

Large Eddy Simulation of Premixed and Stratified Turbulent Combustion

by

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Declaration of Originality

I declare that the work presented in this thesis is the result of my own research and written in my own words except where acknowledged otherwise. Any work by others is referenced appropriately in the text and a list of references is included.

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Abstract

The work presented in this thesis focuses on the modelling of turbulent fully premixed and stratified flames, where stratification refers to the equivalence ratio of the unburned mixture varying in space.

The modelling approach is based on a transported probability density function formulation in the context of Large Eddy Simulation, in conjunction with the fully Eulerian stochastic fields solution method. This method provides detailed statistical information about the flow field and reactive scalars without making assumptions about the combustion regime, maintaining generality.

In the probability density function formulation the chemical reaction rate term appears in closed form and a reduced yet still detailed reaction mechanism is employed to model the methane-air combustion over a range of stratification ratios.

Amendments to the formulation and implementation are proposed. These account properly for the limit case of no sub-grid viscosity, which is important in modelling flames in well resolved and low Reynolds number flow regions as found in the vicinity of flame holders used in many premixed burner configurations.

Two laboratory scale burner configurations are investigated numerically, under various operating conditions and mixture stratification ratios, and results are compared against existing detailed experimental measurements. These configurations are a low Reynolds number slot burner that uses a rod to stabilise a V-shaped flame and a moderate Reynolds number co-annular burner with a central bluff-body to stabilise swirling and non-swirling flames. The equivalence ratio of the mixtures fed in by the slots or annuli were varied to produce different stratification ratios.

Improvements in ability to model low Reynolds number flames and capture stratified flame behaviour are demonstrated. The method is able to predict the flow field as well as the mean and rms values of the reactive scalars to a good degree of accuracy.

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First of all you have to define what that really means, having no results. When you are looking for something and don't find it, that isn't nothing. It means that what you were looking for wasn't there. In other words, it has been disproved. But it doesn't mean that you have found nothing at all. What you have found is that the theory is wrong. It means that you have to set up another theory to explain the phenomenon that the disproved theory had tried to explain. That is a great discovery.

Rolf-Dieter Heuer, Director-General of CERN.

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Nomenclature

Abbreviations

AFT	Artificial Flame Thickening
ARM	Augmented Reduced Mechanism
CFD	Computational Fluid Dynamics
LDA	Laser Doppler Anemometry
LES	Large Eddy Simulation
LIF	Laser-Induced Fluorescence
PDF	Probability Density Function
PIV	Particle Image Velocimetry
PLIF	Planar Laser-Induced Fluorescence
RANS	Reynolds Averaged Navier-Stokes
SFM	Stochastic Field Method
SFR	Swirl Flow Ratio
sgs	sub-grid scale

Greek Upper Case

Δ	characteristic filter width
Λ	integral length scale
Ω	entirety of domain

Greek Lower Case

α	thermal diffusivity
α, β	chemical species
δ_{ij}	Kronecker delta
η	Kolmogorov length scale
η_i^n	dichotomic random vector
λ	thermal conductivity
μ	dynamic viscosity
ν	kinematic viscosity
$\nu'_{\alpha,r}, \nu''_{\alpha,r}$	stoichiometric coefficient of reactants, products
$\dot{\omega}_{\alpha}, \dot{\omega}_{\alpha,r}$	reaction rate of species α , of reaction r
ϕ	scalar variable
ϕ_E	equivalence ratio
ψ	sample space variable
ρ	density
σ	Schmidt number
τ_{ij}	stress tensor
ξ	stochastic field variable

Roman Upper Case

$\mathcal{A}$	advection term
A_α	drift coefficient vector
$B_{\alpha\beta}$	diffusion coefficient matrix
C_d	micro-mixing constant
C_S	Smagorinsky constant
$\mathcal{D}$	diffusion term
D, D_α	diffusivity, of species α
Da	Damköhler number
E	activation energy
$\mathcal{F}$	joint fine-grained probability density function
F	cumulative distribution function
G	Filter function/kernel
J	Joule
$J_{\alpha,i}$	diffusion flux of species α in i -th direction
Ka	Karlovitz number
Le	Lewis number
$\mathcal{M}$	micro-mixing term
M_α	species concentration
N	number of stochastic fields
N_R	number of reactions
N_S	number of chemical species
P	probability density function
Pr	Prandtl number
$\dot{Q}$	rate of external energy input
Q	generic function of ϕ
$\mathcal{R}$	reaction term
R	universal gas constant
Re	Reynolds number
$\mathcal{S}$	stochastic term
S	swirl number
S_L	laminar flame speed
S_{ij}	rate of strain tensor
Sc	Schmidt number
T	temperature
V	volume
$V_{\alpha,i}$	mass diffusion velocity of species α
X_α	mole fraction of species α
Y_α	mass fraction of species α
Z	mixture fraction

Roman Lower Case

a	generic variable
c	progress variable
c_T	progress variable based on temperature
f	test function
f'	fine-grained probability density function

$f_{\alpha,i}$	external force on species α
g	generic function
Δh_{α}^o	enthalpy of formation
h	enthalpy
$k_{f,r}, k_{b,r}$	forward specific rate coefficient, backward
q_r	net reaction rate of reaction r
m	mass
c_p	heat capacity at constant pressure
p	pressure
q_i	i-th component of flux vector
t	time
$\hat{\mathbf{u}}$	sample space variable of $\mathbf{u}$
u_i	velocity component in the i-direction
dW	increment of a Wiener Process
$\mathbf{x}$	spacial coordinate vector

Operators

$-$	spatial filtering
δ	delta function
$\langle \cdot \rangle$	expected value
$\tilde{\cdot}$	Favre filtering/density weighted filtering
∂	partial derivative

Chapter 1

Introduction

Combustion of carbon fuels is the most ubiquitous source of energy consumed world wide. According to the (IEA, 2015) in 2013 91.6% of the worlds total primary energy supply and 78.7% of the final energy consumption (not including 18% electricity of mixed origin) stemmed from carbon-based fuels sources. As such, we are highly dependent on carbon fuels.

The current rate of growth of global demand is estimated at 2% year-on-year and the global outlook shows continued growth at an average rate of 1.5% until 2035 (BP, 2015). At these rates the establishment of alternatives as viable energy sources and the continued improvement of emerging and especially existing technologies is of fundamental importance.

Of particular interest in the context of this thesis is the aviation industry. According to (ATAG, 2015), the aviation industry accounted for 2% of the global CO_2 emissions in 2013. While this figure seems relatively low, on the one hand it is skewed, as most flights are currently taken by residents of wealthier, developed nations (e.g. in 2005 the UK already estimated aviation to account for 6.3% of its CO_2 emissions), on the other hand the aviation sector is amongst the fastest growing of all in terms of greenhouse gas emissions. Further to this, CO_2 alone does not provide a good measure of the aviation industries impact. Other major emissions such as nitrogen oxides NO_x , water vapour H_2O , sulphur oxides SO_x and soot have a large impact on global warming, especially as these emissions are made in the upper troposphere to lower stratosphere.

In terms of passages air traffic is expected to grow to double its 2008 value as soon as 2023 (Rolls-Royce, 2015). This is considered due to ever stronger demand for rapid growth of the industry in large developing nations and sustained growth in developed nations.

In 2012 35% (and increasing) of the total operating costs of airlines was attributed to the cost of fuel. Thus there is a large financial incentive and any savings that can be made through e.g. improvements in fuel efficiency of engines are highly sought after.

Of particular interest for this thesis is the technological challenge of improving aero gas turbines engine efficiency.

Legislation governing pollutant emissions has promoted a development trend away from high temperature stoichiometric combustion towards lean premixed combustion. This mode delivers lower temperatures and complete combustion, resulting in lower emissions of e.g. carbon monoxide and oxides of nitrogen. To date however, the aviation industry has enjoyed lenient regulation due to failure to incorporate it in the Kyoto Protocol and again more recently in the Paris Agreement.

One of the major challenges for aviation is that compared with greener cars the potential for environmentally friendly flying are limited. Technologies designed to reduce the environmental impact of flying are being developed and implemented and there are further gains in engine efficiency to be made e.g. the shift away from non-premixed combustion. However, moving towards hybrid and/or electric alternatives as the automotive industry is currently doing are not feasible in aviation. The energy density of liquid fuels such as Kerosene is around 50MJ/kg while that of a lithium-ion battery ranges around 0.5MJ/kg . Further, typical electric motors have power to weight ratios of 0.6kW/kg (e.g. Toyota Prius 2009 MG2 with 60kW at 104kg).

One of the most advertised ways to curb demand is the large scale production and use of aviation bio-fuels, which are however not without challenge themselves (OECD, 2015). Even with these alternative fuel it would appear as though aviation at the current and future scales cannot be sustained without the use of combustion.

The International Air Transport Association has set out three ambitious targets for aircraft designers to tackle: 1.5% average annual fuel efficiency improvement

between 2010 and 2020, Carbon neutral growth from 2020 and a reduction in net emissions of 50% by 2050 compared to 2005 levels

In the aeronautics industry computational fluid dynamics (CFD) is becoming increasingly more important in research and development and is being relied on to investigate methods to reduce the quantity of pollutants emitted by aircraft engines, their noise emissions and the quantity of fuel they consume. To achieve this ambitious goal, finer and more complex models are required, in particular to simulate combustion chamber performance with greater precision. This is in part made feasible due to the proliferation of powerful and simultaneously cheaper computing resources.

While this thesis is presented primarily in the context of aviation, the above is relevant on a much larger scale also: combustion processes are responsible for more than 90% of the worlds energy. Although this is decreasing and renewable sources are becoming more mainstream, it is on the order of decades that the dependency on energy from combustion will significantly reduce.

For the work presented in this thesis, Large-Eddy Simulation, the transported probability density function and stochastic field solution method were used; some of the most power full tools at our disposal for combustion modelling in order to further investigate and validate them in the context of application to premixed and stratified combustion. The goal is to demonstrate the applied methods capabilities, but also that a subject as well studied as combustion and the pdf method are not fully matured and incremental improvement are still being made.

1.1 Premixed and Stratified Combustion

Lean premixed combustion is widely used in combustion technologies as it can deliver very low pollutant emissions at high efficiencies. Lower temperatures and complete combustion result in low emissions of oxides of nitrogen and unburned hydrocarbons, as illustrated in Figure 1.1 for internal combustion engines. However, this mode of combustion is prone to, for example instabilities, extinction and flash-back. Furthermore, with the long term goal of burning liquid fuels at the emissions levels of

natural gas, as is potentially the case with kerosene in aviation, this is further complicated by the need to pre-vaporise the fuel and mix it with the oxidiser upstream of the flame front.

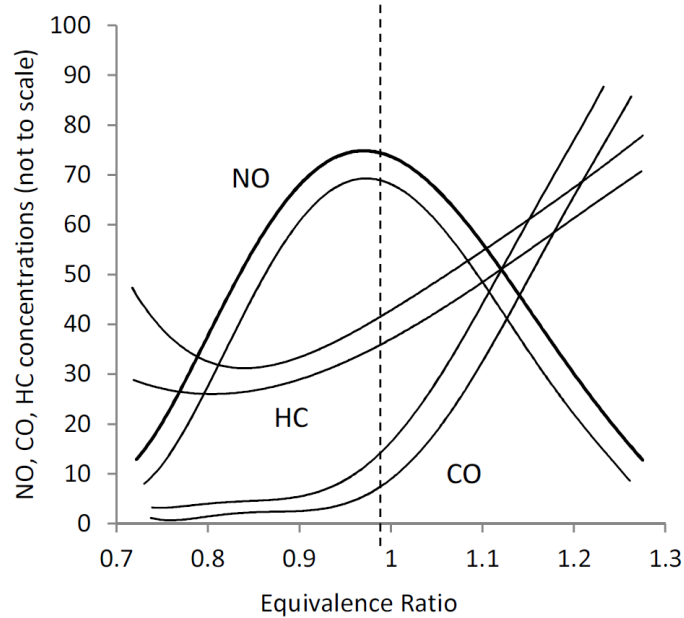


Figure 1.1: Variation of concentrations with equivalence ratio. Pollutant emissions against equivalence ratio for spark ignition engines (Heywood, 1988).

The constraints of many practical combustion applications, in particular the design of Lean Premixed Pre-vaporised combustors, can lead to an inhomogeneous mixture of fuel and oxidiser resulting in combustion taking place under partially premixed conditions (Charest, 2005). In general, this mode of combustion can include both premixed and non-premixed modes, while in its basic form it only includes premixed combustion where the equivalence ratio of the mixture exhibits spatial gradients. Thus, in most premixed burners the flame will encounter stratification as the dilution of combustible mixture with co-flowing air creates stratified conditions. Stratified combustion is commonly categorised as either “back-” or “front-supported” combustion depending on the angle between constant lines of the gradients of the reaction progress variable and gradients of the mixtures equivalence ratio. Back-supported combustion generally takes place when a flame burns from a higher towards a lower equivalence ratio. The fundamental properties of stratified combustion remain relatively poorly characterised and understood compared to other combustion regimes,

(Sweeney, 2011).

Figure 1.2 shows instantaneous (left) and mean (right) contour lines of progress variable c (blue) and equivalence ratio ϕ_E (red) on a plane containing the centreline for the stratified swirl burner discussed in Chapter 6. When the gradients of c and ϕ_E are aligned stratification is at its maximum with the flame propagating across different equivalence ratios. According to (Masri, 2015) “back-supported” stratification takes place when excess heat and radicals produced in the reaction zone feed a mixture of different equivalence ratio ahead of the flame, as is the case when burning takes place from stoichiometric to lean. In rich mixtures, as in Figure 1.2 with $\phi_{E,inner} = 1.12$, the flame propagates from rich to stoichiometric, “back-supported” burning may still exist, not due to temperature which increases, but to the diffusion of reactive species from the rich side alone. Conversely, when the flame propagates from stoichiometric to rich, “back-supported” burning may again still exist due to the excess heat.

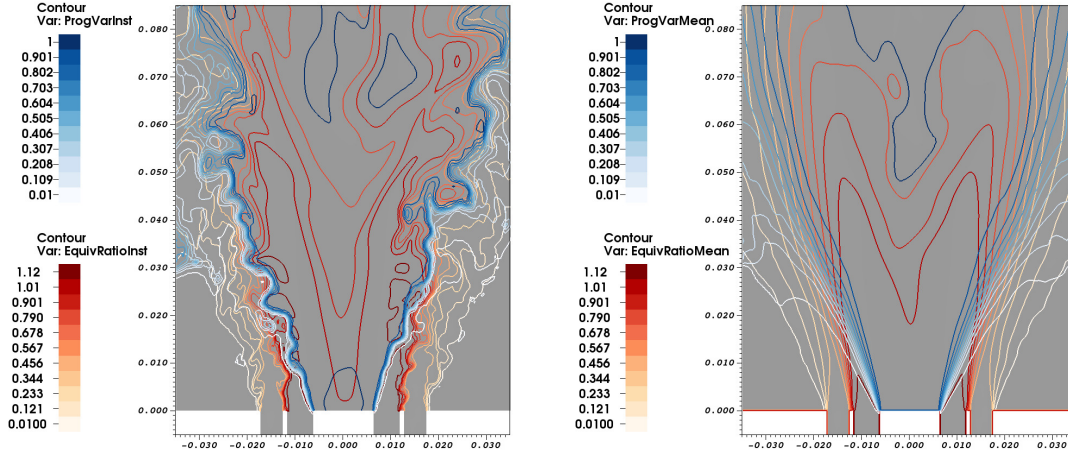


Figure 1.2: Contours of constant lines of c and ϕ_E . Instantaneous on the left, mean on the right

Findings from studies on stratified combustion have shown deviations from homogeneous systems with increased lean flammability limits, increased variations in burning velocity, higher flame propagation rates along with increased flame wrinkling and flame thinning.

