (solid line) and Flame-high (dashed line).

this will be discussed later in this section when examining the correlation between turbulence and flame curvature. More instances of flame-flame interaction are observed at downstream locations, where flame fronts can merge and can results in pockets of

reactants separating from the main flame, as seen around $z/D \approx 4.5$ in Figure 4.11a.

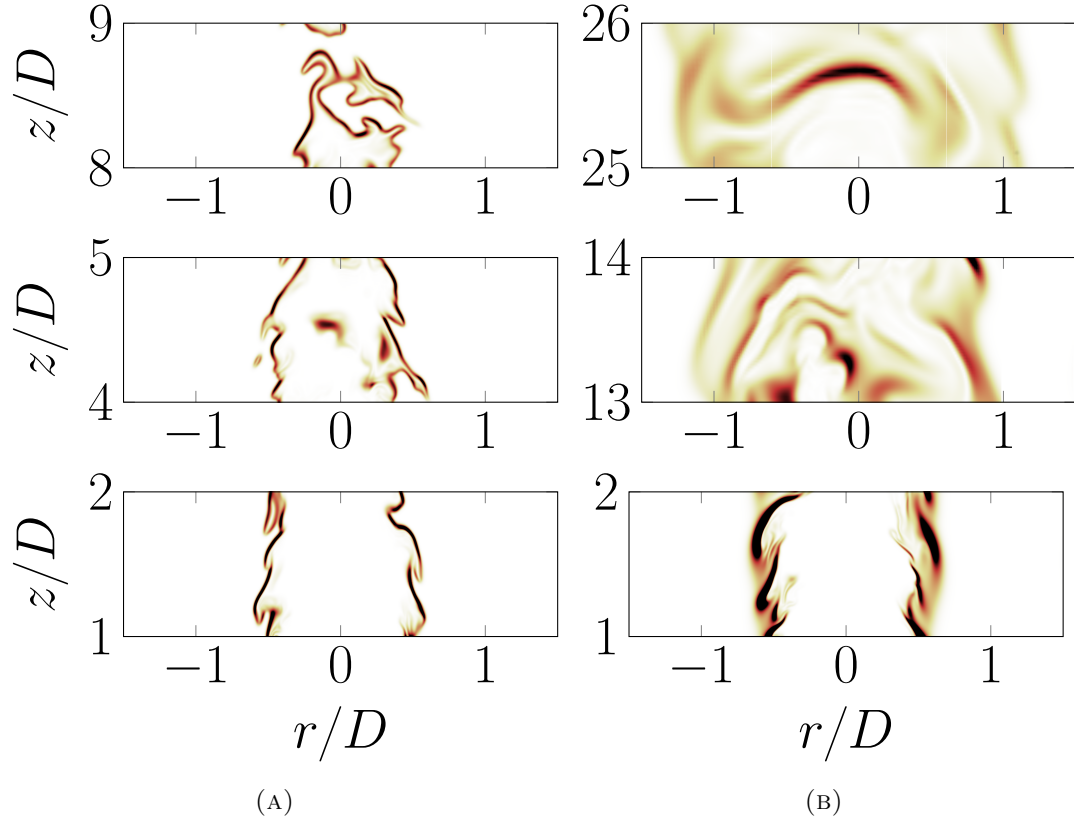


FIGURE 4.11: $z - r$ slices of local scalar gradient $|\nabla c|$ for (A) Flame-low and (B) Flame-high.

The temporally and azimuthally averaged scalar gradient fields, $\langle |\nabla c| \rangle$, are shown in Figure 4.12. Consistent with the observations from the instantaneous $|\nabla c|$, the magnitudes of $\langle |\nabla c| \rangle$ are lower in Flame-high, indicative of a thicker mean flame front. For both flames, the mean flame is thinner in the near nozzle region, quantified by the highest values of mean $\langle |\nabla c| \rangle$.

To further quantify the evolution of the scalar gradient of the two flames, the profiles of $|\nabla c|$ conditionally averaged on c are shown in Figure 4.13 for several streamwise locations, along with their joint PDFs. Additionally, these profiles are compared to the profiles of the respective laminar flames. For both flames, $|\nabla c|$ is observed to be significantly higher than the laminar scalar gradient close to the inlet at $z/L_f = 0.04$, with the largest difference primarily in the preheat zone. The higher gradients in the preheat zone at upstream locations have also been observed by Wang et al. (2017a). At the three locations further downstream, the conditional mean of Flame-low is close to the laminar profile, meaning that the turbulence does not significantly affect the inner flame structure. In contrast, Flame-high shows progressively lower magnitudes of $|\nabla c|$ with increasing streamwise distance. At $z/L_f \geq 0.65$, noticeable thickening of the flame relative to a laminar flame in the preheat zone is observed. It can also be seen that

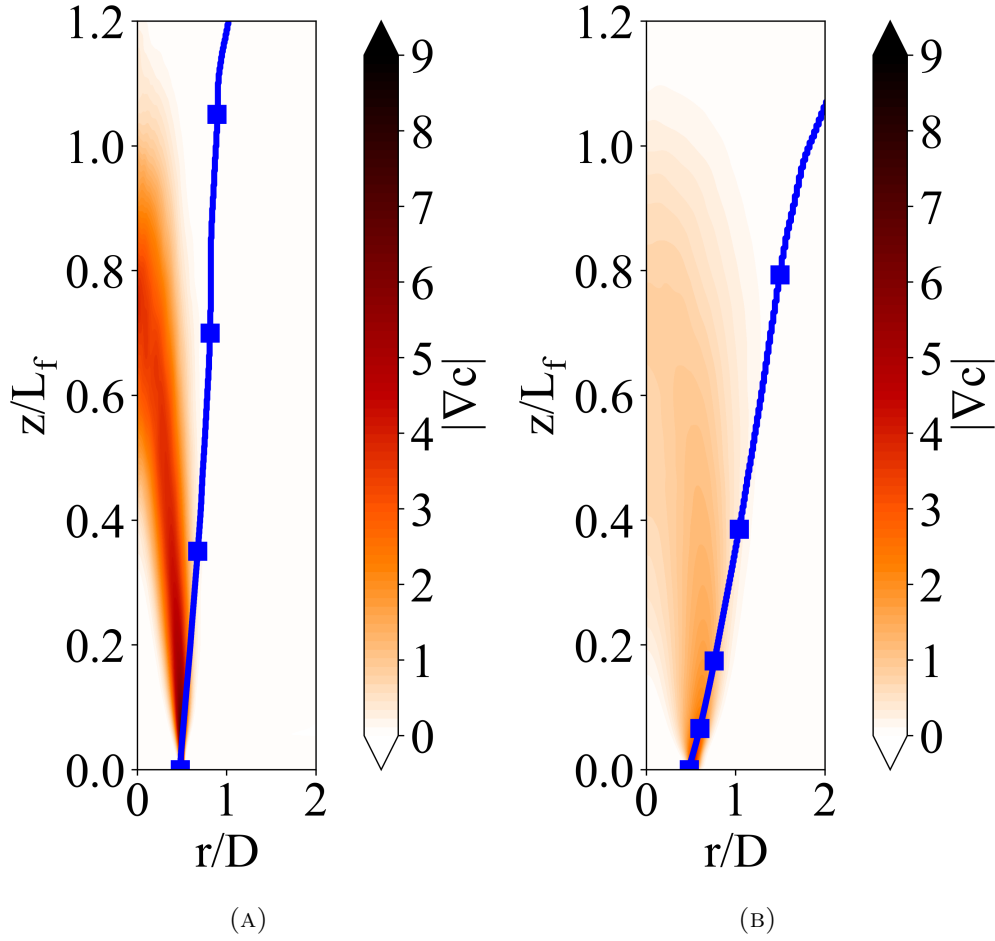


FIGURE 4.12: Time and azimuthally averaged surface density function for A) Flame-low and B) Flame-high. Jet half width $r_{1/2}$ is shown by the solid line.

$\langle |\nabla c| |c \rangle = 0$ at $z/L_f = 0.65$ for low c values, which confirms that reactants are at least partially burnt ($c > 0$) by this streamwise location. The joint PDFs for both flames show the greatest variance for intermediate values of c . For Flame-low, the c value which corresponds to the peak of the upper 10^{-5} contours is slightly lower than the c values corresponding to the peak of the laminar conditional profile. Meanwhile, the c value which corresponds to the peak of the upper 10^{-5} contours for Flame-high is much lower in comparison, indicating significant variations of the gradient in the preheat zone.

4.4.1 Tangential strain rate

The above observations show clear differences of $|\nabla c|$ with spatial and Ka variation. Studies have shown contradicting observations as to the thickening or thinning of the flame under the influence of turbulence. Some have reported mean flame thickening, while others have reported mean flame thinning. The analysis of the flames in this

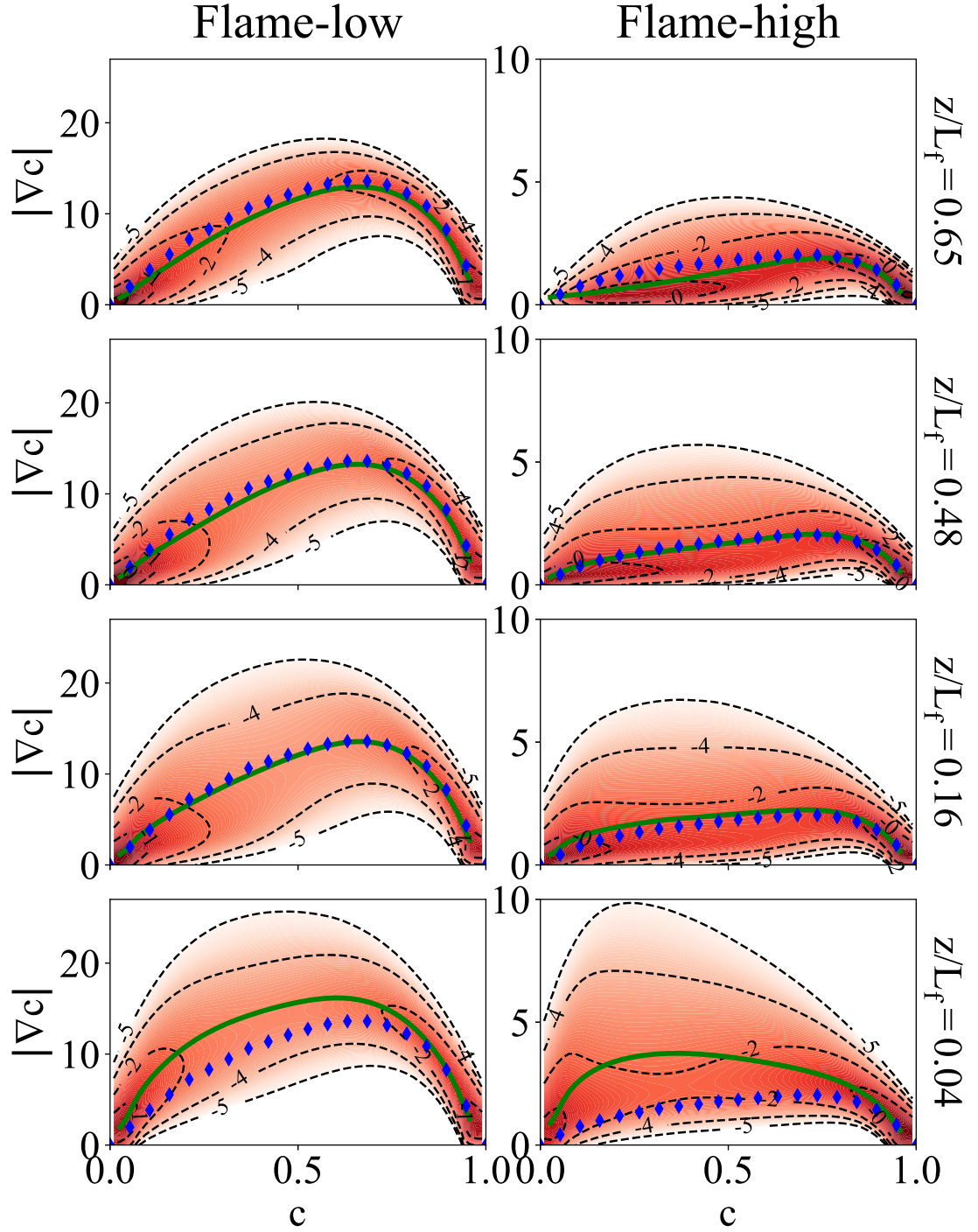


FIGURE 4.13: Joint PDFs of progress variable and surface density function for Flame-low and Flame-high (coloured by red). Contour lines (dashed) are in log scale. Also plotted are the conditionally averaged SDF $\langle |\nabla c| |c \rangle$ (green solid line) along with the profile for the corresponding laminar unstrained flame (blue diamonds).

study showed that flame thickening was mainly observed for Flame-high, while Flame-low showed a relatively constant thickness, except close to the inflow where the flame was found to be thinner than the laminar flame thickness. As the flow conditions for these studies differ, it suggests that the mean evolution of the SDF is not only dependent on

local turbulent structures, but also flow conditions such as the presence of mean shear or high pressures (Sandeep et al., 2018). The SDF is then a product of competing factors. To further understand the mechanisms influencing the SDF results observed for the two flames, the transport equation for SDF is examined (Candel and Poinso, 1990):

$$\frac{\partial |\nabla c|}{\partial t} + \frac{\partial u_k |\nabla c|}{\partial x_k} = (\delta_{ij} - n_i n_j) \frac{\partial u_i}{\partial x_j} |\nabla c| + S_d \frac{\partial n_i}{\partial x_i} |\nabla c| - \frac{\partial n_k S_d |\nabla c|}{\partial x_k}. \quad (4.3)$$

The first term on the right-hand side is the strain rate term where the tangential strain rate is:

$$a_t = (\delta_{ij} - n_i n_j) \frac{\partial u_i}{\partial x_j}. \quad (4.4)$$

The second term on the right-hand side is the curvature term where the curvature is:

$$k_m = \nabla \cdot \mathbf{n}, \quad (4.5)$$

and S_d is the displacement speed. The third term on the right-hand side is the propagation term. The combined effect of tangential flame strain rate and flame curvature is also known as flame stretch defined by the rate of change of a Lagrangian flame surface element δA (Candel and Poinso, 1990):

$$\kappa = \frac{1}{\delta A} \frac{d(\delta A)}{dt} = a_t + S_d k_m. \quad (4.6)$$

Firstly, the tangential strain rate is examined. Figure 4.14 shows the joint PDFs of a_t and $|\nabla c|$ for c^* along with the conditional profiles for several streamwise locations. In both cases, a positive correlation is observed between a_t and $|\nabla c|$ close to the inlet. This shows that increasing a_t leads to the decrease of flame thickness. Further downstream, while the correlation remains strong for Flame-high, it becomes weaker for Flame-low. This shows the important effect of strain rate on the flame structure for Flame-high.

Figure 4.15 shows the conditionally averaged tangential strain rate $\langle a_t | c \rangle$. The $\langle a_t | c \rangle$ for Flame-high varies with c , decreasing from the reactants side to the products side, a trend which was also observed experimentally by Steinberg et al. (2012). With increasing streamwise location, the variation with c decreases. In contrast, $\langle a_t | c \rangle$ tends to be higher on the product side for Flame-low, though the c dependence is weak compared to Flame-high. Globally, $\langle a_t | c \rangle$ is positive, indicating that tangential straining on average acts to decrease the flame thickness.

The tangential strain from Eq. 4.4 can also be written as,

$$a_t = \nabla \cdot \mathbf{u} - \left(\lambda_1 |\mathbf{n} \cdot \mathbf{e}_1|^2 + \lambda_2 |\mathbf{n} \cdot \mathbf{e}_2|^2 + \lambda_3 |\mathbf{n} \cdot \mathbf{e}_3|^2 \right). \quad (4.7)$$