The recent work by (Masri, 2015) provides a detailed summary and extensive review of both experimental and numerical work performed by various research groups

on partially premixed and stratified combustion. For the purpose of this work the focus will be solely on stratified combustion. Previous experimental studies of stratification have been conducted by a number of workers, (Manickam et al., 2010), (Sweeney et al., 2011a), (Sweeney et al., 2012a), (Seffrin et al., 2010) on a variety of experimental configurations including rod-, swirl- and bluff-body stabilised flames. These studies show deviations from homogeneous premixed combustion, reporting that stratification can increase the lean flammability limits in comparison to fully premixed combustion. This is reported in particular for back supported flames and the effect is attributed to the diffusion of heat and/or radicals from the richer region into the leaner region. The degree of stratification, or the ratio of richer to leaner equivalence ratio, is reported also to increase the flammability limit by the same mechanism.

As well as increasing the variation of burning velocity, leading to increased flame wrinkling, stratification can also lead to an increase in the flame propagation rate, further supporting the reported increase in lean flammability limit.

In V-flames stratification is observed to cause flame thinning, again due to the variation in burning velocity causing stretching and an increase in flame surface density, (Barlow et al., 2009).

Numerical studies have been conducted amongst others by e.g. (Bell et al., 2005), (Manickam et al., 2010), (Wu et al., 2011), (Nambully et al., 2014a) and (Proch&Kempf, 2014), and will be reviewed in more depth in Chapter 2.

1.2 Bluff Body and Swirling Flows

A bluff body is an object placed inside a flow field, be it by design or not, that induces a disturbance to the flow in its vicinity and down stream region. The cause of the disturbance are pressure gradients acting opposed to the flow, which results in a deceleration or even a reversal of the flow downstream of the body, thus causing the formation of a recirculation zone.

This type of flow has been studied extensively for non-reacting flows both experimentally and numerically e.g. (Zdravkovich, 1997). Typically, in non-reacting

bluff body flows the down stream regions exhibit different behaviours depending on the Reynolds number: laminar without flow detachment, laminar with bound vortices/recirculation zone attached to the trailing edge of the body, laminar to turbulent with vortex shedding behind the body and turbulent with a fully turbulent wake.

In most combustion devices the flow velocity is significantly higher than the flame speed and the temperature of the inflow/reactants is significantly lower than the auto-ignition temperature. Bluff bodies and swirl are used to hold/stabilise the flame. The flame is initiated and sustained in the free shear layer which starts from the separation points or edges of the bluff body. The flame generally stabilizes a short distance downstream of the bluff body due to ignition delay. Additionally the bluff body creates a recirculation zone that provides the fresh mixture with high temperature products and radicals, the mixing of which can be enhanced by the shear layer.

The stability of the flame is dominated by the incoming velocity and the mixture equivalence ratio. The Damköhler number can be seen as a measure of stability as it compares the characteristic time scale of a flow to that of the chemistry. Taking the ignition delay time as the chemistry time scale and the reactants residence time near the hot products as the flow time scale, it is evident that for sustained combustion the residence time must be long enough for combustion to take place. Volumetric expansions from heat release helps increase the length of the recirculation zone, leading to longer residence time, while higher inlet velocities lead to lower residence times. The equivalence ratio can affect the stability as it is linked directly to the highest flame temperature; equivalence ratios close to 1 result in high temperatures i.e. faster reactions and thus longer residence time, while lower temperatures result in larger chemical times compared to residence time (Poufflet, 2006).

Flame extinction can occur when the fresh reactants do not spend sufficient time in the shear layer to allow ignition to take place or when the rate of heat release from the combustion zone is insufficient to raise the temperature of the unburned gases to the auto-ignition temperature. Flame blowout can occur when unburned mixture penetrates the flame front and disrupts the recirculation zone and its supply

of hot products.

In many premixed burner configurations, such as the two under investigation in this work, the effect of the bluff body is used to stabilise the flame. The slot burner uses a rod/wire placed above and across the burner exit. For the swirl burner a closed tube with a ceramic cap on the end is placed centrally inside two co-annular pipes, where trailing edge acts as a bluff body at the burner exit. The wake of the bluff body together with the swirling flow are used to stabilise the flame.

Combustion and the presents of hot reaction products change the dynamics of the flow in the wake of a bluff body significantly compared to an isothermal flow. Across a premixed flame the viscosity rises sharply from the unburned to the burnt side, for methane-air combustion typically by a factor of around 3. Furthermore, at the same time the density decreases, for methane-air typically by a factor of 10, and the working fluid expands. The increase in viscosity can dampen the turbulent wake and suppress vortex shedding otherwise observed in non-reacting flows.

Swirl adds additional complexity and benefits to the flow. Swirling flows are used in many practical combustion devices to stabilise the flame and enhance mixing. In lean premixed technology high degrees of swirl are applied for stabilisation and achieving compact flames with high power density and good burnout (Benim&Syed, 2014). The strength of swirl is usually characterized by a swirl number S , which is defined as the ratio tangential momentum to axial momentum of the axial flow.

A critical swirl number can be defined, typically $0.4 < S_c < 1$ depending on the application, above which Vortex Breakdown can occur. This sees the vortex swell in size and form a stagnation point on the axis of rotation downstream of which flow reversal occurs. The recirculation zone formed enhances mixing and acts as an aerodynamic flame holder. Generally it is said that Vortex Breakdown occurs when the swirl number transitions from below the critical value to above it.

A region of low pressure is generated at the centre of the swirling flow as a result of centrifugal forces acting on the flow. The low pressure persists as further swirling flow is supplied by the swirl generator resulting in an adverse axial pressure gradient. At high strengths of swirl, the fluid momentum cannot overcome the pressure gradient, leading to vortex breakdown and the reversal of flow along the axis of rotation

of the swirl. Heat release additionally increases the acceleration of the flow, causing stronger recirculation and steeper velocity gradients at the shear layer (Bulat, 2012). Swirl and Vortex Breakdown can influence the flow in a similar way to an aerodynamic blockage. Thus, a flame can be stabilised without the use of a centerbody / bluff body. The Cambridge Stratified Swirl burner however does include a bluff body which extends through the axis of rotation. In this case the recirculation in the wake of the bluff body merges with the recirculation created by the swirling flow.

1.3 Computational Fluid Dynamics

With Computation Fluid Dynamics (CFD) one can to a certain degree predict the behaviour of a fluid, for example in a combustion system, and gain insight into the thermo-chemical processes taking place, that experiments cannot deliver. In particular Large Eddy Simulation is now a feasible tool for such investigations, thanks to the steady increase of computational power, forming the middle ground between affordable low detail Reynolds Averaged Navier Stokes and supercomputing very high detail Direct Numerical Simulations.

1.4 Objectives and Thesis Overview

The thesis has the following structure: Chapter 2 will cover fundamentals of Large Eddy Simulation (LES), governing equations, filtering and turbulence modelling followed by discussion of application to turbulent reacting flows and a review of existing LES models for premixed and stratified combustion. In Chapter 3 the transported probability density function (PDF) approach will be introduced along with a discussion of solution methods focussing predominantly on the Eulerian Stochastic Fields method. Chapter 4 covers some aspects of the numerical implementation with a focus on the interaction of the stochastic and the micro-mixing terms. A reformulation of the PDF equation and adjustment to the stochastic field solution algorithm to ensure correct behaviour in the absence of turbulence are proposed and discussed. In

Chapters 5 and 6 two burners that can be operated under both fully-premixed and stratified conditions are investigated numerically. Results for 3 flames of the Cambridge Stratified Slot Burner, a rod-stabilised low turbulence device, are presented in Chapter 5. The Cambridge Stratified Swirl Burner, a bluff-body-stabilised moderate turbulence device, is presented in Chapter 6, with results for 3 non-swirling and 3 swirling cases. The Appendixes contain some additional details on the derivation of the PDF equation and the stochastic field method.

Chapter 2

Large Eddy Simulation of Turbulent Reacting Flows

In large eddy simulation (LES) the large scale energetic structures of the flow are resolved while the small scale structures, commonly referred to as sub-grid scale (sgs) structures are modelled. The separation of scales is achieved by spatial filtering. Typically the LES filter width is on the order of $1mm$, while the flame thickness of a turbulent premixed flame is on the order of $0.1mm$. Thus even in a high fidelity LES combustion takes place predominantly on the sub-grid level and requires modelling. In this chapter the governing equations required to describe a reacting flow are presented, the concept of spacial filtering is discussed and some LES combustion models are introduced.

2.1 General Governing Equations

The incompressible conservation equations for mass and momentum for variable density flows can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (2.1.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} \quad (2.1.2)$$

Where the gravity/body force term has been omitted, p is the pressure and τ_{ji} is the stress tensor defined as:

$$\tau_{ji} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (2.1.3)$$

The fluid is assumed to be Newtonian (Stokes hypothesis for bulk viscosity) and μ is the kinematic viscosity and δ_{ij} the Kronecker delta, indicating the isotropic part is absorbed into the pressure term.

The enthalpy, h , defining the energetic state of the mixture, is here defined as the sum of sensible and chemical enthalpy.

$$h = \int_{T_o}^T c_P dT + \sum_{\alpha=1}^{N_s} \Delta h_{\alpha}^o Y_{\alpha} \quad (2.1.4)$$

c_P is the average heat capacity of the mixture, Δh_{α}^o is the enthalpy of formation, Y_{α} is the species mass fraction and N_s is the number of species considered to be making up the mixture. The non-linear integral term in Equation 2.1.4 is commonly approximated by JANAF polynomials (Chase, 1998).

The conservation equations for enthalpy can be written as e.g. (Kuo&Acharya, 2012):

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{Dp}{Dt} - \frac{\partial q_i}{\partial x_i} + \tau_{ji} \frac{\partial u_j}{\partial x_i} + \dot{Q} + \rho \sum_{\alpha=1}^{N_s} Y_{\alpha} f_{\alpha,i} V_{\alpha,i} \quad (2.1.5)$$

Where D/Dt is the substantial derivative, $\dot{Q}$ rate of external energy input and the final term is the body force work on each species α . q_i is the i-th component of the flux vector defined as:

$$q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{\alpha=1}^{N_s} h_{\alpha} Y_{\alpha} V_{\alpha,i} (+ q_{Dufour}) \quad (2.1.6)$$

Where λ is the thermal conductivity and the second term the interdiffusion term. The final term q_{Dufour} , the energy flux due to a mass concentration gradient, is generally neglected as it is small compared to the other terms.

A common assumption made in incompressible turbulent combustion modelling is

that the Lewis number, defined as ratio of Schmidt number to Prandtl number, $Le \equiv Sc/Pr = 1$. The Schmidt number is defined as the ratio of momentum to scalar diffusivity, $Sc \equiv \sigma = \nu/D = \mu/\rho D$. The Prandtl number is defined as the ratio of momentum to thermal diffusivity, $Pr \equiv \nu/\alpha = c_P \mu/\lambda$ with α , here the thermal diffusivity, $\alpha = \lambda/\rho c_P$. With $Le = 1$, assuming a low Mach number, which cancels the surface stress and pressure terms, omitting body forces and using Fick's law for diffusion fluxes it can be show (Appendix A.1) that the enthalpy equation reduces to:

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu}{Pr} \frac{\partial h}{\partial x_i} \right) + \dot{Q} \quad (2.1.7)$$

The conservation equation for each reacting species α can be written as:

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_i Y_\alpha}{\partial x_i} = -\frac{\partial J_{\alpha,i}}{\partial x_i} + \rho \dot{\omega}_\alpha \quad (2.1.8)$$

The diffusion flux term $J_{\alpha,i}$ is treated similarly to the the flux term in Equation 2.1.5 and is modelled using Fick's law for the diffusion fluxes while neglecting the Soret effect (the mass diffusion flux due to temperature gradients) and assuming a low Mach number thus cancelling the pressure term, resulting in:

$$J_{\alpha,i} = -\rho D_\alpha \frac{\partial Y_\alpha}{\partial x_i} \quad (2.1.9)$$

Where D_α is the diffusion coefficient of species α into the rest of the mixture. Another commonly made assumption, specifically in turbulent/moderate to high Reynolds number combustion modelling, is that the diffusion coefficients are equal for all species. Thus both the enthalpy and the species transport equations can be formulated in terms of a general reactive scalar $\phi = [\phi_1, \dots, \phi_{N_s}, h]$:

$$\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_i \phi_\alpha}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \right) + \rho \dot{\omega}_\alpha \quad (2.1.10)$$

Different values of σ have been used in literature, however most commonly it is assumed to be $\sigma = 0.7$. Additional constitutive relation ships for the viscosity and the density are required to close the Navier-Stokes equations. Formulas for viscosity can be found in e.g. (Bird et al., 2006) and the ideal gas law for single species and

mixtures, at low to moderate pressures (Kuo&Acharya, 2012) is:

$$pV = mRT \quad (2.1.11)$$

2.2 Spatial Filtering

The present work is performed in the context of LES and spatial filtering of a variable is commonly defined as (John, 2003):

$$\bar{\phi}(\mathbf{x}, t) = \int_{\Omega} \phi(\mathbf{x}', t) G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) d\mathbf{x}' \quad (2.2.1)$$

Where $\phi(\mathbf{x}', t)$ is an instantaneous flow variable and G is a filter kernel. This kernel depends on the filter width $\Delta(\mathbf{x})$, which is here chosen to be linked to the local mesh spacing $\Delta \approx (\Delta_x \Delta_y \Delta_z)^{1/3}$. The box or “top-hat” filter is used and is defined as:

$$G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) = \begin{cases} 1/\Delta^3 & \text{if } |\mathbf{x} - \mathbf{x}'| < \Delta/2. \\ 0 & \text{otherwise.} \end{cases} \quad (2.2.2)$$

Which denotes the average within the local control volume.

A variety of different filter kernels exist and an in depth discussion of filtering in the LES context and analysis of various filter functions can be found in e.g. (Sagaut, 2006). In LES the equations are generally only filtered implicitly i.e. the computational mesh is assumed to be the filter and when the filter width is required for computation, it is taken to be the cubed root of the local mesh volume. (Generally no distinction is made between the terms “sub-filter” and “sub-grid”, although they are technically not the same). Filtering will not be discussed beyond the properties required for the LES-PDF method, as no explicit filtering of the equations is performed during the computations.

The filtering operation is required to have the following properties (Jaberi et al., 1999):

- normalisation: $\int_{-\infty}^{\infty} G(\mathbf{x}) d\mathbf{x} = 1$
- commutation of filtering and spatial differentiation: $\overline{\frac{\partial \phi}{\partial x_i}} = \frac{\partial \bar{\phi}}{\partial x_i}$
- positive definite filter function for which moments, with $m > 0$, $\int_{-\infty}^{\infty} \mathbf{x}^m G(\mathbf{x}) d\mathbf{x}$ exist.
- compact support

From the normalisation property and the choice of “top-hat” filter, which is a positive function, it follows that G defines a pdf. Property two is treated as an assumption and is generally not true, as the filter width is a function of space. This introduces a commutation error, the effect of which has been investigated by e.g. (Ghosal&Moin, 1995) and shown to be negligible compared to the effect of the closures introduced for unknowns as a consequence of filtering. (Restrictions on the computational mesh growth rates and aspect ratios can help minimise the error.) The third property is a requirement for pdf methods; a pdf and a positive definite filter kernel G have the same properties in the sense of distributions. (This rules out the use of a spectral filter in this context.)

For variable density flows density weighted filtering, called Favre filtering, is used and defined as:

$$\tilde{\phi}(\mathbf{x}, t) = \frac{\overline{\rho(\mathbf{x}, t) \phi(\mathbf{x}, t)}}{\bar{\rho}(\mathbf{x}, t)} = \frac{1}{\bar{\rho}(\mathbf{x}, t)} \int_{\Omega} \rho(\mathbf{x}', t) \phi(\mathbf{x}', t) G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) d\mathbf{x}' \quad (2.2.3)$$

2.3 Filtered Governing Equations

Using density weighted Favre filtering to account for the variation of density as a consequence of combustion, the continuity, momentum and general reactive scalar transport equations become:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0 \quad (2.3.1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \bar{\mu} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right) - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} \quad (2.3.2)$$

$$\frac{\partial \bar{\rho} \tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\bar{\rho} D \frac{\partial \tilde{\phi}_\alpha}{\partial x_j} \right) + \overline{\rho \dot{\omega}_\alpha(\phi_\alpha, T)} - \frac{\partial J_{\alpha, j}^{sgs}}{\partial x_j} \quad (2.3.3)$$

Where $\bar{\rho}$ is the filtered density, p the pressure, τ_{ij}^{sgs} the sub-grid stress, $\bar{\mu}$ the filtered viscosity and δ the Kronecker delta. The sub-grid scale (sgs) stress, $\tau_{ij}^{sgs} = \bar{\rho}(\widetilde{u_i u_j} - \widetilde{u_i} \widetilde{u_j})$. In Equation 2.3.3 D is the diffusion coefficient and $J_{\alpha,j}^{sgs} = \bar{\rho}(\widetilde{u_j \phi_\alpha} - \widetilde{u_j} \widetilde{\phi_\alpha})$ is the sub-grid scalar flux. Quantities $\bar{\rho}$, $\bar{\mu}$ and $\bar{\omega}$ are filtered regularly while others which are functions of space are filtered with the density weighted filter.

Equation 2.3.2 requires a closure for the unknown sub-grid stress term, while Equation 2.3.3 contains two unknown terms which require closure; the sub-grid scalar flux J^{sgs} and the filtered net formation rate.

In the present work equation (2.3.3) is not solved directly. This is due to the difficulty in attempting to close the reaction rate term which includes $\bar{\omega}$. Instead it can be used to derive a transport equation for the joint pdf of the species concentration and enthalpy needed to describe a reaction.

2.3.1 Sub-Grid Stress Term

The sub-grid scale stresses τ_{ij}^{sgs} in Equation 2.3.2 (specifically the anisotropic part) are modelled using the Smagorinsky-Lilly model (Smagorinsky, 1963), (Lilly, 1967), which can be dynamically calibrated following (Germano et al., 1991) and (Piomelli&Liu, 1995).

Without going into much detail, the sgs-stress term is modelled under the assumption that its contribution is small, as the large energetic scales are resolved, and that the effect of the small scales is to dissipate energy, specifically turbulent kinetic energy. It is therefore assumed to remove energy from the large sales and is generally modelled in a diffusion-like manner, where a sub-grid viscosity is related to the sub-grid stress by:

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = 2\rho C_S \Delta^2 ||\tilde{S}_{ij}|| \tilde{S}_{ij} \quad (2.3.4)$$

$$= 2\mu_{sgs} \tilde{S}_{ij} \quad (2.3.5)$$

Where C_S is a model parameter (Smagorinsky coefficient), $\tilde{S}_{ij} = \frac{1}{2}(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i})$ is the large scale rate of strain tensor and μ_{sgs} is the sub-grid viscosity. $||\tilde{S}_{ij}||_F = (\sum_i^m \sum_j^n |s_{ij}|^2)^{\frac{1}{2}}$ is the Forbenius norm of the strain tensor (Weisstein, a). Orig-

nally C_S was proposed as a constant, however this can produce unsatisfactory results for flows that exhibit many different flow regimes e.g. using the same C_S for the free stream as well as in the near boundary flow. The dynamic determination of the coefficient C_S is based on the assumption that C_S can be determined locally (i.e. $C_S = C_S(\mathbf{x}, t)$) and that the information provided by the resolved scales is sufficient to infer a model for the sub-grid scales. Additionally it is assumed that the coefficient is scale invariant. A comparison can then be made between filtered quantities at the grid level (conventional filtering) and filtered quantities at a second, explicitly filtered, test filter level generally chosen to be twice the filter width. The relationship between the two can then be used to calibrate the local Smagorinsky coefficient, allowing for improved prediction of the turbulence statistics as well as improved model behaviour in quiescent flow and wall proximity (Piomelli&Liu, 1995). The procedure is prone to producing extreme values and is thus generally clipped.

2.4 Chemical Reaction Modelling

Combustion is an exothermic process that convert chemical energy stored in a fuel source into heat by chemical reaction with an oxidiser. Its popularity/ubiquity is in part due to the energy density of carbon fuels, which is on the order of $50MJ/kg$ compared to e.g. $0.5MJ/kg$ for a typical battery. For even the shortest of organic fuels, methane CH_4 , reacting with standard atmospheric air, the detailed reaction mechanism becomes large and complex; the GRI-Mech 3.0 contains 53 species and 325 reaction steps (Smith et al.). Chemical reactions depend predominantly on the species concentrations and the temperature (although they can also be influenced by other conditions e.g. pressure or radiation). For a system of m reactions a stoichiometric relation describing the reactions can be expressed as (Glassmann&Yetter, 2010):

$$\sum_{\alpha=1}^{N_s} \nu'_{\alpha,r}(M_\alpha) \rightleftharpoons \sum_{\alpha=1}^{N_s} \nu''_{\alpha,r}(M_\alpha), \quad r = 1, \dots, N_R \quad (2.4.1)$$

Where $\nu'_{\alpha,r}$ and $\nu''_{\alpha,r}$ are the stoichiometric coefficients of the reactants and the products respectively, N_s is the total number of species, N_R is the number of reactions of the mechanism and M_α are the species concentrations. The net reaction rate for each of the r reactions is defined as:

$$q_r = k_{f,r} \prod_{\alpha=1}^{N_s} (M_\alpha)^{\nu'_{\alpha,r}} - k_{b,r} \prod_{\alpha=1}^{N_s} (M_\alpha)^{\nu''_{\alpha,r}} \quad (2.4.2)$$

Where $k_{f,r}$ and $k_{b,r}$ are the specific rate coefficients for the forward and backward reactions of each of the r reactions respectively. The rate of change of each species α due to each of the r reactions is then given by:

$$\dot{\omega}_{\alpha,r} = (\nu''_{\alpha,r} - \nu'_{\alpha,r}) q_r = \nu_{\alpha,r} q_r \quad (2.4.3)$$

Finally, the equation for the net formation rate $\dot{\omega}_\alpha$, present in the transport equations of each of the α species described by the reaction mechanism, e.g. Equation 2.1.8, can be expressed as:

$$\dot{\omega}_\alpha = \sum_{r=1}^R \nu_{\alpha,r} q_r \quad (2.4.4)$$

The above equations show the dependency on the species concentrations through M_α , the dependency on temperature enters the equations through the rate coefficients k which are determined the Arrhenius rate expression:

$$k = A e^{(-E/RT)} \quad (2.4.5)$$

Where A is the so called pre-exponential factor that takes into account the collision frequency and the likelihood of a reaction taking place. E is the activation energy, R is the universal gas constant and T the temperature. A can be determined experimentally or mathematically from kinetic theory.

According to (Glassmann&Yetter, 2010) the lean flammability limit of methane in air is 5% by volume or an equivalence ration of $\phi_E = 0.5$ and the rich limit is 15% or an equivalence ratio of $\phi_E = 1.7$.

2.4.1 Equivalence Ratio and Progress Variable

Describing the evolution of various quantities within a flame is often done working in terms of a progress variable c . The progress variable is defined such that it is zero in unburned reactants $c_u = 0$ and has a value of unity in the burned products $c_b = 1$. Different measures of progress variable can be defined, the most frequently employed normalizations using temperature or chemical species concentration to define c .

The thermal progress variable $c(T)$ is often used in experimental literature. As pointed out by (Sweeney et al., 2012b) $c(T)$ is strictly only valid in adiabatic, incompressible flows with near-unity Lewis number. Care must also be taken when comparing progress variables based on different scalar quantities, as their result can be markedly different. For the present work a modified form of a temperature defined progress variable is used which allows it to be applied to stratified flames. Using the same definition employed by (Sweeney et al., 2012b), which yields similar values to those calculated using the scaled Bilger mixture fraction Z :

$$\phi_E = \frac{X_{CO_2} + 2X_{CH_4} + X_{CO} + 0.5(X_{H_2O} + X_{H_2})}{X_{CO_2} + X_{O_2} + 0.5(X_{CO} + X_{H_2O})} \quad (2.4.6)$$

Where X is the mole fraction of the corresponding species.

In order to use a temperature defined progress variable in the context of stratified flames, the adiabatic flame temperature T_a used in the calculation must be allowed to vary with local equivalence ratio:

$$c_T(\mathbf{x}, \phi_E) = \frac{T(\mathbf{x}) - T_u}{T_a(\phi_E(\mathbf{x})) - T_u} \quad (2.4.7)$$

Where $T(\mathbf{x})$ is the temperature at $\mathbf{x}$ and is T_u is the unburned temperature. Values of $T_a(\phi_E)$ were obtained for a range of equivalence ratios using software provided by (CERFACS) based on GRI-Mech3.0 (Smith et al.). For the purpose of post-processing the values have been fit with a polynomial with a maximum deviation of less than $\pm 1\%$ over the range of $\phi_E = [0.35, 1.16]$ (see Appendix A.2)

2.5 Premixed Flame Structure and Characteristics

The structure of premixed flames is said to be made up of three zones: the preheat zone, the inner layer and the oxidation layer. Figure 2.1 is taken from a flame of the Cambridge Stratified Slot Burner discussed in Chapter 5 and shows approximate locations of these zones from left to right, separated by dashed lines. The flame propagates towards and heats up the mixture in the preheat zone in front of it, by conduction and radiation. This zone is still considered to be chemically inert, i.e. chemical reaction and heat release are negligible. The preheat zone is followed by the inner layer in which the fuel is consumed and most of the heat release takes place; there is a steep change in temperature and density across and also in the close proximity of it. This layer keeps the process going and also determines the rate of combustion along with the coefficients of diffusion. The third zone is the oxidation layer in which the oxidation of radicals formed in the inner layer is completed. The level of interaction of turbulence with the inner layer, i.e. the relation of smallest turbulent length and time scales to those of the inner layer determine the regime of premixed combustion. These regimes will be discussed in Section 2.5.2.

2.5.1 Parameters

In order to discuss these regimes and some of the combustion model assumptions in the following sections it is useful to define relevant non-dimensional numbers and characteristics which are frequently used.

Kolmogorov Scales

Kolmogorov scales are the smallest scale in turbulence at which viscous effects are dominant and the inertial energy of the smallest eddies is dissipated completely, which would imply a local Reynolds number of 1. The length scale, η , and the time scale, τ , which are used in categorising combustion regimes, were arrived at through dimensional analysis and are defined only in terms of kinematic viscosity, ν , and

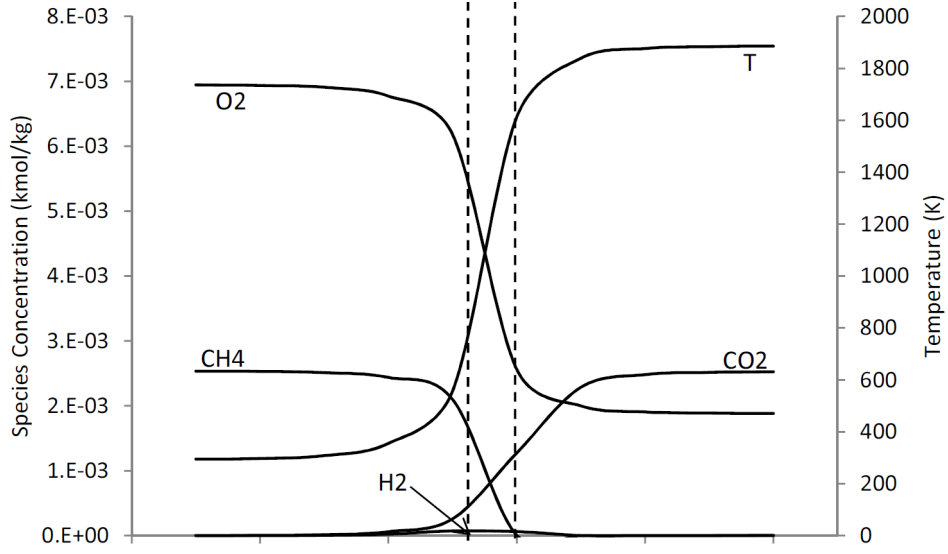


Figure 2.1: Instantaneous flame structure if a premixed methane-air flame. Example species concentrations and temperature through a low Reynolds number premixed methane-air flame taken from a V-Flame simulation.

turbulent kinetic energy dissipation rate, ε . They are as follows:

$$\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{1/4}, \quad \tau = \left(\frac{\nu}{\varepsilon} \right)^{1/2} \quad (2.5.1)$$

Integral length scale

The Integral length scale refers to the large scale eddies containing the most energy. This quantity is established from a two-point velocity correlation. An estimate can also be derived from observed characteristic length, time and velocity scales linked to the r.m.s. turbulence intensity and be shown to be:

$$l_0 \cong \frac{k^{2/3}}{\varepsilon} \quad (2.5.2)$$

Taylor micro-scale

The Taylor micro-scales fall in the region between the Kolmogorov and Integral length scales. Eddies of this scale pass kinetic energy down to the smallest scales. One interpretation of this length scale is that it represents the largest scale at which viscosity significantly affects the dynamics of turbulent eddies. The general defini-

tion is used as a measure of the size of eddies in the inertial sub range and in LES as a guide line for filter size:

$$\lambda = \left(\frac{10vk}{\varepsilon} \right)^{1/2} \quad (2.5.3)$$

Reynolds number

The Reynolds, Re , number is defined as the ratio of inertia forces to viscous forces and is generally used as an indicator of whether a flow is laminar or turbulent.

$$Re = \frac{\rho UL}{\mu} \quad (2.5.4)$$

Where U and L are a characteristic velocity and length scale, respectively. A turbulent Reynolds number can also be defined as:

$$Re_t = \frac{v_t l_t}{\nu} \quad (2.5.5)$$

Where v_t and l_t are the velocity fluctuation and a turbulent length scale. Thus Re_t is the ratio of the turbulent (eddy) viscosity and molecular viscosity. Additionally, in the context of premixed turbulent combustion (Peters, 2000) defines Re_t as the ratio of turbulent eddy viscosity to the characteristic flame thickness l_F and flame time t_F :

$$Re_t = \frac{v' l_t}{s_L l_F} \quad (2.5.6)$$

Where v' is the turbulent intensity and l the integral length scale. Here σ , Pr and Le have been assumed to be unity by (Peters, 2000), which is not always the case.

Damköhler number

The Damköhler number, Da , has several definitions, however in turbulent combustion it is a measure that compares characteristic time scales of turbulence (integral time scale), τ , and chemistry, τ_c . An alternate expression for Da can be found using the correlations $\tau = l_t/v'$, i.e. integral length scale and velocity fluctuation, and

$\tau_c = l_F/s_L$ i.e. flame thickness and laminar flame speed:

$$Da = \frac{\tau}{\tau_c} = \frac{l_t l_F}{v' s_L} \quad (2.5.7)$$

Thus Da can be understood as a measure of whether combustion is diffusion or chemistry controlled. Alternatively, τ can be defined in terms of LES i.e. the filter width Δ as length scale and the sub-grid velocity fluctuation u'_Δ

Karlovitz number

The Karlovitz number, Ka , is also a ratio of time scales, however of the Kolmogorov time scale to the chemical time scale and is a measure of the flow and chemistry interaction of the smallest turbulent scales. It is thus the same as the inverse Damköhler number using the Kolmogorov rather than the integral time scale, describing chemistry/turbulence interaction taking place at the smallest scales. Ka can be expressed in several ways (Peters, 2000):

$$Ka = \frac{\tau_c}{\tau_\eta} = \frac{l_F^2}{\eta^2} = \frac{v_\eta^2}{s_L^2} \quad (2.5.8)$$

Ka may also be expressed in terms relating it to the reaction zone thickness, l_δ , where at atmospheric pressure $l_\delta \cong 0.1 l_F$ and:

$$Ka_\delta = \delta^2 Ka \quad (2.5.9)$$

The significance of Ka and its application to categorising flame regimes will be discussed in the following section.