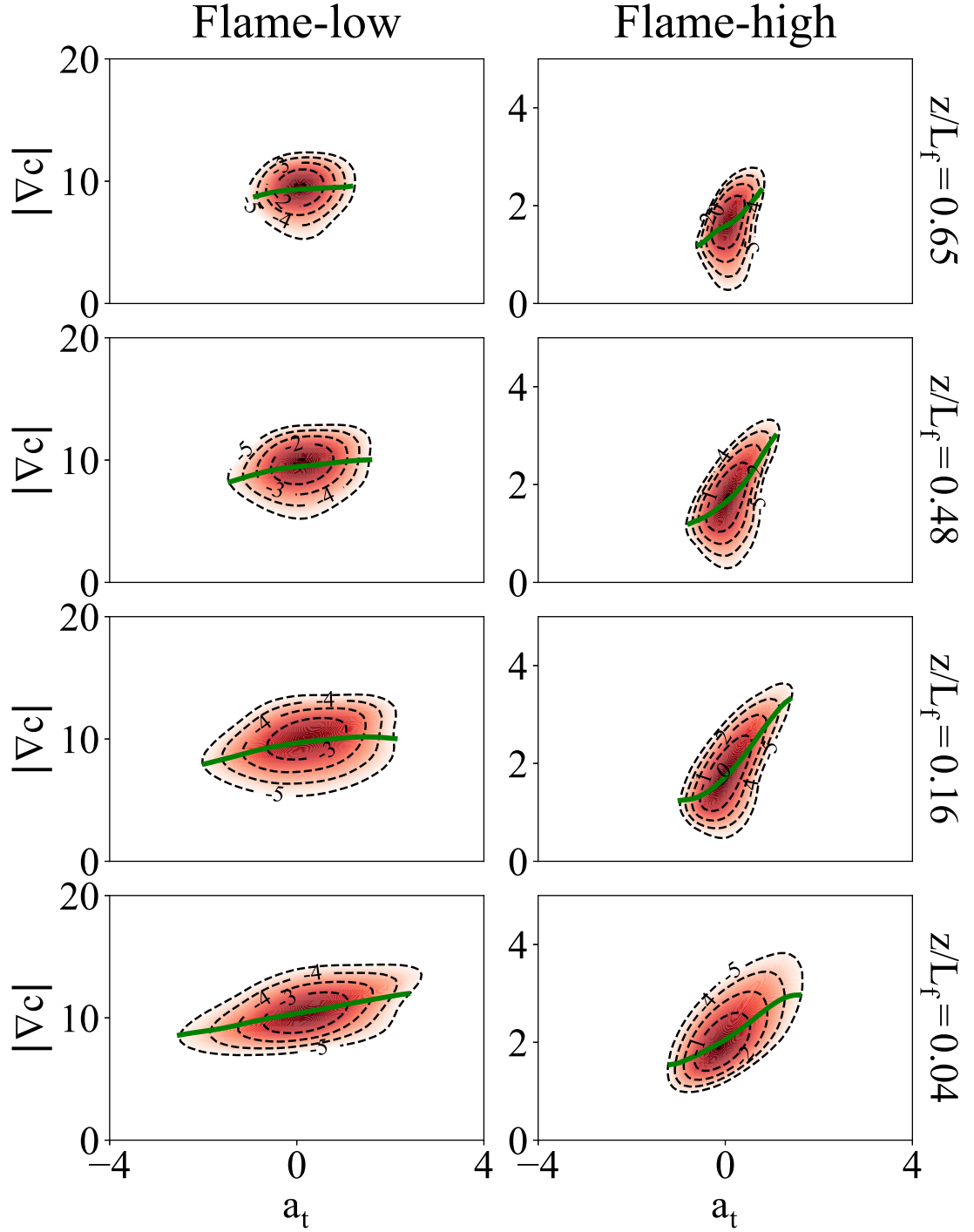


FIGURE 4.14: Joint PDF of surface density function and tangential strain rate for Flame-low and Flame-high.

The PDFs of the eigenvalues λ_1 , λ_2 , and λ_3 are shown in Figure 4.16. The eigenvalue of the extensive strain rate, λ_1 , mostly has a positive value, which indicates that alignment of the flame normal with $\mathbf{e}_1$ tends to decrease a_t , while the eigenvalue of the compressive strain rate, λ_3 , mostly has a negative value, which indicates that alignment of the flame normal with the $\mathbf{e}_3$ tends to increase a_t . For flames with $Ka > 1$, studies have observed

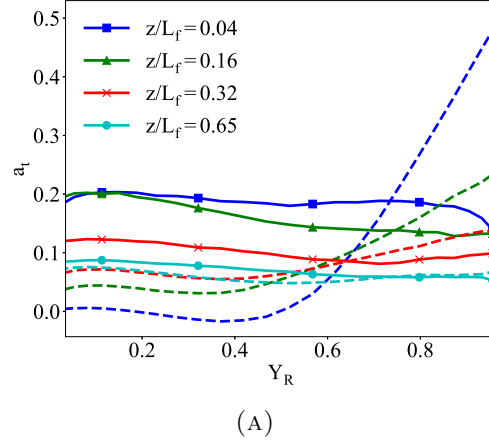


FIGURE 4.15: Conditional mean of tangential strain rate a_t with Y_R for Flame-low (solid line) and Flame-high (dashed line).

that there is a preferential alignment of the flame normal vector to the compressive strain rate eigenvector $\mathbf{e}_3$ (Chakraborty and Cant, 2007; Wang et al., 2016). The tangential strain rate increases as the flame normal aligns with the direction of compressive principal flow strain rate.

The alignment between the flame normal vector and the three eigenvectors of the strain rate tensor are shown in Figure 4.17. For both flames, $|\mathbf{n} \cdot \mathbf{e}_3|$ approaches 1 with increasing streamwise distance. Similar to the observations in Figure 3.17, Flame-low and Flame-high show preferences to values close to 0.7 (45°) at $z/L_f = 0.04$. In the reaction zone, there is a higher probability towards certain values of alignment, whereas the preheat zone shows greater spreading of the PDFs, indicated by the lower peaks of the PDFs.

Despite the weaker alignment of $\mathbf{n}$ with $\mathbf{e}_3$ at $z/L_f = 0.04$ compared to downstream locations, higher mean strain rates were observed in Figure 4.15. The higher strain rate can be attributed to mean shear. Wang et al. (2018) had showed for their high Karlovitz number jet flame that the mean shear is the largest contributing factor to tangential strain rate, dominating the effects of small scale turbulence. Therefore, as the flame coincides with the shear layer of the jet close to the nozzle exit, the mean shear is expected to play a major role, contributing to the thinning of the flame brush despite the higher local Ka values estimated near the nozzle exit in Figure 4.6. The mean tangential strain rate can be decomposed into a contribution from straining due to turbulence and a strain due to mean flow field as (Candel and Poinso, 1990; Trounev and Poinso, 1994),

$$\langle a_t \rangle = \langle a_{t,f} \rangle + \langle A_t \rangle, \quad (4.8)$$

where $\langle a_{t,f} \rangle$ is the strain rate due to turbulence:

$$\langle a_{t,f} \rangle = \langle \nabla \cdot \mathbf{u}'' - \mathbf{nn} : \nabla \mathbf{u}'' \rangle. \quad (4.9)$$

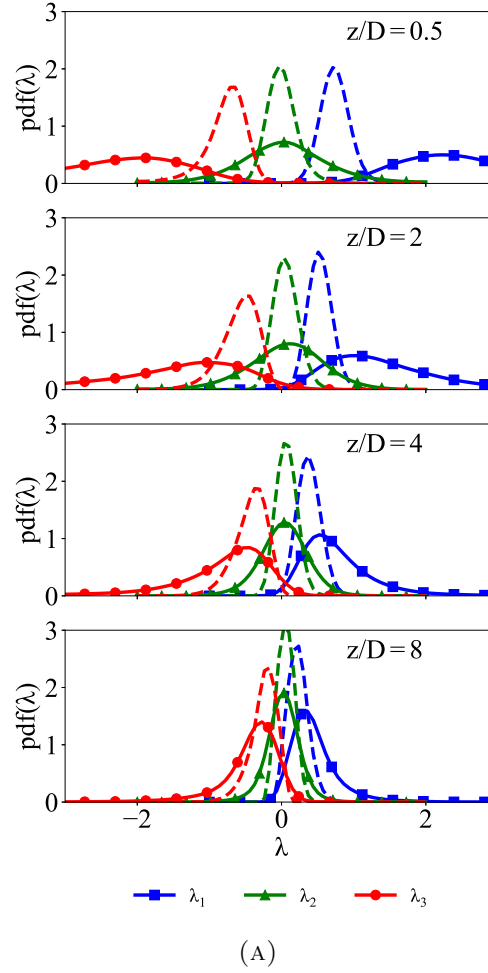


FIGURE 4.16: PDFs of strain rate eigenvalues at c^* for Flame-low (solid line) and Flame-high (dashed line).