Schmidt and Prandtl numbers

The Schmidt number, σ , and the Prandtl number, Pr , are ratios of diffusivity; the Schmidt number of momentum diffusivity, given by the kinematic viscosity, $\nu = \mu/\rho$, to mass diffusivity, D , and the Prandtl number to thermal diffusivity $\alpha = \lambda/\rho c_P$:

$$\sigma = \frac{\nu}{D}, \quad Pr = \frac{\nu}{\alpha} \quad (2.5.10)$$

A low Prandtl number, $Pr < 1$, signifies that conductive transport dominates over convective transport, and vice versa for high Pr .

Lewis number

Le is the Lewis number and is defined as the ratio of thermal to mass diffusivity and thus can also be expressed in terms of the Schmidt and Prandtl numbers:

$$Le = \frac{\alpha}{D} = \frac{\sigma}{Pr} \quad (2.5.11)$$

2.5.2 Premixed Regimes

Premixed combustion is generally categorised as one of four regimes: wrinkled flamelet, corrugated flamelet, thin reaction and broken reaction, as seen in 2.2. It should be noted that in practice most flames generally stretch across multiple regimes. The diagram is typically known as a Borghi diagram where the ratio of velocity fluctuation to laminar flame speed is plotted over the ratio of integral length scale to laminar flame thickness, as y and x coordinates respectively. The lines of significance, which separate combustion regimes, are $Re_t = 1$, $Ka = 1$ and $Ka_\delta = 1$. Also of interest are the lines where $v'/s_L = 1$, $Da = 1$ and $Da \gg 1$.

It should be noted that in the context of LES an alternative diagram could be used with the filter width as a length scale and the sub-grid velocity fluctuations instead of just v' , see e.g. (Pitsch, 2006).

Laminar

The region under the line $Re_t = 1$ signifies the laminar combustion regime.

Wrinkled

The wrinkled flamelet zone falls below the lines $Ka < 1$ as well as $v'/s_L < 1$. $Ka < 1$ indicates that the time and length scales associated with the flame are smaller than the smallest scales of turbulence. The velocity of the flame is higher than that associated with eddies, which means they are too large and slow to penetrate the

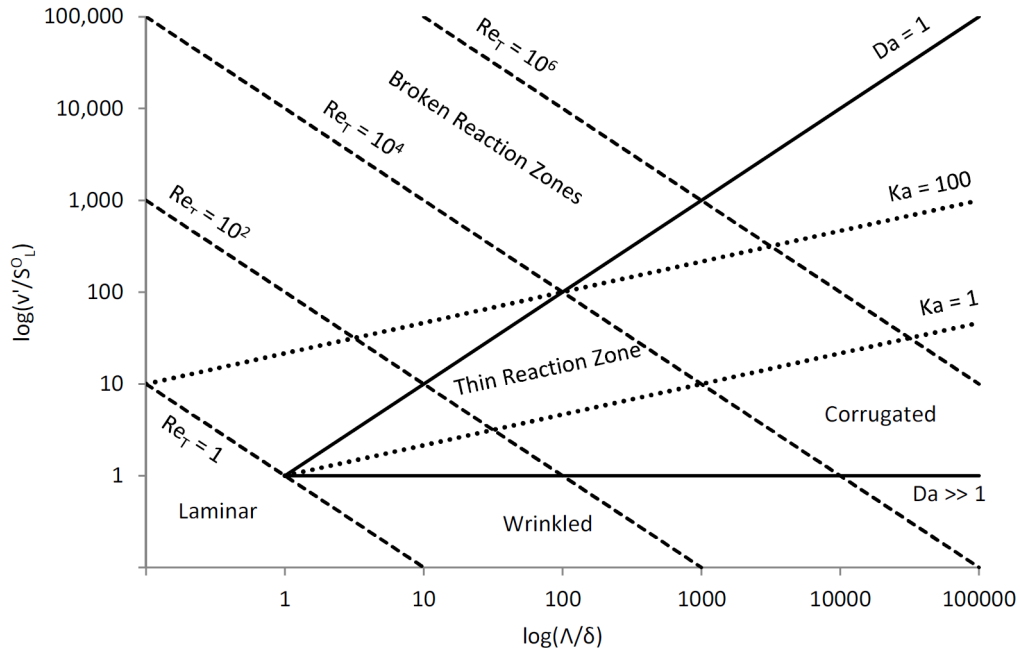


Figure 2.2: Borghi Diagram - Turbulent premixed combustion regime diagram

flame; the flame front is only wrinkled by the turbulence.

Corrugated

The corrugated flamelet zone also lies below $Ka < 1$, however above $v'/s_L > 1$. The eddy velocity is larger than the flame speed, eddies corresponding to that velocity are able to interact more intensely with the flame structure causing it to corrugate and entrap burned or unburned gas. Together the wrinkled and corrugated zones make up the laminar flamelet regime.

Thin

The thin reaction zone falls between $Ka_\delta < 1$ and $Ka > 1$. $Ka > 1$ indicates that the turbulence scales are smaller than those of the flame structure making it possible for small eddies to enter into the flame zone and distort it. However, these eddies are still larger than the thickness of the inner layer, which is approximately 1/10th of the flame thickness, therefore any interaction occurs in the preheat zone. In this regime eddies are able to enhance mixing and transport and further distort the flame structure in the preheat zone.

Broken

The last zone is the broken reaction zone and is characterised by the inequality $Ka_\delta < 1$. In this region the small eddies can disrupt the not just the preheat zone but also the inner layer of the flame itself, causing local extinction. In practical devices this regime is avoided.

According to (Swaminathan&Bray, 2011), most internal combustion engines operate in the region overlapping the corrugated and thin reaction zones at lower turbulence levels and aero gas turbines do the same but at higher levels of turbulence. Gas turbines used for power generation mostly operate at turbulence levels comparable to IC engines, however in the wrinkled combustion region. (Swaminathan&Bray, 2011) also point out that there is a trend moving away from the flamelet regime towards the thin reaction zone i.e. higher Karlowitz numbers. This indicates that models that are not limited to the flamelet assumption will most likely be required for future development.

2.6 Overview of Premixed Combustion Models

A variety of models have been proposed by various research groups in order to tackle turbulence, chemistry and their interaction in combustion. Most of these models are developed and optimised for a specific purpose and are therefore often limited to a particular combustion regime. Additionally, the state of modelling for stratified combustion is still less advanced than that of non- and premixed combustion (Sweeney et al., 2011a). One of the main challenges in developing combustion models for LES is that of the finding a closure for the filtered reaction rates which appear in the species, mixture fraction or progress variable transport equations. This originates from the highly non-linear dependency of the chemical reaction rates on temperature and species mass fractions. In the context of premixed combustion there is the added challenge of small flame thickness over which thermochemical properties experience steep gradients. The flame thickness of a premixed flame is generally smaller than the LES filter width, such that it is not possible to resolve the flame

Table 2.1: Combustion Model Classification

	Premixed	Non-Premixed
Infinitely Fast Chemistry	Bray-Moss-Libby Coherent Flame Eddy Break-up	Conserved Scalar Equilibrium
Finite Rate Chemistry	Transported PDF Models	
	Flamelet Based on G-Eqn Flame Surface Density Artificial Flame Thickening	Flamelet Based on Mixture Fraction Conditional Moment Closure
	Linear Eddy Model	

front. Some of the most commonly used models to address these difficulties for premixed combustion are outlined briefly in the following section: Flame Surface Density (FSD), G-Equation (level set), and Artificial Flame Thickening (AFT). A modified overview of models is provided in Table 2.1 (Peters, 2000).

The focus of the following Chapter will be on the probability density function approach and stochastic field solution method. This approach is capable of providing a general description of a flame, bridging combustion regimes and flame types and making it a promising approach for stratified combustion.

Flamelet assumption based Models

The flamelet assumption states that a flame can be considered to be made up of many smaller one-dimensional laminar flames. Further flamelet assumptions are as follows: quick chemistry; the chemical time scale is shorter than the turbulence scale, thin reaction layer that is smaller than any turbulent eddies; the structure of the reaction zone remains predominantly laminar and is embedded in a turbulent field and diffusive transport occurs essentially normal to the flame surface (Warnatz et al., 1996). This approach allows the local structure of the flame sheet to be treated as laminar and chemistry and turbulence can be handled separately.

Assuming equal diffusivity and constant pressure combustion without heat loss, thermo-chemical properties can be determined completely by the local state of mixing given by the mixture fraction. Under the assumption of widely separated time scales, the combustion chemistry is in a quasi-steady state and adapts to local flow

condition instantaneously. In order to extend the flamelet approach beyond assuming infinitely fast chemistry the scalar dissipation rate can be used to describe the extent of non-equilibrium. The physical flame coordinate can then be transformed into mixture fraction space and temperature and species can be determined by the balance of diffusion to chemical reaction. Using different equivalence ratios and scalar dissipation rates one can then generate a library (table) of flamelets in which thermo-chemical properties are expressed as functions of mixture fraction and the scalar dissipation rate. Solving Navier-Stokes, the conservation equation for the mixture fraction and evaluating the local scalar dissipation rate one can obtain density, temperature, and species concentrations from the flamelet library using linear interpolation.

For premixed flames it is necessary to also incorporate a progress variable c in the tabulation process. While the mixture fraction describes the state of mixing of the fuel and the oxidiser, for premixed flames the progress variable describes the extent of the transition from the unburned to the fully burned state.

Eddy Break-up Model

One of the most straightforward combustion modelling approaches attempts to directly estimate the filtered chemical reaction rate term. Assuming combustion is dominated by the processes of chemical reaction and scalar mixing, the rate of combustion will be controlled by the slower of the two.

A mixing rate term can be introduced that is proportional to the minimum reactant mass fraction and another reaction rate term that is proportional to the chemical reaction rate given by simple 1-step reaction mechanism. The slowest of these two rates is used to represent the filtered reaction rate.

Extensions to and examples applications of the Eddy Break-up Model can be found e.g. in (Pouyrou, 2006).

G -Equation

The G -equation approach attempts to model the behaviour of the flame without resolving it and instead treats the flame as a sheet that separates unburned from burnt

gases. G is a non-reacting scalar and the G -equation, a so called level-set equation, describes the behaviour of the iso-surface of constant $G = G_0$, generally chosen to describe the flame front. G can be chosen such that $G_0 = 0$ at the flame front, $G > G_0$ in the burned gasses and $G < G_0$ in the unburned mixture. The quantity represented by G is chosen to be a constant value of e.g. temperature or a reaction progress variable. RANS formulations for the G -Equation were proposed by (Bray et al., 1985) and further developed by (Peters, 2000). More recently adaptations of the method for LES valid in the corrugated flamelets and the thin reaction zone regimes have been developed by e.g. (Hawkes&Cant, 2000) and (Pitsch, 2005).

Artificial Flame Thickening

Artificial Flame Thickening (AFT) models attempt to resolve the flame, thickening it by increasing the thermal diffusivity of the flame and simultaneously reducing the rate of reaction in order to maintain the laminar flame speed. Dynamic approaches are generally used to only thicken in the immediate vicinity of the flame.

When the flame is thickened, the chemistry turbulence interaction (i.e. Damköhler Number) is affected and must be compensated by the model. Generally a efficiency function is introduced to account for the flame thickening effects in the sub-grid scale model via a sub-grid wrinkling term.

LES models have been developed in combination with flamelet libraries amongst others by (Legier et al., 2000) and (Colin et al., 2000).

Flame Surface Density

The Flame Surface Density (FSD) approach attempts to model premixed flames by combining the diffusion term and the reaction term to form a flame propagation term. Early work in the RANS context was conducted by (Cant et al., 1991), and the method has more recently been adapted by e.g. (Chakraborty&Cant, 2009) with a summary of models provided by (Lin, 2010).

The propagation term is proportional to a propagation velocity and a measure of flame surface density. The FDS model uses the density of iso-surface per unit volume, Σ , or in the context of LES the sub-grid flames surface density, Σ_{sgs} , per unit filtered

volume. Considering a LES filter volume, the probability density function of finding $\psi = \psi^*$ can be determined and a general expression for the filtered FSD can be arrived at (Swaminathan&Bray, 2011):

$$\bar{\Sigma}(\mathbf{x}, t) = \int_0^1 \Sigma(\psi^*; \mathbf{x}, t) d\psi^* = \overline{|\nabla \psi|} \quad (2.6.1)$$

ψ^* represents a progress variable, which can be linked to tabulated chemistry enabling the filtered FSD, $\bar{\Sigma}$, to be used in modelling the filtered reaction rate $\overline{\dot{\omega}_\psi}$.

Most FSD models use one of two methods in order to determine $\bar{\Sigma}$: assume the reaction rate to be proportional to the scalar dissipation rate and develop algebraic expressions, or use a modelled transport equation for the FSD.

F-TACLES

The Filtered Tabulated Chemistry for Large Eddy Simulation approach (F-TACLES) tabulates chemistry from explicitly filtered flamelets. This information is used in order to provide closure for the combined filtered source term and sub-grid flux term of a progress variable transport equation. Additionally an algebraic flame wrinkling model is used. Flamelets are filtered at different filter widths and tabulated quantities are stored as functions of filtered progress variable and filter width (Fiorina et al., 2010).

Probability Density Function Methods

In general terms there are two types of probability density function methods, those that make use of flamelet tabulation and those that make use of composition or composition-velocity pdfs.

The flamelet based PDF methods tabulate thermo-chemical quantities as functions of e.g. unfiltered progress variable and mixture fraction. Their filtered counterparts from a LES can be related to the flamelet table variables through use of sub-grid pdfs. For the mixture fraction this pdf describes the mixing of fuel and oxidiser, for the progress variable the degree of transition from unburned to burned. These pdfs can be arrived at by solving transport equations for the pdfs and their second moment

or by assuming the shape of the pdf itself, e.g. that of a beta-function frequently used for the mixture fraction. Other quantities can also be tabulated against in order to implement more complex combustion models. The filtered source term can then be arrived at by convolution of the tabulated term with the pdfs.

In composition PDF methods scalars are interpreted as random variables and their pdf essentially describes the probability of finding a certain species concentration at a given point in the computational domain. A transport equation for the entire composition pdf can be derived, which will be discussed in detail in Chapter 3, for which several different solution approaches exist.

Lagrangian approaches use particles to solving the transported pdf equation. So called notional particles are employed, whose one-point, one-time pdf evolve in space and composition space according to a set of stochastic equations which are equivalent to the modelled transported pdf equation. This requires the coupling of the Lagrangian particles with a Eulerian CFD solver. Care must then be taken to ensure proper particle tracking and sufficient spacial distribution / number density of particles in order to control statistical error over the domain and in particular near points of interest.

Eulerian approaches avoid this by using multiple instances of each variable in form of fields which are combined in a manner specific to the method. An alternative Eulerian PDF method to the one used in this work is the multi-environment pdf method, which is a deterministic approach. Here each scalar is represented by N_E environments and equations are solved for the weight i.e. the contribution of each environment as well as weighted species concentration of each species for each environment.

The stochastic field method makes use of the similarity of the transported composition pdf equation to the Fokker-Planck equation and it's relationship with stochastic differential equations, see Chapter 3.

A very extensive review of numerous pdf methods and solution approaches is provided in (Haworth, 2010).

2.7 Existing LES Models for Premixed and Extensions to Stratified Combustion

The following section presents a more detailed review of the existing literature on modelling of stratified premixed combustion in the context of Large Eddy Simulation. Within this scope all existing work used flamelet based approaches which were extensions and variations on the methods outlined in Section 2.6.

Duwig & Fureby (2007)

(Duwig&Fureby, 2007) were among the first to investigate stratified combustion using LES. They investigated two flames of the ORACLES Burner, C1 & C3, by extending two flamelet based methods to account for varying equivalence ratios. Both used progress variable / mixture fraction formulations with a flame wrinkling model. The chemistry was pre-computed, parametrized by reactive scalar c , based on fuel mass fraction, and mixture fraction z , assuming equal diffusivities.