The superscript " indicates density-weighted fluctuations and $\langle A_t \rangle_S$ is the strain rate due to the mean shear:

$$\langle A_t \rangle = (\delta_{ij} - \langle n_i n_j \rangle) \langle S_{ij} \rangle. \quad (4.10)$$

Figure 4.18 shows $\langle A_t \rangle$ conditionally averaged on Y_R . For both flames, the greatest magnitudes of $\langle A_t \rangle$ are found at $z/L_f = 0.04$, showing that the contribution of the mean shear to tangential strain rate is greatest close to the nozzle where the shear layer coincides with the flame. At this location, a difference is observed between the profiles of the two flames, where higher values of $\langle A_t \rangle$ are observed for Flame-low compared to Flame-high for $Y_R < 0.9$. This observation may be due to the difference in the flame thickness. With the thinner flame of Flame-low, the entire flame brush lies within the shear layer, as observed visually in Figure 4.7. In Flame-high, only part of the flame brush lie in the shear layer, resulting in the variation of $\langle A_t \rangle$ across the flame brush.

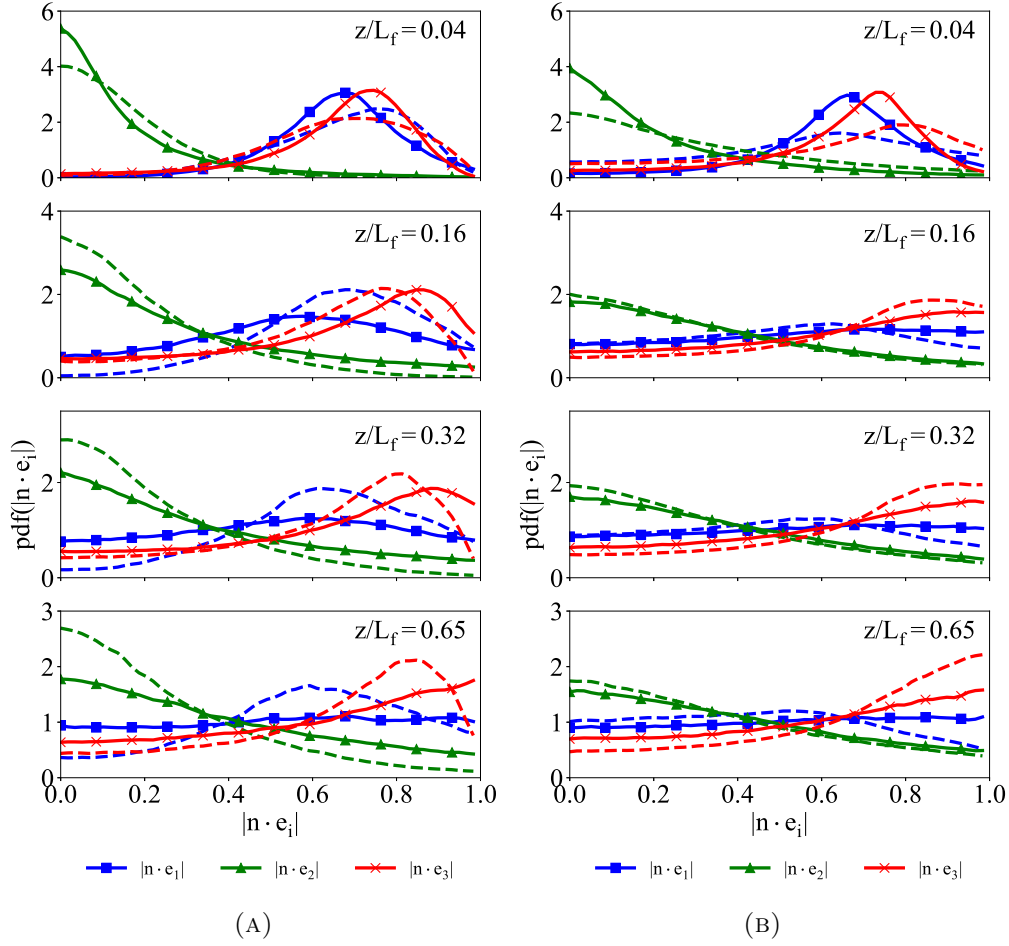


FIGURE 4.17: Alignment of flame normal vector and strain rate eigenvectors at (A) $Y_R = 0.134$ and (B) $Y_R = 0.85$ for Flame-low (solid line) and Flame-high (dashed line).

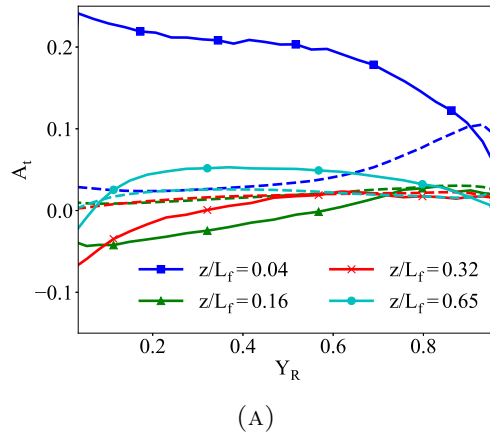


FIGURE 4.18: Conditional averaged of the contribution of mean flow to tangential strain rate for Flame-low (solid line) and Flame-high (dashed line).

4.4.2 Flame curvature

Next, the contribution of flame curvature is examined. A higher magnitude of flame curvature contributes to an increase in flame thickness. Figure 4.19 shows the conditionally

averaged flame curvature on Y_R . For Flame-low, a positive mean curvature is observed close to the products side indicating concave curvature towards the reactants, while negative mean curvature is found on the reactants side indicating convex curvature towards the reactants side. The magnitudes of curvature increases with streamwise location for Flame-low. In contrast, Flame-high exhibits lower magnitudes of mean curvature since it features a much larger flame thickness. As a result, the flame is less wrinkled in response to turbulence.

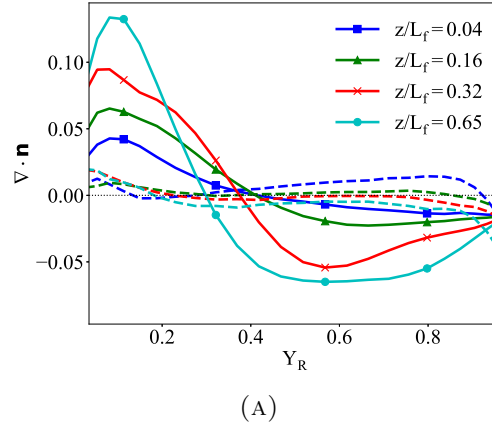


FIGURE 4.19: Conditional mean of flame curvature $\nabla \cdot \mathbf{n}$ with Y_R .

4.4.3 Flame stretch

As discussed in Section 1.2.4.2, the basis of most algebraic FSD models is an assumption equilibrium between the production and destruction of FSD. In the context of Eq. 4.6, this means that the tangential strain rate and flame curvature terms are assumed to balance. Therefore, it is useful to determine the correlation of the two terms with respect to each other for the present flames, to examine the validity of this assumption.

Figure 4.20 shows the conditional average of tangential flame strain rate with the curvature term for $Y_R = 0.134$, normalised by the flame time scale τ_L . The results for Flame-low show that the conditional mean coincides with the line of $a_t = -S_d(\nabla \cdot \mathbf{n})$ for certain values of $S_d(\nabla \cdot \mathbf{n})$. On the other hand, the results of Flame-high show that the mean is skewed towards positive values of the tangential strain rate term and does not coincide with the line of $a_t = -S_d(\nabla \cdot \mathbf{n})$. This shows that for the two flames in this study, the assumption of balance between the production and destruction of FSD is less applicable to Flame-high compared to Flame-low due to the greater tangential strain rate contribution.

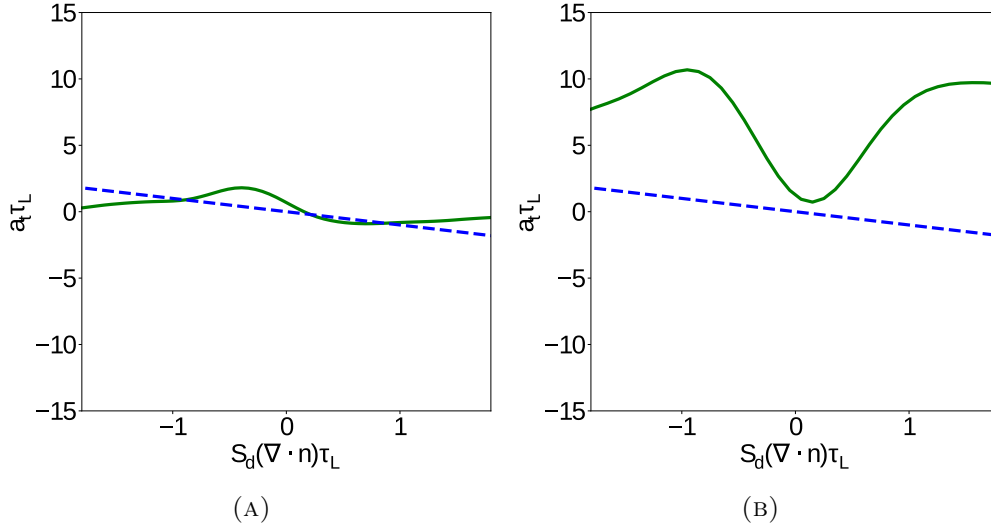


FIGURE 4.20: Conditional mean of tangential strain rate term with curvature term normalized by for (A) Flame-low and (B) Flame-high. Blue dashed line indicates $a_t = -S_d(\nabla \cdot \mathbf{n})$.

4.5 Conclusions

A comparison of DNS of two turbulent premixed flames in a pipe/jet configuration with different Karlovitz numbers was presented in this chapter. One flame lies on the lower range of the Thin Reaction Zone regime close to the corrugated regime, while the other lies on the higher range of the Thin Reaction Zone regime close to the broken reaction zone regime. Differences were observed in both the global and local flame structure. The higher Karlovitz number flame was significantly longer in length, which also affected the evolution of the turbulent jet. Locally, the flame front of the higher Ka flame is thicker, quantified by lower progress variable gradients.

The spatial dependence of the flame structure and TFI were also observed. Visualisation of both flames shows that the vortex structures are affected by the presence of the flame front, with small randomly oriented structure in the reactant stream and larger structures outside of the flame. The higher dilatation due to heat release in the preheat zone for the lower Ka flame results in lower enstrophy production compared to the higher Ka flame.

Flame strain rates and flame curvature in both flames were compared. The effect of the flame strain rate on SDF was found to be especially important near the inflow, including a significant contribution to the flame strain rate from the the mean shear resulting from the shear layer development. The above factors are deemed to be important as they affect the SDF. Comparison of the terms in the SDF transport equation showed that

the modelling assumption of a balance between the production and destruction of SDF is less viable for the higher Ka flame.

Chapter 5

Flame-surface density models using Gene Expression Programming

5.1 Introduction

This chapter presents the development of algebraic Flame Surface Density (FSD) models using the approach of Gene-Expression Programming (GEP) described in Section 2.5. The database of the DNS of the two turbulent premixed jet flames with different inlet Karlovitz numbers analysed in Chapter 4 is used as the training data for the GEP algorithm by applying explicit filtering with different filter sizes. This study serves as a proof of concept to generate FSD models using this technique. The performance of the models is evaluated *a-priori*. The sensitivity of the method to the choice of the training data is also investigated by developing models using different subsets of the DNS database.

5.2 GEP parameters

For this study, the independent variables used for generating the models were the length ratio Δ/δ_z and the velocity ratio u'_Δ/S_L . The Zel'dovich flame thickness is calculated by $\delta_z = 1/PrRe_SLe$, such that $\delta_z/D = 0.0167$ for Flame-low and $\delta_z/D = 0.0463$ for Flame-high. The Σ_{gen} was also restricted to the gradient based model using the Ξ_{gen} ,

such that the models is of the form:

$$\Sigma_{gen} = \Xi_{gen} |\nabla \bar{c}| = f \left(\frac{\Delta}{\delta_z}, \frac{u'_\Delta}{S_L} \right) |\nabla \bar{c}|, \quad (5.1)$$

where f is the functional form obtained from GEP. Since the expected value of Σ_{gen} for the unburnt and burnt mixtures was zero ($|\nabla \bar{c}| = 0$), only the data within the range of $0.01 < \bar{c} < 0.99$ was used for the target data.

To prevent premature convergence to sub-optimal solutions, conditions are imposed such that individuals which do not satisfy these conditions have their cost value artificially increased so that they will not survive during the selection process. The definition of suboptimal solutions is a design choice, and justification of the choices made here are discussed. Following Weatheritt and Sandberg (2017b), the first criterion is that shorter functions are considered suboptimal. In this setup, six symbols is chosen as the lower limit on the length of the individuals. This specific value is chosen because the functionally simplest reference model, the Boger model, can be expressed with a gene of six elements. The second criterion, which has also been considered by Weatheritt and Sandberg (2017b), is to limit the number of nested operators (i.e. $\exp(\exp(\sin(\exp(\dots))))$) allowed. This is to prevent overly complicated functions. The chosen limit is a maximum of three nested operators. The condition is chosen by accessing the complexity of the reference models. Lastly, a criterion is imposed such that all the independent variables chosen to represent the functional form must appear at least once in the individuals.

The fitness of each individuals was evaluated using the cost function:

$$fit = \frac{1}{n_\Delta} \sum_{\Delta} \int \frac{(\langle \Sigma_{gen} | \bar{c}, \Delta \rangle - \langle \Sigma_{gen}^{DNS} | \bar{c}, \Delta \rangle)^2}{\langle \Sigma_{gen}^{DNS} | \bar{c}, \Delta \rangle^2} d\bar{c}, \quad (5.2)$$

where n_Δ is the number of filter sizes used for the training data. Equation 5.2 aims to minimum the error in the conditional averaged of Σ_{gen} with respect to $\bar{c}$ and Δ .

5.3 Training Data

The data for training the GEP algorithm and for the *a-priori* assessment of models are extracted from the DNS datasets of Flame-low and Flame-high. The filtered quantities are obtained by applying the Gaussian filter discussed in Section 2.4.1 in all three dimensions. The filter sizes used are $\Delta/\delta_z = 1.7, 2.2, 4.4, 8.8$ for Flame-low and $\Delta/\delta_z = 1.6, 3.2, 4.3, 6.4$ for Flame-high. Due to computational cost of conducting multiple runs of the GEP algorithm, the training data was reduce to selected regions. Slices on the r - θ plane were included for seven chosen streamwise positions for each flame corresponding

to 4%, 16%, 32%, 48%, 65%, 80%, and 96% of their respective mean flame length L_f/D . A sampling of 100 time instants were used for training.

Since the expected value of Σ_{gen} for the unburnt and burnt mixtures was zero ($|\nabla \bar{c}| = 0$), only the data within the range of $0.01 < \bar{c} < 0.99$ was used for the training data. In total, the number of data points in the training dataset was approximately 66 million.

The variable u'_Δ was calculated from the sub-grid turbulent kinetic energy as,

$$u'_\Delta = \sqrt{(\widetilde{u_i u_i} - \widetilde{u_i} \widetilde{u_i})/3}. \quad (5.3)$$

Figure 5.1 shows slices of Σ_{gen} extracted from the DNS for one streamwise location at $z/L_f = 0.32$. With increasing filter size, the resolution of the flame brush is observed to weaken. Particularly, the flame brush in the regions of high wrinkling can be seen to blur together, decreasing the magnitudes of flame wrinkling.

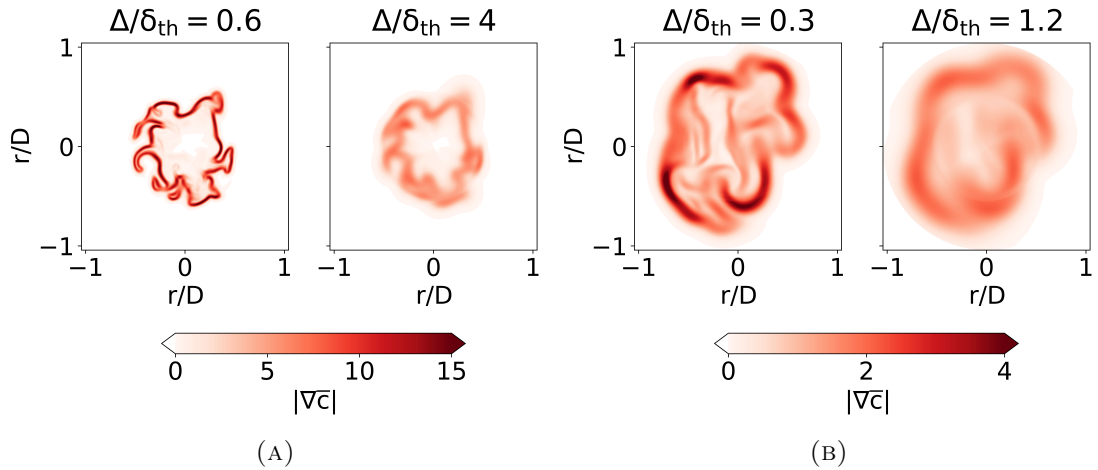


FIGURE 5.1: Filtered streamwise slice at $0.32L_f$ of (A) Flame-low and (B) Flame-high.