Two different LES codes were used, one Finite Volume, the other Finite Differences. Both use formulations designed for (restricted to) lean premixed combustion. The Finite Volume code used a propagation formulation where the diffusive term and the source term were regrouped as a filtered flame front displacement term that was closed using a flame wrinkling model. The sub-grid flux was closed using the so called mixed model which is a one-equation eddy viscosity model with wall extension. The Finite Difference code used an explicitly filtered flame approach. All unclosed terms in the filtered progress variable equation, the filtered diffusion term, sub-grid flux and filtered source term, were grouped together and closed with a Gaussian distribution model for heat release and a flame wrinkling model.

The mixture fraction/progress variable formulation further requires closure of a cross scalar dissipation rate like term which is closed with an effective diffusivity in analogy to scalar dissipation rate closures from non-premixed combustion modelling.

The ORACLES burner operates on a propane air mixture with equivalence ratios of 0.75 for the C1 flame and 0.65 – 0.85, i.e. stratification ratio of 1.3, for the C3 flame. Under these conditions the burner exhibits large amplitude fluctuating inlet

velocity pulsations which were attempted to be simulated. The Reynolds number is $Re \cong 25000$, and the Karlovitz number is $Ka \cong 1.5$. Several computational grids were used with 1-4 million cells/points.

Reasonable agreement with the experimental data is reported for the mean axial velocity of the non-reacting case for both codes, while larger discrepancies are reported for the rms velocity fluctuations. For the fully premixed case symmetric flapping of the flame was observed, while for the stratified case asymmetric flapping and modified flow were observed and attributed to the presents of higher equivalence ratios increasing flame speeds and product temperatures. Good agreement of both mean and rms axial velocities are reported for both codes for the fully premixed case and reasonable agreement for the stratified case.

Species concentrations were not shown, with mostly qualitative analysis/comparisons and the main focus on capturing and analysing flame dynamics using proper orthogonal decomposition, as they are exposed to strongly varying boundary conditions with time. However, the modelling approach and closures used in this work form the basis of other numerical studies on the effect of stratified equivalence ratios in more recent work.

Auzillon, Veynante et al (2012)

(Auzillon et al., 2012) investigated the MOLECULES combustor, in which a swirling flame is stabilised behind a TURBOMECA injector. The numerical approach used was the Filtered Tabulated Chemistry for LES (F-TACLES) method, which was adapted to account for stratified combustion.

The chemical subspaces are mapped by a collection of 1-D laminar premixed flames computed for equivalence ratios within the flammability limits using detailed chemistry. This excludes the possible combustion outside the limits i.e. extensions of limits by mixture stratification. Laminar thermochemical quantities are stored in look-up tables as a function of three coordinates: progress variable, mixture fraction and its variance. The orientation of progress variable iso-surfaces to mixture fraction iso-surfaces is related to the cross-scalar dissipation rate $\mathcal{X}_{zc} = \rho D \nabla c \cdot \nabla z$ and can influence the chemical flame structure. In this work it was assumed to be

0, i.e. constant and perpendicular (at the sub-grid scale level).

The transport equation for the filtered non-normalized progress variable is solved which requires modelling closure for sub-grid transport, filtered laminar diffusion, and filtered source terms. Parts of each term were precomputed and stored in four dimensional look-up tables (progress variable, mixture fraction, unmixedness factor and filter width). The tabulation process used GRI 3.0 to generate a collection of 1-D methane-air flamelets, assuming unity Lewis number.

The burner consists of a plenum chamber, a swirl-injector and the combustion chamber. The global equivalence ratio is 0.8, the operating pressure is 2 bar and the Reynolds number for air is $Re \cong 46000$.

Good agreement was achieved for the non-reacting case in comparisons with experimental data for mean and rms velocity components as well as the methane mass fraction. Good agreement was also achieved for the reacting case for velocities and methane mass fraction, however with deviations of up to 30% at two measurement locations in the vicinity of the inlet. The lift-off height and flame envelope were captured and OH mass fraction compares well to PLIF images. Further comparisons demonstrated the sensitivity and importance of the sub-grid wrinkling model in reproducing results. Simulations not accounting for the sub-grid scale mixture fraction inhomogeneity (stratification) are also performed. Omitting this lead to significantly increased displacement speeds, demonstrating a strong dependence of the flame dynamics on sub-grid mixture fraction variance.

Kuenne, Dreizler et al (2012)

In several joint experimental and numerical papers (Kuenne et al., 2012) investigated the Darmstadt Stratified burner using a progress variable / mixture fraction approach combined with Artificial Flame Thickening (ATF) and Flamelet Generated Manifolds (FGM) (lookup tables). Combustion modelling was based on two-dimensional tabulated chemistry via the FGM technique using the mixture fraction z and a progress variable based on the CO_2 mass fraction. CHEM1D and the GRI3.0 mechanism for methane air combustion were used assuming a Lewis number of $Le = 1$. Outside of the flammability limits extrapolation was applied. An Artificial

Flame Thickening procedure is applied with a grid-adaptive thickening factor and an efficiency function combined with a flame sensor based on the progress variable. Thickening was applied to both scalars.

The burner has a central rod-stabilized pilot flame surrounded by two concentric tubes placed into a shielding co-flow, and the flame is stabilised without swirl. With a Karlowitz number range of $1 < Ka < 2.1$, the flames are estimated to fall within the thickened-wrinkled flamelet regime near the corrugated flamelet regime. Two grids were investigated one coarse with 0.8 million and one fine with 6.5 million control volumes. Part of the burner is included and the velocity measurements closest to the burner exit are imposed on the computational domain inlet.

Mean and rms results from the simulations are compared against the experimental measurement data for the flame configuration TSF-A with a stratification ratio of 1.5 i.e. $\phi_{E,1} = 0.9$ & $\phi_{E,2} = 0.6$. Temperatures results presented show over-prediction near burner centre line. This was attributed to the assumption of adiabatic walls and demonstrates the importance of heat loss modelling in achieving accurate predictions for this burner.

Marincola, Kempf et al (2013)

(Marincola et al., 2013) also investigate the Darmstadt turbulent stratified flame burner. For this purpose they used the same method as (Duwig&Fureby, 2007): a progress variable / mixture fraction approach with reaction rate modelling using a flame surface density / wrinkling model (without use of lookup tables) and a laminar flame speed based on the mixture fraction. The molecular diffusion term and the reaction rate reaction are joined together and expressed as a generalised flame surface density $\overline{(\rho S_d)}_s \Sigma_{gen}$. The overlined part of the term is modelled using the laminar flame speed. The second part of the term is modelled with fractal flame wrinkling model that is proportional to an efficiency function, a fractal dimension and the sgs-velocity fluctuations. The efficiency function accounts for the net sgs straining effects on the flame and is modelled, as is the fractal dimension, as a function of sgs-velocity and laminar flame speed.

The code used is called PsiPhi, a Cartesian code with uniform, cubic cells. One non-

reactive and two burning cases are investigated; premixed no-shear and stratified no-shear. Two grids with resolutions of $1mm$ and $0.5mm$ are used, corresponding to 12.7 and 101.4 million cells.

Velocities are reproduced well for isothermal and burning cases. Mixture fraction and temperature mean and rms are in very good agreement with experimental data. Statistics of a cross-scalar dissipation rate are investigated and used to identify where the term is significant, finding it accounts for less than 6% of the total source term. It is also concluded that there is no need for a sgs-model for the filtered laminar flame speed. Analysis of scatter plot of ∇z and ∇c showed predominantly back-supported burning for the stratified configuration of the burner.

Nambully, Vervisch et al (2014)

(Nambully et al., 2014a) were amongst the first to investigate the Cambridge Stratified Swirl Burner numerically. They use a progress variable / mixture fraction formulation that also includes transport equations for their variances and uses a filtered laminar flame-pdf closure (four dimensional lookup tables). This formulation has 12 terms which require closure: 8 sgs stresses, 2 reaction rate source terms and 2 scalar dissipation rates. This is achieved using a number of different techniques such as a presumed β -pdf for the mixture fraction, a sgs-wrinkling factor, flame resolution sensor or a mapping from location along a laminar flamelet and the filter width to filtered progress variable and unmixedness. This allows the flamelet filter size to be determined using both the characteristic mesh size and the scalar fluctuations. A model based on the gradient of residence times is used to account for global differential diffusion (accumulation of carbon in recirculation zone) with a Hirsch-Felder and Curtiss like model for diffusivity of the progress variable.

The YALES2 code is used with a local dynamic sgs-viscosity model and two grids, one with 50 million tetrahedral and 0.3-0.4mm resolution and a very fine grid with 400 million cells and a resolution of 0.15-0.2mm in the reaction zone.

For the non-swirling, fully premixed case, SwB1, the velocity and temperature results are in good agreement both for mean and rms quantities. CH_4 profiles are in very good agreement for the mean and slight under-predicted for the rms values.

Very good agreement was achieved for mixture fraction mean and rms values. Good agreement was also achieved for species such as CO_2 , however for e.g. CO only the trend is captured while the magnitudes, particularly in the vicinity of the bluff body, are under-predicted.

In the second part of their paper (Nambully et al., 2014b) investigate the moderately and highly stratified non-swirling flames of the Cambridge Stratified Swirl Burner, SwB5 and SwB9. Overall good agreement is achieved for reactants, slightly less so for products and the following observations are made:

There is lower accumulation of mixture fraction in the recirculation zone for the stratified cases compared to the fully premixed case; CO however sees increased accumulation. This is attributed to lower O_2 concentrations due to stoichiometric or rich conditions of the inner annuli stream as opposed to the lean conditions for the fully premixed case. It is also observed that temperatures along the centre line, especially near the bluff body, are over-predicted. This is attributed to heat loss to the bluff body which reduces flame speeds, resulting in slight radial shifts of measurement profiles.

It is report that flamelet based models work well in the case of lean stratification, but do not account well for staged combustion when the equivalence ration crosses the stoichiometric line and non-premixed combustion of partially burner products occurs.

(Nambully et al., 2014b) demonstrate that for SwB5 and SwB9 stratification occurs on a length scale much larger than the typical reaction layer thickness of $\delta \approx 0.1mm$. Furthermore, they demonstrate predominantly premixed flamelet behaviour occurring, with negligible presents of diffusion flamelets and minor but non-negligible amounts of partially premixed flamelet behaviour. The flames exhibit characteristics from multiple reaction zones from wrinkled up to thin reaction zones and thus a model is needed that can account for each dynamically.

These findings suggest that detailed modelling of differential diffusion and heat loss can be important for this type of burner and that a more general modelling approach can be beneficial.

Proch & Kempf (2014)

(Proch&Kempf, 2014) also investigate the Cambridge Stratified Swirl Burner using a progress variable / mixture fraction approach coupled with an Artificial Flame Thickening (AFT) and Premixed Flamelet Generated Manifolds (PFGM) (lookup tables) method. The chemical state of a 1d propagating premixed flame is tabulated over a progress variable based on CO_2 , CO and H_2O . This is extended to be suitable for stratified conditions by tabulating multiple flames at different equivalence ratios, assuming stratified combustion consists of an ensemble of premixed flames. The Lewis number is assumed to be $Le = 1$ and results in constant mixture fraction across flames, simplifying tabulation. The manifold is stored in a 2D lookup-table as function of mixture fraction and progress variable. It also contains laminar viscosity, density and progress variable reaction rate and post-processing information.

Artificial Flame Thickening is applied through a factor F , efficiency function E and flame sensor Ω in the progress variable equation. The sensor is based on the normalised gradient of the progress variable and stored in manifold. Using F and the sensor the flame thickness is resolved by a given number of grid-points. A joint filtered sgs-pdf for progress variable and mixture fraction, assumed to have a top-hat shape, is used to account for unknown sub-filter distributions. Progress variable and mixture fraction are assumed to be statistically independent and can thus be evaluated separately. The method is integrated into the Cartesian PsiPhi code.

Basic trends captured by all meshes, with improved accuracy with each grid refinement. Radial velocities are slightly over-predicted with otherwise good agreement on the finer meshes. Agreements are good for other mean and rms quantities, with the same observations made as for the radial velocities appearing in the results. The authors linked this to the asymmetry of the experimental results and the AFT model under performing in wall proximity.

Good agreement is achieved for species with discrepancies in the recirculation zone in particular near the bluff body. These are attributed to possible effects of differential-diffusion and heat-loss, both of which are not accounted for by the model.

Trisjono, Pitsch et al (2014)

(Trisjono et al., 2014) numerically investigate the Darmstadt Turbulent Flame Burner using a progress variable / mixture fraction formulation that uses a Level-Set (G -Equation) approach and accounts for possible heat-loss to walls via an enthalpy defect. The modelling approach also includes a radiation model.

The progress variable is used for the combustion process and turbulence-chemistry interaction while the level-set provides for the correct flame propagation velocity. The two are coupled via a progress variable source term using a blended exponential function. The source term then depends on the level-set near the flame and on the progress variable away from flame, ensuring a thin reaction zone. Filtered and unfiltered quantities are related using a joint pdf for mixture fraction and progress variable, approximated by a β -pdf. Differential diffusion is accounted for in flamelet space using a non-unity Lewis number for each species. In order to avoid expanding flamelet manifold by a third variable, it is proposed instead to project the reference flamelet onto flamelets of different enthalpy levels through scaling using a correction function for the relevant thermochemical quantities in the governing equations.

Only velocity and temperature results are presented with good agreement reported for the mean velocities, slightly less so for the rms quantities. The same is observed for temperature with improved agreement for simulations including heat loss to the burner. The inclusion of a radiation model is reported to improve results at downstream locations.

Fiorina et al (2015)

Most recently (Fiorina et al., 2015) collated results of 5 research groups for the Darmstadt Stratified Burner. All results are based on variations of the above flamelet models, with the addition of a "no combustion model" for comparison. All models were extended to take into account heat loss to the burner near the pilot.

Comparisons are made for temperature, mixture fraction and major species mass fractions. The importance of heat-loss is emphasised in reproducing flame lift off and flame brush position for the burner.

All methods are able to achieve reasonable agreement with the experimental data (ignoring the "no combustion model" results), however differences of up to 40% are observed between the approaches and simulations.

Most flamelet based approaches were designed for a specific purpose, e.g. premixed or non-premixed combustion modelling, and then extended in some way in order to be able to account for a new combustion phenomenon. Models derived to handle e.g. thin premixed flames might not be able to also account for non-premixed or partially premixed combustion. In practical combustion devices, such as gas turbine combustion chambers, generally one mode of combustion dominates, however other modes will also be present and can play important roles. In such cases it is necessary to use more general approaches that do not make assumptions about the combustion regime, such as the transported probability density function approach.

Chapter 3

Transported Probability Density Function and Stochastic Fields method

The present work is based on the composition probability density function and its transport equation. This pdf is a one-point, one-time joint pdf for all the variables required to describe the thermochemical state of a reacting process. The primary advantage of the transported pdf method is that the chemical reaction rate term, which describes a one-point process, appears in a closed form and thus the term does not require any modelling beyond the specification of a reaction mechanism of choice. The main disadvantage of the method is the high dimensionality of the pdf, with dependency on space, time and composition space, rendering it infeasible to model using e.g. finite difference methods. Thus generally Monte Carlo methods are employed in the solution of the pdf equation. Initially Lagrangian methods were predominantly used e.g. (Pope, 1985), where the pdf is represented by an ensemble from a large number of notional particles. More recently, fully Eulerian methods have emerged as feasible and convenient solution approaches to the modelled pdf equation e.g. (Valiño, 1998) (RANS), (Mustata et al., 2006) (LES), where the pdf is represented by continuous Eulerian fields. The present work makes use of the Eulerian Stochastic Fields method (SFM) to solve for the modelled sub-grid composition pdf transport equation.

3.1 Probability Density Function Properties

Some fundamentals of probability theory as well as the properties of a pdf are worth recalling before delving into the transported pdf-method.