5.4 Results

5.4.1 Evaluation of GEP models

Models were developed using three datasets. For each subset, the GEP algorithm executed 10 times and the best model (lowest *fit*) from each are analysed below. The models are shown in Table 5.1, where “GEP_{low}” was the result of using a dataset with only the data from Flame-low, “GEP_{high}” from a dataset with only the data from Flame-high, and “GEP_{all}” from a dataset with the data from both flames. Each run of the GEP algorithm was performed with a population size of 5000 individuals and results were obtained after 5000 generations. The algorithm was run using Intel Xeon

E5-2643 CPUs, and the total data points were divided such that approximately 800,000 data points per CPUs were used. The computational cost for 66 million data points was approximately 607.824 seconds per generation per CPU.

Name	Model formulation	<i>fit</i>
GEPlow	$\Sigma_{gen} = 0.636 \left(u'_{\Delta}/S_L + (2.189 + \Delta/\delta_z)^3 + (u'_{\Delta}/S_L + 3.934)^{1.5} \right)^{1/9} \nabla \bar{c} $	0.0031
GEPhigh	$\Sigma_{gen} = 1.413 \exp \left(1.742 u'_{\Delta}/S_L^2/f_1^2 \right) \nabla \bar{c} $ where $f_1 = 2u'_{\Delta}/S_L - \Delta/\delta_z + \left((\Delta/\delta_z - 2.718)^3 + 2.478 \right)^{0.5} + (u'_{\Delta}/S_L/(\Delta/\delta_z - 1))^2$	0.0224
GEPall	$\Sigma_{gen} = \exp \left(\frac{((1-\Delta/\delta_z)^2}{\Delta/\delta_z (14.301 + (\Delta/\delta_z + u'_{\Delta}/S_L^3)^{1/3})} \right) \nabla \bar{c} $	0.0115
Charlette2	$\Sigma_{gen} = \left(1 + \min \left[\frac{\Delta}{\delta_L}, \Gamma_{\Delta} \left(\frac{u'_{\Delta}}{S_L} \right) \right] \right)_1^{\beta} \nabla \bar{c} $ where $\Gamma_{\Delta} = \left[\left((f_u^{-a_1} + f_{\Delta}^{-a_1})^{-1/a_1} \right)^{-b_1} + f_{Re}^{-b_1} \right]^{-1/b_1}$, $Re_{\Delta} = \frac{u'_{\Delta} \Delta}{\nu}$, $b_1 = 1.4$, $\beta_1 = 0.5$, $C_k = 1.5$, $a_1 = 0.60 + 0.2 \exp \left[-0.1 \frac{u'_{\Delta}}{S_L} \right] - 0.20 \exp \left[-0.01 \frac{\Delta}{\delta_L} \right]$, $f_u = 4 \left(\frac{27}{110} C_k \right)^{1/2} \left(\frac{18}{55} C_k \right) \left(\frac{u'_{\Delta}}{S_L} \right)^2$, $f_{\Delta} = \left\{ \left(\frac{27}{110} C_k \pi^{4/3} \right) \left[\left(\frac{\Delta}{\delta_L} \right)^{4/3} - 1 \right] \right\}^{1/2}$, $f_{Re} = \left[\frac{9}{55} \exp \left(-1.5 C_k \pi^{4/3} Re_{\Delta}^{-1} \right) \right]^{1/2} Re_{\Delta}^{1/2}$	
Fureby	$\Sigma_{gen} = \left[\Gamma \left(\frac{u'_{\Delta}}{S_L} \right) \right]^{D-2} \cdot \nabla \bar{c} $ where $D = 2.05/(u'_{\Delta}/S_L + 1) + 2.35/(S_L/u'_{\Delta} + 1)$	
Zimont	$\left[1 + 0.51 \frac{u'_{\Delta}}{S_L} \frac{\Delta}{\delta_L} \right] \nabla \bar{c} $	

TABLE 5.1: GEP generated models and selected reference models

Chakraborty and Klein (2008) assessed the performance of algebraic FSD models using three criteria: the variation volume-averaged value $\langle \Sigma_{gen} \rangle$ with filter size, the correlation coefficient between the modelled FSD and FSD from the DNS, and the conditionally averaged values $\langle \Sigma_{gen} | \bar{c} \rangle$. These criteria are used here to assess the performance of the GEP generated models and compare to selected models from the literature. The models from the literature are the models of Charlette et al. (2002), Fureby (2005), and Zimont and Lipatnikov (1995). The models which use dynamic formulation, adjustable constants, or additional variables are excluded as these features are not included in the current GEP formulations.

The models are evaluated at streamwise locations and filter sizes different from the training data set: at locations corresponding to 10%, 40%, and 70% of the respective mean flame length, and at filter sizes $\Delta/\delta_z = 3, 9$, and 12. The GEP models are compared to models of similar form to Eq. 1.14, which include the models Charlette (Charlette et al., 2002), FurebyM (Fureby, 2005; Ma et al., 2013), and Zimont (Zimont

and Lipatnikov, 1995). Models which use dynamic formulation, adjustable constants, or additional variables are excluded as these features are not included in the current GEP formulations.

Figure 5.2 shows the variation of $\langle \Sigma_{gen} \rangle$ with Δ/δ_z which represents the total flame surface area. The reference models generally overestimate $\langle \Sigma_{gen} \rangle$ for both flames. For Flame-low, Fureby model provides better estimates than the other reference models, and give reasonable estimates at $z/L_f = 0.4$ and 0.7 , but overestimates for larger filter sizes at $z/L_f = 0.1$. The Zimont model consistently overestimates the most out of the reference models. The GEP models are generally able to give better estimates of $\langle \Sigma_{gen} \rangle$ compared to the reference models for both flames. However, GEPhigh is observed to underpredict $\langle \Sigma_{gen} \rangle$ for $\Delta/\delta_z = 3$ for $z/L_f = 0.4$ and 0.7 when applied to Flame-low. This is likely because GEPhigh was developed from the data subset of Flame-high which exhibits a different range of u'_Δ/S_L . For Flame-high, all three GEP models give similar estimates for $\langle \Sigma_{gen} \rangle$.

Figure 5.3 shows the correlation coefficient between the DNS and the modelled FSD $\text{corr}(\Sigma_{gen}, \Sigma_{gen}^{DNS})$, where a unity value is desired. The GEP models show $\text{corr}(\Sigma_{gen}, \Sigma_{gen}^{DNS})$ closest to unity for increasing filter sizes, except for results of Flame-low obtained with GEPhigh. The reference models in general also provide reasonable values for $\text{corr}(\Sigma_{gen}, \Sigma_{gen}^{DNS})$. The comparable $\text{corr}(\Sigma_{gen}, \Sigma_{gen}^{DNS})$ for the models have been attributed to the fact that all the models are dependent on $|\nabla \bar{c}|$ through Eq. 1.14 Chakraborty and Klein (2008).

Figure 5.4 and 5.5 shows the values of Σ_{gen} conditionally averaged on $\bar{c}$ for Flame-low and Flame-high, respectively. The Charlette2 and Zimont models are found to be consistently overestimating $\langle \Sigma_{gen} | \bar{c} \rangle$ for both flames. Consistent with $\langle \Sigma_{gen} \rangle$ results in Fig. 5.2, Fureby model provides the best estimates of the reference models for Flame-low at downstream locations. GEPlow and GEPall show good predictions for all streamwise locations and filter sizes, while GEPhigh is found to underestimate $\langle \Sigma_{gen} | \bar{c} \rangle$, especially for $\Delta/\delta_z = 3$ for downstream locations.

The reference models are observed to all overestimate $\langle \Sigma_{gen} | \bar{c} \rangle$ for Flame-high. In contrast, the GEP models provide much better performance in predicting $\langle \Sigma_{gen} | \bar{c} \rangle$. Minor underprediction for $\langle \Sigma_{gen} | \bar{c} \rangle$ is observed for GEPhigh and GEPall in the region of the preheat zone for larger filter sizes. This may indicate the increased difficulty in capturing the unresolved turbulent eddies which penetrate the preheat zone and their effect on the flame structure.