Probability density functions have the following three properties (Papoulis&Pillai, 2002):

- positive $P(\boldsymbol{\psi}) \geq 0$
- normalisation $\int_{-\infty}^{\infty} P(\boldsymbol{\psi}) d\boldsymbol{\psi} = 1$
- compact support i.e. $\lim_{\boldsymbol{\psi} \rightarrow \pm\infty} P(\boldsymbol{\psi}) = 0$

These are similar properties to the filter properties outlined in Section 2.2 and are used in defining the filtered pdf in the following sections.

Recap of some probability theory for continuous variables, that will be required in the following sections, before delving into the derivation of the transported pdf equation. The integration limits of the following equations are from $-\infty \rightarrow \infty$ unless stated otherwise. The expected value of a continuous random variable ϕ , where $\langle \dots \rangle$ denotes the expectation is defined as:

$$\langle \phi \rangle = \int \psi P(\psi) d\psi \quad (3.1.1)$$

Where ψ is the sample space variable of ϕ . The expected value of a function $Q = Q(\phi)$ is thus defined as:

$$\langle Q(\phi) \rangle = \int Q(\psi) P(\psi) d\psi \quad (3.1.2)$$

If the pdf is a joint pdf of the random variables in $\boldsymbol{\phi}$ then the marginal pdf for a single random variable from the joint pdf P is defined as:

$$P_{\phi_{\alpha}}(\psi_{\alpha}) = \int P(\boldsymbol{\psi}) d\psi_1 \dots d\psi_{\alpha-1} d\psi_{\alpha+1} d\psi_{N_S} \quad (\text{not including } \alpha) \quad (3.1.3)$$

Key to the derivation of the transport equation for the composition pdf, which is the pdf in question in the present work, are the conditional pdf and the conditional expected value. This is due to the composition pdf not containing any information

about the velocity vector $\mathbf{u}$. Following (Gerlinger, 2005) let $P = P(\hat{\mathbf{u}}, \boldsymbol{\psi})$, be the joint pdf of the velocity vector $\mathbf{u}$ and the composition vector $\boldsymbol{\phi}$, and $\hat{\mathbf{u}}$ and $\boldsymbol{\psi}$ be their corresponding sample space variables. Then, Bayes' Theorem describes the relationship between the conditional ($P_{\mathbf{u}|\boldsymbol{\phi}}$), marginal (composition pdf) ($P_{\boldsymbol{\phi}}$) and joint (P) pdfs as follows:

$$P_{\mathbf{u}|\boldsymbol{\phi}} = P_{\mathbf{u}|\boldsymbol{\phi}}(\hat{\mathbf{u}}|\boldsymbol{\phi}(\mathbf{x}, t) = \boldsymbol{\psi}; \mathbf{x}, t) = \frac{P(\hat{\mathbf{u}}, \boldsymbol{\psi}; \mathbf{x}, t)}{P_{\boldsymbol{\phi}}(\boldsymbol{\psi}; \mathbf{x}, t)} \quad (3.1.4)$$

This describes the probability of event $\hat{\mathbf{u}}$ occurring, given the condition that $\boldsymbol{\phi} = \boldsymbol{\psi}$ and allows the expected value of a variable not described by the marginal pdf $P_{\boldsymbol{\phi}}$ to still be expressed in terms of $P_{\boldsymbol{\phi}}$, albeit involving the conditional pdf. The expected value of $\mathbf{u}$ can thus be expressed as (dropping the dependencies on space and time for compactness):

$$\begin{aligned} \langle \mathbf{u} \rangle &= \iint \hat{\mathbf{u}} P_{\mathbf{u}|\boldsymbol{\phi}}(\hat{\mathbf{u}}|\boldsymbol{\phi} = \boldsymbol{\psi}) P_{\boldsymbol{\phi}}(\boldsymbol{\psi}) d\hat{\mathbf{u}} d\boldsymbol{\psi} \\ &= \int \langle \mathbf{u}|\boldsymbol{\phi} = \boldsymbol{\psi} \rangle P_{\boldsymbol{\phi}}(\boldsymbol{\psi}) d\boldsymbol{\psi} \end{aligned} \quad (3.1.5)$$

The conditional expected value for a function $Q = Q(\mathbf{u}, \boldsymbol{\phi})$ is then:

$$\langle Q(\mathbf{u}, \boldsymbol{\phi})|\boldsymbol{\phi} = \boldsymbol{\psi} \rangle = \langle Q|\boldsymbol{\phi} = \boldsymbol{\psi} \rangle = \int Q(\hat{\mathbf{u}}, \boldsymbol{\psi}) P_{\mathbf{u}|\boldsymbol{\phi}} d\hat{\mathbf{u}} \quad (3.1.6)$$

Combining Equations 3.1.4 and 3.1.5 allows for a relation between the conditional and unconditional expected values for the function Q to be formulated (in short hand notation) as:

$$\langle Q \rangle = \int \langle Q|\boldsymbol{\phi} = \boldsymbol{\psi} \rangle P_{\boldsymbol{\phi}} d\boldsymbol{\psi} \quad (3.1.7)$$

If Q is fully determined by $\boldsymbol{\phi}$, as for example it will be seen that the density is, then:

$$\langle Q|\boldsymbol{\phi} = \boldsymbol{\psi} \rangle = Q(\boldsymbol{\psi}) \quad (3.1.8)$$

3.1.1 δ -Functions

The δ -function and its properties are used extensively in the derivation process. The δ -function is a generalised function, also referred to as an “improper” function, that itself does not have a well-defined value; however, when it occurs as a factor in an integrand the integral is well defined (Dirac, 1958). The δ -function has several key properties that will be made use of (Lighthill, 1959), (Weisstein, b):

$$\delta(x - a) = 0 \quad , \quad \text{for } x \neq a \quad (3.1.9)$$

$$\int_{-\infty}^{\infty} \delta(x - a) dx = 1 \quad (3.1.10)$$

$$\int_{-\infty}^{\infty} f(x) \delta(x - a) dx = f(a) \quad (3.1.11)$$

$$\int_{-\infty}^{\infty} f(x) \delta'(x - a) dx = -f'(a) \quad (3.1.12)$$

$$\frac{\partial \delta(x - a)}{\partial x} = -\frac{\partial \delta(x - a)}{\partial a} \quad (3.1.13)$$

The first property (3.1.9) states that for the case that $x = a$, the δ -function is thought to have either an infinite value or to be undefined. The second (3.1.10) is a normalisation condition which implies that the δ -function can be interpreted as a density, in the sense of a probability density function (pdf). The corresponding cumulative distribution function is the Heavyside function. This property is used to define so called “fine-grained” pdfs (used in (3.2.1)). (3.1.11) refers to the sifting or sampling property of the δ -function, as the integral sifts out the value $f(a)$. The function $f(x)$ is a so-called good- (or test-) function that is continuous, differentiable and vanishes approaching $\pm\infty$. Furthermore, (3.1.12) states that the derivative of the delta function sifts out the negative value of the derivative of the test function f at a . (3.1.13) is strictly only valid in the context of multiplication with a test function e.g. $f(x)$ and integration, as in (3.1.12). In the context of pdfs and the “fine-grained” pdf, (3.1.13) allows for the switching of the realizations with the sample space variable. Further details can be found e.g. in the appendices of (Pope, 2000).

3.2 Filtered Density Functions

Under the previously mentioned assumptions of a low Mach number and an ideal gas containing N_s chemical species, the species concentrations and the mixtures enthalpy (as well as for incompressible flows the reference pressure) are sufficient to determine all properties required to describe a reacting flow (density, viscosity, chemical reaction rates).

In the following the variable ϕ is a vector containing the species to be accounted for in the pdf as well as the enthalpy. These variables are treated as random variables with the corresponding sample space vector ψ .

3.2.1 Marginal/Fine Grained pdf

The implication of (3.1.11) is that a “fine-grained” pdf for a single scalar (marginal) may be defined as (Libby&Williams, 1980):

$$\mathcal{F}_\alpha(\psi_\alpha; \mathbf{x}, t) = \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}, t)) \quad (3.2.1)$$

where ψ denotes the sample space of the scalar ϕ and $\phi(\mathbf{x}, t)$ is a realisation of the scalar. For the δ -function ψ is the independent variable, while ϕ is a “constant”. “Fine-grained” refers to the pdf being “spiky” in that the pdf only gives a non-vanishing probability density if $\phi(\mathbf{x}, t)$ is exactly equal to ψ or rather of finding ϕ on an infinitesimal interval $\psi < \phi < \psi + d\psi$. Thereby, the knowledge of the fine-grained pdf for each point $\mathbf{x}$ of a particular realization at time t , is equivalent to the knowledge of the realization. An analogy can be made to producing a histogram with fixed bin sizes; a pdf can be build from δ -functions by binning realisations with infinitesimal bin sizes, as the number of realisations tends to ∞ .

Key properties of the “fine-grained” pdf are (where the brackets denote an expectation) (Pope, 2000):

$$\langle \mathcal{F}_\alpha(\psi_\alpha; \mathbf{x}, t) \rangle = P_\alpha(\psi_\alpha; \mathbf{x}, t) \quad (3.2.2)$$

$$\langle g(\mathbf{x}, t) \mathcal{F}_\alpha(\psi_\alpha; \mathbf{x}, t) \rangle = \langle g(\mathbf{x}, t) | \phi_\alpha(\mathbf{x}, t) = \psi_\alpha \rangle P_\alpha(\psi_\alpha; \mathbf{x}, t) \quad (3.2.3)$$

From (3.2.2) it follows that the expected value (or ensemble average of realisations) of the "fine-grained" pdf is the pdf itself. (Further details in Appendix A.3). For a set of N_S scalars $\boldsymbol{\phi} = [\phi_1, \dots, \phi_{N_S}]$ a joint fine grained pdf can be defined as:

$$\mathcal{F}(\boldsymbol{\psi}; \mathbf{x}, t) = \delta(\boldsymbol{\psi} - \boldsymbol{\phi}(\mathbf{x}, t)) = \prod_{\alpha=1}^{N_S} \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}, t)) \quad (3.2.4)$$

3.2.2 Sub-Grid Probability Density Function

Applying conventional filtering to equation (3.2.4) the filtered joint sub-grid pdf $\bar{P}_{sgs}$ can be defined as (Jaberi et al., 1999):

$$\bar{P}_{sgs}(\boldsymbol{\psi}; \mathbf{x}, t) = \int_{\Omega} \mathcal{F} G d\mathbf{x}' = \int_{\Omega} \prod_{\alpha=1}^{N_S} \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}', t)) G(\mathbf{x} - \mathbf{x}', \Delta(\mathbf{x})) d\mathbf{x}' \quad (3.2.5)$$

Applying Favre filtering to equation (3.2.4), in order to take into account variable density flows, the density weighted joint sub-grid pdf $\tilde{P}_{sgs}$ can be defined as (Jones&Navarro-Martinez, 2007):

$$\bar{\rho} \tilde{P}_{sgs}(\boldsymbol{\psi}; \mathbf{x}, t) = \int_{\Omega} \rho \mathcal{F} G d\mathbf{x}' = \int_{\Omega} \rho(\boldsymbol{\psi}) \prod_{\alpha=1}^{N_S} \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}', t)) G(\mathbf{x} - \mathbf{x}', \Delta(\mathbf{x})) d\mathbf{x}' \quad (3.2.6)$$

The relationship between Favre filtered and conventional filtered pdf is given by:

$$\tilde{P}_{sgs} = \frac{\rho(\boldsymbol{\psi})}{\bar{\rho}} \bar{P} \quad (3.2.7)$$

Since the filter function G has the same properties as a pdf, filtering of the fine grained joint pdf can be interpreted as the sifting out of possible values of ϕ_α from within the filter volume $\mathbf{x}'$ at $(\mathbf{x}, t)$. Thus $\tilde{P}_{sgs}$ describes the probability of finding values of ϕ_α on the infinitesimal interval $\psi_\alpha < \phi_\alpha < \psi_\alpha + d\psi_\alpha$. Using Equation 3.2.6 together with the definition of a conditional pdf, Equation 3.1.4, and the conditional expected value for a function Q , Equation 3.1.5, a conditional filtering operations

can be introduced:

$$\overline{(Q|\phi = \psi)} = \frac{\int_{\Omega} Q \mathcal{F} G d\mathbf{x}'}{\bar{P}_{sgs}} \quad (3.2.8)$$

$$\bar{\rho}(Q|\widetilde{\phi = \psi}) = \frac{\int_{\Omega} \rho Q \mathcal{F} G d\mathbf{x}'}{\widetilde{P}_{sgs}} \quad (3.2.9)$$

3.2.3 Fine Grained PDF Transport Equation

Definition 3.2.6 and 3.2.9 are used to derive the transport equation of $\tilde{P}_{sgs}$ from the transport equation of a joint fine grained pdf $\mathcal{F}$. Such an equation can be arrived at starting from the substantial derivative of $\mathcal{F}$:

$$\frac{D\mathcal{F}}{Dt} = \frac{\partial \mathcal{F}}{\partial t} + u_i \frac{\partial \mathcal{F}}{\partial x_i} = - \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \frac{\partial \phi_{\alpha}}{\partial t} - u_i \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \frac{\partial \phi_{\alpha}}{\partial x_i} \quad (3.2.10)$$

Equation 3.2.10 is a result of the properties of the delta function, some details of which can be found in the Appendix (A.3). Multiplying by the density and taking into account the continuity equation, Equation 3.2.10 can be rearranged to:

$$\frac{\partial \rho \mathcal{F}}{\partial t} + \frac{\partial \rho u_i \mathcal{F}}{\partial x_i} = - \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \left(\rho \frac{\partial \phi_{\alpha}}{\partial t} + \rho u_i \frac{\partial \phi_{\alpha}}{\partial x_i} \right) \quad (3.2.11)$$

The right hand side of Equation 2.1.10 can now be substituted into the bracketed term above. (Alternatively the right hand side of Equation 2.1.8, without any modelling can be substituted instead) This brings the flux term, modelled with Fick's law, and the reaction rate term into the equation, resulting in:

$$\frac{\partial \rho \mathcal{F}}{\partial t} + \frac{\partial \rho u_i \mathcal{F}}{\partial x_i} = - \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \left(\frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \right) + \rho \dot{\omega}_{\alpha} \right) \quad (3.2.12)$$

Through use of the product rule (and rearranging its terms) the first term on the right hand side of Equation 3.2.12 can be recast into two more convenient terms (see Appendix, A.4), one a diffusion term, the other a scalar dissipation rate term:

$$- \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \left(\frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \right) \right) = \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \mathcal{F}}{\partial x_i} \right) - \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_{\alpha} \partial \psi_{\beta}} \left(\mathcal{F} \frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \frac{\partial \phi_{\beta}}{\partial x_i} \right) \quad (3.2.13)$$

Thus the transport equation for the joint one point one time fine grained pdf is:

$$\frac{\partial \rho \mathcal{F}}{\partial t} + \frac{\partial \rho u_i \mathcal{F}}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \mathcal{F}}{\partial x_i} \right) = - \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\mathcal{F} \frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \right) - \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_\alpha} \rho \dot{\omega}_\alpha \quad (3.2.14)$$

3.3 Sub-grid PDF Transport Equation

Filtering Equation 3.2.14 using definitions 3.2.6 and 3.2.9 the transport equation describing the evolution of the joint pdf can be written, dropping the dependencies on space and time for compactness, as (e.g. (Pope, 1985)):

$$\begin{aligned} & \frac{\partial \bar{\rho} \tilde{P}_{sgs}(\psi)}{\partial t} + \frac{\partial \bar{\rho}(u_j | \widetilde{\phi = \psi}) \tilde{P}_{sgs}(\psi)}{\partial x_j} - \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\bar{\rho}}{\rho(\psi)} \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_i} \right) = \\ & - \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\frac{\bar{\rho}}{\rho(\psi)} \tilde{P}_{sgs}(\psi) \frac{\mu}{\sigma} \left(\frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \Big|_{\phi = \psi} \right) \right) \\ & - \sum_{\alpha=1}^N \frac{\partial}{\partial \psi_\alpha} \left(\dot{\omega}_\alpha(\psi) \bar{\rho} \tilde{P}_{sgs}(\psi) \right) \end{aligned} \quad (3.3.1)$$

In this equation the chemical reaction term is in closed form. The sgs-convection and -mixing terms are unclosed due to the conditional filtering and require modelling, which will be outlined in the following sections. An additional minor modelling assumption that will be made for the diffusion term and the scalar dissipation term is that $\bar{\rho} = \rho(\psi)$ (Jaberi et al., 1999).

3.3.1 Convection Term

It is common practice to split the sgs-convection term in two and approximate part of it in a similar manner to the sgs-stress of the filtered momentum equation, with a gradient approximation in analogy to the Smagorinsky model.

$$\bar{\rho}(u_j | \widetilde{\phi = \psi}) \tilde{P}_{sgs}(\psi) = \bar{\rho} \tilde{u}_j \tilde{P}_{sgs}(\psi) + T_{sgs} \quad (3.3.2)$$

Where the first term on the rhs is the convective transport by the filtered velocity and the second term, T_{sgs} , is the scalar conditioned transport by sgs fluctuations, modelled as:

$$T_{sgs} = \bar{\rho}(\widetilde{(u_j|\phi = \psi)} - \tilde{u}_j)\tilde{P}_{sgs}(\psi) = -\frac{\mu_{sgs}}{\sigma_{sgs}}\frac{\partial\tilde{P}_{sgs}(\psi)}{\partial x_j} \quad (3.3.3)$$

3.3.2 Micro-Mixing Term

The first term on the rhs of Equation 3.3.1 is commonly referred to as the micro-mixing term and describes the effect of molecular diffusion of the pdf $P(\psi)$ i.e. transport in composition space. Its cross derivatives describe the conditional molecular mixing which cause scalar fluctuations to decay. It requires closure due to the conditionally filtered scalar covariance dissipation rate term (Prasad, 2011). A very detailed discussion of the term and different existing models is provided by (Fox, 2003). The most commonly used closure, based on its performance, implementation, the fact that at high Reynolds numbers it should have a low impact (in particular in the LES context) and the lack of evidence that more complex models yield any advantage (Prasad, 2011), is the Linear Mean Square Estimation (LMSE) closure originally developed by (Dopazo&O'Brien, 1974).

The unclosed term is replaced by:

$$\frac{C_d}{\tau_{sgs}} \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} \left[(\psi_{\alpha} - \tilde{\phi}_{\alpha}(\mathbf{x}, t)) \bar{\rho} \tilde{P}_{sgs}(\psi) \right] \quad (3.3.4)$$

As pointed out in (Brauner et al., 2016), it should be noted that the LMSE model does not satisfy the limiting property of approaching zero as the variation in ϕ over the filter volume become linear; the construction of such a model appears difficult and is beyond the scope of this work. Also the model for the micro-mixing term should be such that the pdf collapses to a Dirac δ -function in the limit of the sgs variations approaching zero, i.e. in well resolved regions of the flow or where the DNS limit is achieved and thus there is no sub-grid viscosity. In this limiting case the time scale τ_{sgs} should tend to zero. The sgs viscosity provides a measure of sgs fluctuations and this can be used to ensure the desired limiting behaviour. A

dynamic model for the sub-grid viscosity is used to determine C_s and a zero value of this implies no sgs variations. Thus analogous to (Jones et al., 2012) a modified time scale is employed:

$$\tau_{sgs} = \frac{\bar{\rho}\Delta^2}{\mu + \mu_{sgs}}(1 - \exp(-R^2)) \quad (3.3.5)$$

Where R is defined as the ratio of sub-grid to molecular viscosity, $R = \mu_{sgs}/\mu$. This modified time scale has the desired limiting behaviour $\tau_{sgs} \rightarrow 0$ as $\mu_{sgs} \rightarrow 0$ for well resolved and low turbulence areas, with the consequence that the pdf will tend towards a Dirac δ -function. The model provides increased micro-mixing in regions where the sgs fluctuations are small although the modification becomes effective only if the sgs viscosity is comparable with or small compared to the molecular viscosity.

3.3.3 Sub-grid PDF Transport Equation

With all unclosed terms modelled the transported sub-grid pdf equations finally becomes:

$$\begin{aligned} & \frac{\partial \bar{\rho} \tilde{P}_{sgs}(\boldsymbol{\psi})}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{P}_{sgs}(\boldsymbol{\psi})}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\left(\frac{\mu}{\sigma} + \frac{\mu_{sgs}}{\sigma_{sgs}} \right) \frac{\partial \tilde{P}_{sgs}(\boldsymbol{\psi})}{\partial x_i} \right) = \\ & - \frac{C_d}{\tau_{sgs}} \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left[(\psi_\alpha - \tilde{\phi}_\alpha(\mathbf{x}, t)) \bar{\rho} \tilde{P}_{sgs}(\boldsymbol{\psi}) \right] - \sum_{\alpha=1}^N \frac{\partial}{\partial \psi_\alpha} \left(\dot{\omega}_\alpha(\boldsymbol{\psi}) \bar{\rho} \tilde{P}_{sgs}(\boldsymbol{\psi}) \right) \end{aligned} \quad (3.3.6)$$

3.3.4 Modified Treatment of the Micro-Mixing Term

The flames considered in the present work have low to moderate Reynolds numbers ($Re \approx 1500-10000$). The sgs-fluctuations can be very small or absent in some regions of the flow, in particular in the immediate vicinity of bluff-bodies/flame holders and flame attachment locations. In these circumstances it is important that the sgs-pdf behaves correctly in the limit of small and zero sgs-fluctuations. Motivation and necessity of a reformulation of the sgs-pdf equation will be illustrated in chapter 5 in application to the V-flame burner under investigation.

It is proposed to treat the first term on the rhs of Equation 3.3.1 in the same manner as the convection term in Section 3.3.1, by splitting it into resolved and unresolved

parts (Brauner et al., 2016):

$$\begin{aligned} & \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\tilde{P}_{sgs}(\psi) \frac{\mu}{\sigma} \left(\frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \right) \Big| \phi = \psi \right) = \\ & \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\tilde{P}_{sgs}(\psi) \frac{\mu}{\sigma} \frac{\partial \tilde{\phi}_\alpha}{\partial x_i} \frac{\partial \tilde{\phi}_\beta}{\partial x_i} \right) + M_{sgs} \end{aligned} \quad (3.3.7)$$

Thus only M_{sgs} , rather than the whole term, is modelled using the LMSE in Equation 3.3.4.

In the derivation of the stochastic field method the molecular viscosity term of Equation 3.3.6 is associated with the stochastic term. The sum of the molecular and sub-grid viscosities appear in the stochastic term and have the effect that it does not vanish even when the sub-grid viscosity approaches zero. This alternate formulation effectively removes the molecular viscosity from the stochastic term in the sfm formulation allowing it vanish with vanishing sgs-viscosity.

3.4 Modified Sub-grid PDF Transport Equation

An alternate formulation of the transport equation for the sub-grid pdf, using the treatment of the micro-mixing term introduced in Equation 3.3.7, can be written as:

$$\begin{aligned} & \frac{\partial \bar{\rho} \tilde{P}_{sgs}(\psi)}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{P}_{sgs}(\psi)}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_i} \right) \\ & + \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\tilde{P}_{sgs}(\psi) \frac{\mu}{\sigma} \frac{\partial \tilde{\phi}_\alpha}{\partial x_i} \frac{\partial \tilde{\phi}_\beta}{\partial x_i} \right) + \sum_{\alpha=1}^N \frac{\partial}{\partial \psi_\alpha} \left(\dot{\omega}_\alpha(\psi) \bar{\rho} \tilde{P}_{sgs}(\psi) \right) = \\ & - \frac{\partial}{\partial x_i} \left(\frac{\mu_{sgs}}{\sigma_{sgs}} \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_i} \right) - \frac{C_d}{\tau_{sgs}} \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left[(\psi_\alpha - \tilde{\phi}_\alpha(\mathbf{x}, t)) \bar{\rho} \tilde{P}_{sgs}(\psi) \right] \end{aligned} \quad (3.4.1)$$

Where now $\tau_{sgs} = \frac{\bar{\rho} \Delta^2}{\mu_{sgs}} (1 - e^{-R^2})$.

In Equation 3.4.1 the resolved contributions to the advection and the sgs molecular diffusion/mixing terms have been added to both sides of the equation with the consequence that the rhs of the equation involves contributions from sgs fluctuations

only; identically zero if sgs variations are zero, i.e. the variations in all relevant quantities over the filter volume are negligible. The final term on the rhs of the equation, the diffusive mixing term, approaches zero as the variation of ϕ over the filter volume become linear. The shape of the pdf in this latter limit, and with velocity and density constant over the filter volume, depends on the choice of filter. For the “top-hat” filter presently used the pdf becomes uniformly distributed between the minimum and maximum values arising at the edges of the filter volume. In the DNS limit where the governing equations are solved without approximation the filtering operation has negligible influence and the pdf reduces to the fine-grained pdf. The lhs of the equation involves only known terms whereas the rhs requires modelling in LES. This separation of terms is common practice for the advection term but to date does not seem to have been applied to the diffusive mixing term. A further consequence of the approach is that the $\tilde{P}$ equation becomes exact in the limit that sgs variations are zero.

Also pointed out in (Brauner et al., 2016), a form similar to Equation 3.4.1 is proposed in (Valiño et al., 2015), although without motivation for the necessity of a modification. A Reynolds decomposition is applied to the exact equation for P , effectively separating out the turbulent contribution to diffusive mixing. While the proposal of (Valiño et al., 2015) is consistent with an entirely laminar flow, when extended to the LES context it does not ensure that the pdf collapses to a Dirac delta function in any region of a turbulent flame where the flow becomes laminar, i.e. where sgs fluctuations become negligible.

3.5 Monte-Carlo Solution Methods

The pdf in question is a function of time, 3 spatial dimensions and a number of chemical species, depending on the reaction mechanism, and the enthalpy. This high dimensionality does not permit the use of conventional discretisation methods and instead stochastic solution methods are sought.

Monte-Carlo is a technique using computer generated random numbers to sample a probability density function in order to obtain numerical results.

The key enabling factor, in the context of transported pdf methods, is the possibility of rearranging the pdf transport equation into a Fokker-Planck-like equation. Subsequently the relationship between the Fokker-Planck Equation and Stochastic Differential Equations can be benefited from. The details of this connection are beyond the scope of the present work, however the reader may refer to e.g. (Gardiner, 2009) (Chapters 2-4) for a very detailed derivation. The Fokker-Planck Equation is a special form of the differential Chapman-Kolmogorov equation that describes generalised diffusion processes. While the Chapman-Kolmogorov equation can also be used to model instantaneous jump processes, the Fokker-Planck equation only accounts for drift and diffusion processes. As such it is used to describe the time evolution of a probability density function.

For a pdf $P(\boldsymbol{\psi}; \mathbf{x}, t)$, where as before $\boldsymbol{\psi}$ is a vector of N_s random variables, the Fokker-Planck equation takes the following form (Gardiner, 2009):

$$\begin{aligned} \frac{\partial P(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial t} = & - \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} (A_{\alpha}(\boldsymbol{\psi}; \mathbf{x}, t) P(\boldsymbol{\psi}; \mathbf{x}, t)) \\ & + \frac{1}{2} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_{\alpha} \partial \psi_{\beta}} (B_{\alpha\beta}(\boldsymbol{\psi}; \mathbf{x}, t) B_{\beta\alpha}(\boldsymbol{\psi}; \mathbf{x}, t) P(\boldsymbol{\psi}; \mathbf{x}, t)) \end{aligned} \quad (3.5.1)$$

Where A_{α} is the drift coefficient vector and $B_{\alpha\beta}$ the diffusion coefficient matrix. The equivalent stochastic differential equation to Equation 3.5.1, using the Itô interpretation of the stochastic integral is:

$$d\psi_{\alpha} = A_{\alpha}(\boldsymbol{\psi}; \mathbf{x}, t)dt + B_{\alpha\beta}(\boldsymbol{\psi}; \mathbf{x}, t)dW_{\beta}(t) \quad (3.5.2)$$

In the following section the transported pdf Equation 3.4.1 is recast into Equation 3.6.3, which takes the form of the above Fokker-Planck Equation 3.5.1 (steps are outlined in Appendix A). Then, using just the relationship between the above Fokker-Planck Equations 3.5.1 and stochastic differential Equation 3.5.2, it is already possible to arrive at the terms of the Stochastic Field Equations 3.6.4, equivalent to the transported pdf equation.

3.6 Eulerian Monte-Carlo, the Stochastic Fields method

The closed form of the equation describing the evolution of the pdf, Equation 3.4.1, is solved using the Eulerian stochastic field method, (Valiño, 1998). $\tilde{P}(\boldsymbol{\psi}; \boldsymbol{x}, t)$ is represented by an ensemble of N stochastic fields for each of the N_s scalars namely $\xi_\alpha^n(\boldsymbol{x}, t)$ with $1 \leq n \leq N$; $1 \leq \alpha \leq N_s$.

$$\tilde{P}_{gs}(\boldsymbol{\psi}; \boldsymbol{x}, t) = \frac{1}{N} \sum_{n=1}^N \prod_{\alpha=1}^{N_s} \delta(\psi_\alpha - \xi_\alpha^n(\boldsymbol{x}, t)) \quad (3.6.1)$$

This method was originally proposed by (Valiño, 1998) in the RANS context using the Itô formulation of the stochastic integral. (Sabel'nikov&Soulard, 2005) developed an equivalent method using a different approach and the Stratonovich formulation of the stochastic integral. As pointed out by (Jones, 2012) similar methods have been developed by different researchers e.g.: Configuration field method, (Laso&Öttinger, 1993), Multi-fluid method, (Spalding, 1995). The necessary developments to make use of the Stochastic Fields method in the context of LES were carried out by (Mustata et al., 2006) and (Jones&Navarro-Martinez, 2007).

The idea is to represent the pdf with Eulerian stochastic fields instead of Lagrangian notional particles. According to (Valiño, 1998) these fields have similar length scales to those of the pdf, which in the LES context implies that they do not have any sub-grid contributions i.e. they are smooth at the scale of the filter width. By extension this also means that the stochastic fields do not represent real fields, but rather fields whose statistics are equivalent to those of the pdf being modelled. (Valiño, 1998) goes on to explain, that the relationship between the field ξ^n and the pdf can be expressed as:

$$\xi^n(\boldsymbol{x}, t) = F^{-1}(\nu^n(\boldsymbol{x}, t); \boldsymbol{x}, t) \quad (3.6.2)$$

Where F is the cumulative distribution function of the pdf P and ν are another set of stochastic fields with uniform distribution. Equation 3.6.2 is then the formal statement of generating a random sample ξ^n from a probability distribution P , here

extended to fields rather than individual points. Therefore, the stochastic fields ξ^n represent possible sampling outcomes of the pdf P , which according to (Jones, 2012) are continuous and twice differentiable in space, and continuous, but not differentiable in time. (Non-differentiability is due to the presents of the increment of a Wiener process dW and is also the reason equation 3.6.4 is generally expressed in increment form rather than derivative form.)