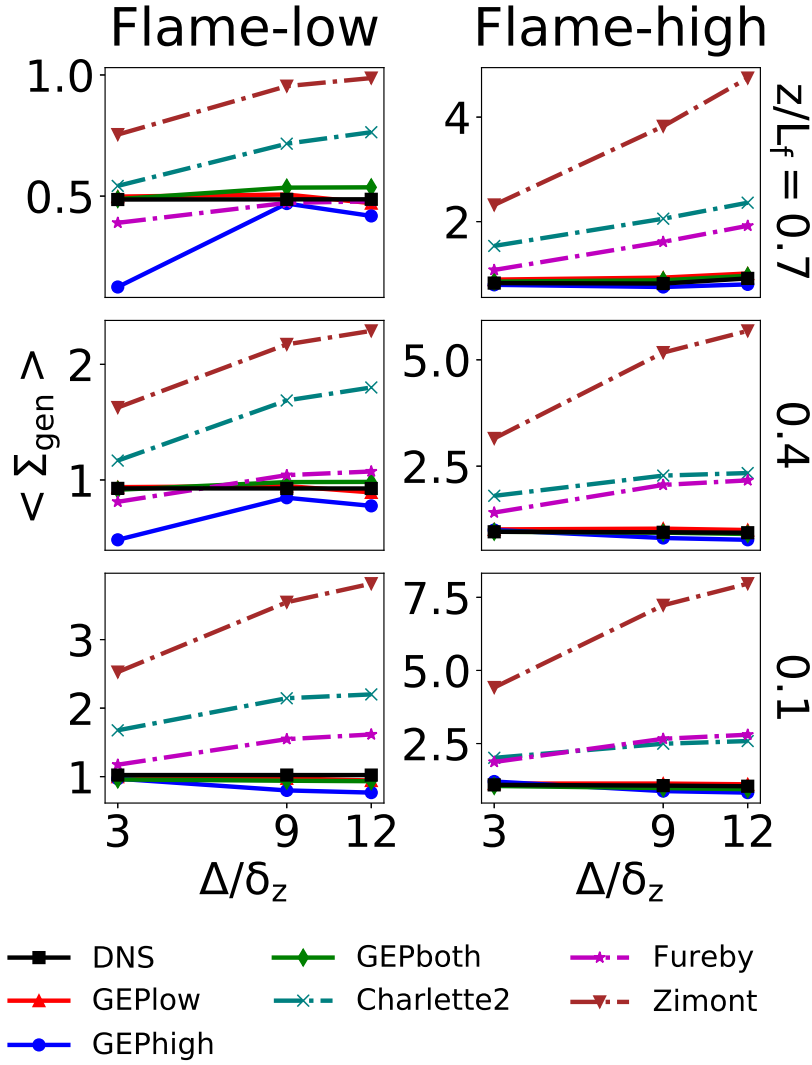


FIGURE 5.2: Variation of volume averaged FSD with filter size.

It is interesting that GEPlow has a wider range of validity compared to GEPhigh both in terms of the Karlovitz number and the filter size. This implies that a larger range of $\langle \Sigma_{gen} | \bar{c} \rangle$ covered by Flame-low makes this case more suitable for training.

5.5 Conclusions

Gene-Expression Programming (GEP), an evolutionary machine learning algorithm, was used to develop Algebraic Flame Surface Density (FSD) models in the Large-Eddy Simulation (LES) context. The algorithm was trained using filtered DNS data from different spatial regions of two turbulent premixed jet flame with different inlet Karlovitz numbers. Different subsets of the data were used to investigate the sensitivity of the choice

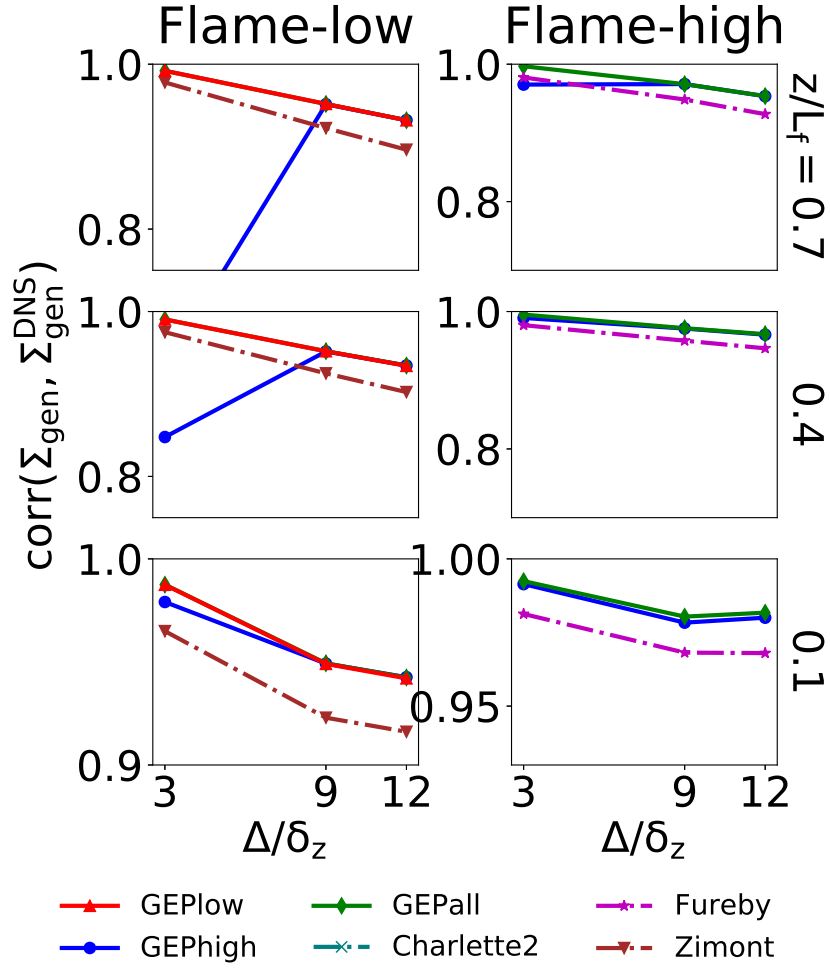
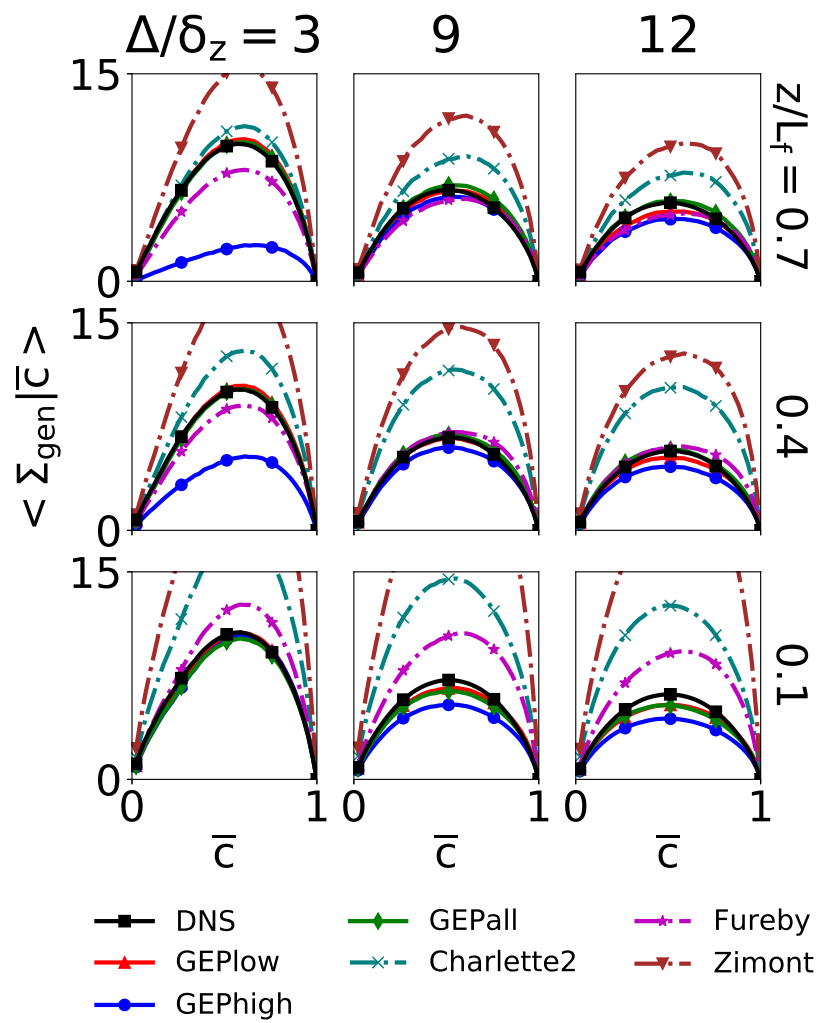
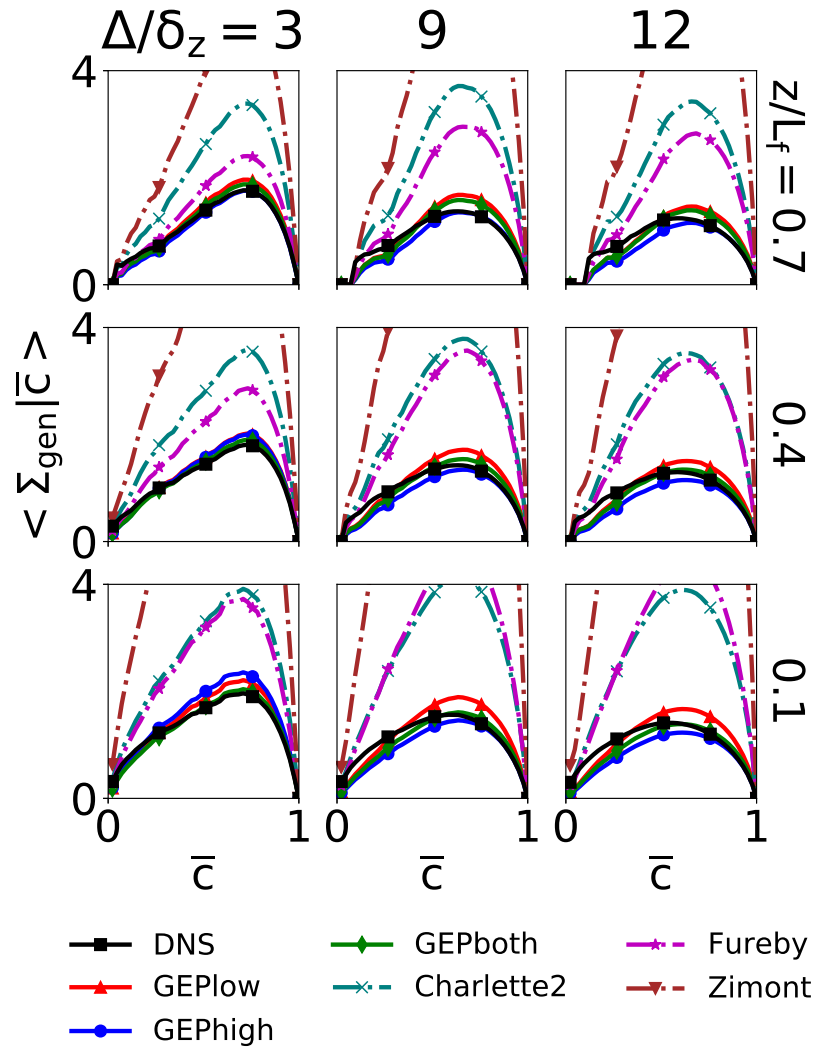


FIGURE 5.3: Correlation coefficient between DNS and modelled FSD in the range of $0.1 < \bar{z} < 0.9$.

of training data. The *a-priori* predictions of FSD by the best GEP models were compared. The models trained on the lower Ka number flame and both flames were found to perform well, comparable or better to the existing Charlette2, Fureby, and Zimont models. The model trained using the higher Ka flame was able to give good estimates when evaluated on the higher Ka flame, but was observed to underpredict FSD when applied to the lower Ka flame. The results of the GEP models showed that the GEP is a promising tool for developing algebraic FSD models for LES, although the choice of training data was shown to be a major factor that can affect the quality of the model.


 FIGURE 5.4: Conditional averaged FSD with $\bar{c}$ for Flame-low.


 FIGURE 5.5: Conditional averaged FSD with $\bar{c}$ for Flame-high.

Chapter 6

Conclusions and recommendations for future work

Direct Numerical Simulation (DNS) was used to analyse and model turbulence-flame interactions (TFI) in turbulent premixed jet flames. New toolsets were developed in order to conduct the simulations and data-driven modelling. Three DNS cases of turbulent premixed round jet flames were considered, two of which featured a computational domain consisting of an upstream long pipe to feed a fully developed turbulent inflow to the jet flame. The two flames are quantified by different inflow Karlovitz numbers (Ka), one in the lower region of the thin reaction zone regime ($Ka = 4$) and the other in the higher region ($Ka = 90$). A third DNS was conducted with the same parameters as the lower Ka flame except without the upstream pipe, instead generating the turbulent inflow synthetically, in order to investigate the influence of inflow turbulence on TFI. Finally, algebraic flame surface density (FSD) models were developed by training a Gene-Expression Programming (GEP) algorithm with the DNS dataset.

The conclusions drawn from these studies are as follows.

- The influence of inflow boundary conditions on TFI were investigated by considering on the simulations with and without an upstream pipe. In the case of the fully developed inflow with the pipe, the mean flame was shorter and the turbulent jet wider than in the case of the synthetic inflow which underestimated the turbulent kinetic energy of the jet. Local statistics related to flame orientation, strain rate, and alignment, were found to exhibit some quantitative differences. When the effects of bulk strain were removed, TFI were found to be similar between the two setups, showing that the differences in the local statistics were due to the bulk strain rate when different turbulent inflow conditions were used. The

bulk strain rates were affected by the global evolution of the jet and flame. The spatial dependence of TFI on the inflow turbulence was considered, and it was determined that close to the inflow, the finite response time between the flame and the inflow lead to weaker coupling between flame and turbulence, while further downstream differences in the turbulence cause by the inflow were no longer sufficient to significantly influence TFI.

- The spatial and Karlovitz number dependence of TFI in turbulent premixed round jet flames were quantified by comparing two simulations with different premixture temperatures. Differences were observed in the global flame structure, where the higher Ka flame was longer and exhibited larger scale wrinkling of the flame surface. The magnitude of the scalar gradient or surface density function, which is an important parameter in TFI modelling, was found to exhibit different behaviour between the two flames. The increased influence of turbulent eddies in the preheat zone with increasing Karlovitz number led to differences in terms which govern scalar gradient evolution, including contributions from tangential strain rate, propagation, and curvature. It was also found that the flame was noticeably thinner near the inflow, due to high straining due to mean shear and weaker coupling between turbulence and flame. Comparison of the tangential strain rate term in the SDF transport equation, which accounts for the production of SDF, and the curvature term, which accounts for the destruction of SDF, show that the modelling assumption of a balance between the two terms is less viable for the higher Ka flame.
- Algebraic FSD models for Large-Eddy Simulation (LES) were developed by a novel application of Gene-Expression Programming (GEP), an evolutionary machine learning algorithm. The *a-priori* evaluation of the models showed that GEP is a promising approach for FSD modelling, as the models were comparable or better to models in literature in estimating FSD in the flames analysed in this study. Interestingly, the model trained on the lower Ka flame was able to give good estimates for both flames, but the model trained on the higher Ka flame results in underprediction when estimating the FSD in the lower Ka flame.

6.1 Recommendations for Future Work

In this study, three DNS of turbulent premixed jet flames were performed to provide a better understanding of turbulence-flame interactions and for model development. Despite the useful findings from these datasets, further insight can be obtained by additional simulations. The additional data would also provide a wider variety of training data for

model development with the GEP algorithm. The following is a list of recommendations for future work that the author considers of interest:

- A wide variety of data is a necessary part in data-driven modelling approaches. It is desirable to obtain additional DNS data for turbulent premixed flames under different configurations and flame parameters to cover a larger range on the combustion regime diagram. The characteristics of the mean flow and flame can also be further extended with different flame configurations, such as a counter-flow flame.
- The algebraic FSD models developed in this study were evaluated *a-priori*. Although the models were evaluated for filter sizes and at streamwise locations different from those chosen for the training data, it will be constructive to conduct *a-posteriori* analysis using these models to further evaluate their performance.
- While the FSD models in this study are trained using the independent variables of Δ/δ_z and u'_Δ/S_L , additional variables may be needed to improve the performance of models obtained from GEP. However, introducing additional variables will increase the number of possible solutions that the GEP algorithm can search through, thereby making convergence to an optimal solution more difficult. Therefore, a systematic approach in the selection of the independent variables is essential.

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