Substituting Equation 3.6.1 for $\tilde{P}(\boldsymbol{\psi}; \mathbf{x}, t)$ in Equation 3.4.1 and rearranging into the form of Equation 3.5.1 (see Appendix A.4 for details), with $\delta_\xi^n = \delta(\boldsymbol{\psi} - \boldsymbol{\xi}^n)$ and $\mu_T = \mu + \mu_{sgs}$, results in:

$$\begin{aligned}
\frac{1}{N} \sum_{n=1}^N \frac{\partial}{\partial t} \bar{\rho} \delta_\xi^n &= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\delta_\xi^n \left(-\bar{\rho} \tilde{u}_i \frac{\partial \xi_\alpha^n}{\partial x_i} + \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \right) \right) \right) \\
&+ \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\delta_\xi^n \left(\frac{\mu_T}{\sigma_T} - \frac{\mu}{\sigma} \right) \frac{\partial \xi_\alpha^n}{\partial x_i} \frac{\partial \xi_\beta^n}{\partial x_i} \right) \right) \\
&- \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\bar{\rho} C_d}{2\tau_{sgs}} (\xi_\alpha^n - \tilde{\phi}_\alpha) \right) \right) \\
&+ \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} (\bar{\rho} \dot{\omega}_\alpha^n(\boldsymbol{\xi}^n)) \right) \tag{3.6.3}
\end{aligned}$$

The first and second terms of the rhs resemble those of Equation 3.5.1, while the last two represent separate contributions to each field in composition space, without explicitly including the pdf. In the present work the Itô formulation of the stochastic integral is adopted, thus as specified by Equation 3.5.2 the stochastic fields evolve according to the following stochastic partial differential equation:

$$\begin{aligned}
\bar{\rho} d\xi_\alpha^n &= -\bar{\rho} \tilde{u}_i \frac{\partial \xi_\alpha^n}{\partial x_i} dt + \frac{\partial}{\partial x_i} \left(\left(\frac{\mu}{\sigma} + \frac{\mu_{sgs}}{\sigma_{sgs}} \right) \frac{\partial \xi_\alpha^n}{\partial x_i} \right) dt + \left(2\bar{\rho} \frac{\mu_{sgs}}{\sigma_{sgs}} \right)^{1/2} \frac{\partial \xi_\alpha^n}{\partial x_i} dW_i^n \\
&- \frac{\bar{\rho} C_d}{2\tau_{sgs}} (\xi_\alpha^n - \tilde{\phi}_\alpha) dt + \bar{\rho} \dot{\omega}_\alpha^n(\boldsymbol{\xi}^n) dt \tag{3.6.4}
\end{aligned}$$

The difference between the above equation and the original proposed by e.g. (Jones&Navarro-Martinez, 2007) is that the stochastic term now only contains the sub-grid viscosity μ_{sgs} .

dW_i^n represents increments of a vector Wiener process, different for each field but

independent of the spatial location x . The factor 2 and the square root in the dW_i^n -term emerge from the relationship with the last term of Equation 3.5.1: The diffusion term in the Fokker-Planck equation is multiplied by 1/2 and the equivalent to $B_{\alpha\beta}B_{\beta\alpha}$ comprises μ_{sgs}/σ_{sgs} as well as the derivatives of the stochastic fields. This stochastic term has no effect on the first moments (or filtered values) of ξ_α^n , but exerts a strong influence on the shape and “width” of the pdf. It has the following properties regarding its mean and variance:

$$\langle d\mathbf{W} \rangle = 0 \quad (3.6.5)$$

$$\langle d\mathbf{W}^2 \rangle = dt \quad (3.6.6)$$

The Wiener process is approximated by time-step increments $\eta_i^n \sqrt{dt}$, where η_i^n is a $\{-1, +1\}$ dichotomic random vector. The solutions of Equation 3.6.4 preserve any bound properties of the scalar in question as the gradient of the scalar will tend to zero as the value of the scalar approaches extrema values, and therefore the stochastic contribution will tend to zero. The solutions for each field will satisfy all the mass conservation and bound properties of the modelled pdf Equation 3.4.1. For each field, for example, the species mass fractions will remain positive and will sum to unity. For a large number of fields the filtered value of the stochastic term will tend to zero. The solutions of the stochastic field Equation 3.6.4 form an equivalent stochastic system (both sets have the same one-point pdf, (Gardiner, 2009) smooth on the scale of the filter width. All the moments resulting from the stochastic differential equations and from the direct solutions of the modelled form of Equation 3.4.1 will be identical. All of the moments of the scalar fields were obtained by averaging over the stochastic fields as appropriate. For example all first moments are obtained, using equation 3.1.1 and 3.1.9, from:

$$\tilde{\phi}_\alpha = \frac{1}{N} \sum_{n=1}^N \int \psi_\alpha \delta(\psi_\alpha - \xi_\alpha^n) d\psi_\alpha = \frac{1}{N} \sum_{n=1}^N \xi_\alpha^n \quad (3.6.7)$$

Chapter 4

Numerical Implementation

The code used and further developed over the course of this work and with which the results in the following chapters were generated is the in-house code BOFFIN-LES (BOundary Fitted Flow INtegrator) (Jones et al., 2002). It has been incrementally been augmented and improved, and validated against a variety of test cases by a number of different colleagues over the years.

4.1 Boffin properties and previous test cases

Boffin implements a Large Eddy Simulation approach using block-structured domain decomposition and finite volume method (FVM) discretisation. In order to account for complex geometries, coordinates are transformed to general curvilinear coordinates that conform with the boundaries. An incompressible low Mach number formulation is used with a SIMPLE-type pressure correction algorithm together with the (Rhie&Chow, 1983) pressure smoothing method on a collocated storage arrangement. The discretisation schemes used are formally second order accurate, using Crank-Nicholson for temporal derivatives and central differences for all spatial terms with exception of the convective terms of the scalar transport equations which use a Total Varying Diminishing scheme.

(Wille, 1997) conducted extensive research in to discretisation, both in space and in time, and the pressure algorithm, validating some of the codes foundation. (Keays, 2006) investigated premixed combustion using a presumed-beta-pdf method. (Bini, 2006) added spray combustion functionalities. (Jones&Navarro-Martinez, 2007) first

introduced the stochastic field solution method (Prasad, 2011) investigated time stepping schemes, performed stability analysis, and was the first to use the SFM in premixed and partially premixed context and introduced the micro-mixing scaling. (Bulat, 2012) applied the SFM to an industrial gas turbine configuration at high Reynolds numbers. More recently (Dodoulas&Navarro-Martinez, 2013), (Noh et al., 2014) and (Jurisch et al., 2015) and expanded on e.g. the spray capabilities or ability to simulate pressure effects.

Owing to the Eulerian nature of the stochastic fields solution method, the scalar transport-like equations can be implemented with relative ease using existing routines, with the additional detail of the implementation of the stochastic and micro-mixing terms.

4.2 Reaction Mechanisms

The fuel and oxidiser used in both burners investigated are methane and standard atmospheric air. Two reaction mechanisms for methane-air combustion were used in the present work: for initial simulations the global mechanism of (Jones&Lindstedt, 1988) involving 7 species and 4 reaction steps was used. However, the results obtained and presented in the subsequent chapters used the Augmented Reduced Mechanism (ARM) by (Sung et al., 2001) based on the GRI-Mech 3.0 (Smith et al.) involving 19 species and 15 reaction steps.

4.3 Interaction of Stochastic Term and Micro-mixing Term

In this section the motivation to alter the formulation of the pdf equation 3.4.1 is discussed along with modifications to the stochastic fields solution algorithm. The necessity is illustrated through the discussion of the relevant parts of the algorithm and through observations made simulating the V-flame discussed in more depth in Chapter 5.

4.3.1 Stochastic Fields Solution Algorithm

Following (Jones et al., 2012) the algorithm implemented for the time advancement of the stochastic fields takes the following three part fractional-step form, in the context of a predictor-corrector algorithm:

$$\bar{\rho}d\xi_\alpha^n = \left(\mathcal{A}(\xi_\alpha^n) + \mathcal{D}(\xi_\alpha^n) + \mathcal{S}(\xi_\alpha^n) \right) + \mathcal{M}(\xi_\alpha^n, \tilde{\phi}_\alpha) + \mathcal{R}(\xi^n) \quad (4.3.1)$$

Where $\mathcal{A}$ is the advection, $\mathcal{D}$ the diffusion, $\mathcal{S}$ the stochastic contribution, $\mathcal{M}$ the micro-mixing and lastly $\mathcal{R}$ the reaction term of Equation 3.6.4. Each field for each species is first advanced collectively by convection, diffusion with the stochastic term as an explicit source term, followed by the separate evaluation of the the micro-mixing term and then the integration of the chemical source term.

Of particular interest are the implementation and interaction of the stochastic term and the micro-mixing term. Essentially, the stochastic term serves to increase the variance of the pdf being modelled while the micro-mixing term serves to reduce the variance by interacting with the mean field value.

In the following, the indices associated with the stochastic fields will be dropped for clarity. $\xi^{(1)}$ refers to the value of ξ as a result of the first fractional step and t_n refers to the current time level as opposed to the n -th stochastic field (Jones et al., 2012). The first fractional step and the stochastic term are implemented as follows:

$$\bar{\rho}\xi^{(1)} = \bar{\rho}\xi(t_n) + \left(\mathcal{A}(\xi^{(1)}) + \mathcal{D}(\xi^{(1)}) \right) \Delta t + \mathcal{S}(\xi(t_n)) \Delta t \quad (4.3.2)$$

The raised (1) indicates that $\mathcal{A}$ and $\mathcal{D}$ are advanced implicitly using a Crank-Nicholson scheme. The increment of the Wiener process is represented by $\eta_i^n \sqrt{dt}$, where η_i^n is a $\{-1, +1\}$ dichotomic random vector, chosen to ensure that the mean and variance of the random vector are zero and unity respectively. In the conventional formulation of the pdf equation the stochastic term scales with the square root of the sum of molecular and sub-grid viscosities. The new formulation, Equation 3.4.1 and correspondingly Equation 3.6.4, only contains the square root of the sub-grid viscosity alone.

The micro-mixing term is implemented as follows (Prasad, 2011):

$$\xi^{(2)} = \frac{\xi^{(1)} + \beta \Delta t \tilde{\phi}^{(1)}}{1 + \beta \Delta t} \quad (4.3.3)$$

Where $\beta = 0.5C_d/\tau_{sgs}$. The mean field $\tilde{\phi}$ is chosen to be the intermediate mean field $\tilde{\phi}^{(1)}$, formed by averaging over the individual stochastic fields after the first fractional step. This was chosen in order to avoid the need for complex algebraic systems, under the assumption that the micro-mixing term is of stabilising nature, driving the solution back towards the mean. The scaling of beta (Chapter 3) is implemented as follows:

$$\beta^* = \beta \frac{1 + \frac{\mu_{sgs}}{\mu}}{\frac{\mu_{sgs}}{\mu}} \quad (4.3.4)$$

Crucially however, particularly in low Reynolds number situations, this implementation does not permit the micro-mixing term to properly counteract the stochastic term if necessary, even with the previously mentioned scaling in place. While the desired effect of driving the individual fields to the mean as $\mu_{sgs} \rightarrow 0$ is achieved, the intermediate mean $\tilde{\phi}^{(1)}$ itself can have been shifted due to the non-vanishing and non-zero-mean stochastic terms and the use of a finite number of fields.

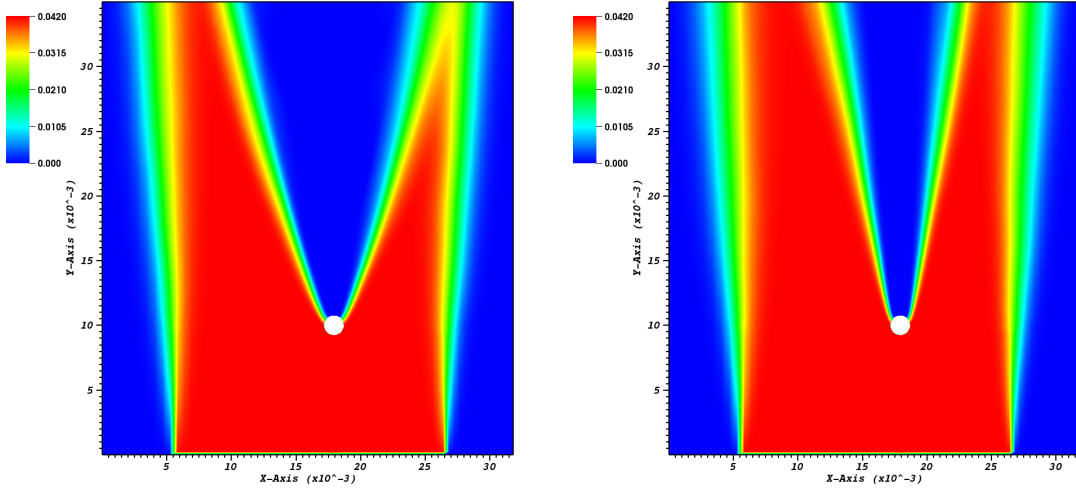


Figure 4.1: Mean methane concentration with 8 stochastic fields for the fully premixed V-flame fs1. On the left the original, and on the right the new and improved formulation and implementation

The effect is pronounced and manifests itself e.g. in over-predicted flame angles/burning velocities for the V-flame configuration, in particular in the vicinity of the flame

holder. This is illustrated in Figure 4.1 for the fully premixed V-flame. The image on the left show the time averaged concentration of CH_4 with 8 stochastic fields to characterise the sub-grid contributions and the old formulation and implementation of the stochastic and micro-mixing terms. The flame angle is $\theta \approx 17^\circ$ relative to the centreline; a significant over-prediction of flame angle/burning velocity compared to the experimental data. From the experimentally measured profiles of (Anselmo-Filho, 2008) the mean flame angle for the flame in Figure 4.1 can be computed to be $\theta_{fs1} \approx 11^\circ$. A more detailed discussion of the V-flame will follow in Chapter 5; however, the images serve to illustrate the effect of a non-vanishing stochastic term in a configuration with low Reynolds number $Re \approx 2000$ and ratios of sub-grid to molecular viscosity of $\mu_{sgs}/\mu < 1$. The image on the right shows the same flame also with 8 stochastic fields, however with the new formulation as well as a modified solution algorithm detailed in the following section. Here, the flame angle is $\theta \approx 9^\circ$; much closer to the experimental data.

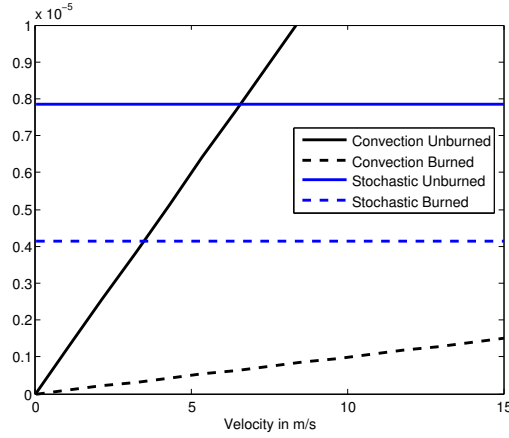


Figure 4.2: Competition of convection and stochastic terms

A notional comparison of the magnitudes of advection and non-vanishing stochastic terms is shown in Figure 4.2. Listed in Table 4.1 are typical values contained in the advection and stochastic terms, as they are encountered in the fresh and burned mixtures of a premixed methane-air flame. The sloped lines are functions of the velocity in the advection term. The plots show clearly that for a large range of velocities the stochastic term can dominate the convection term in magnitude. Thus, if it affects the mean field it can do so in a significant manner.

Table 4.1: Typical values of density, molecular viscosity and time step encountered in premixed flames

dt	ρ_U	ρ_B	μ_U	μ_B	σ
$1e-6$	1.2	0.1	$1.8e-5$	$6.5e-5$	0.7

4.3.2 Modified Solution Algorithm

In the following “mean field” refers to the mean of the stochastic fields, as per Equation 3.6.7, not the time averaged fields. The choice of intermediate mean field $\tilde{\phi}^{(1)}$ in Equation 4.3.3, towards which the fields are driven by the micro-mixing term at low sub-grid viscosities, was initially the cause of discrepancies. A quick solution to this, is to either lag the mean field by one time step or to use the mean field for which auxiliary transport equations are solved for stochastic noise reduction purposes (see (Prasad, 2011) Chapter 4).

While this improves results greatly, it does not address the behaviour of the intermediate mean field after time advancement due to convection, diffusion and the stochastic term. The stochastic term is only meant to affect the variance for the simulated quantity, not the mean field. It is for this purpose that the Wiener process is represented as a dichotomic random vector with zero mean and unity variance. It is however assumed that the following relation holds:

$$\lim_{N \rightarrow \infty} \sum_{n=1}^N b^n dW_i^n = \sum_{n=1}^N b^n \times \sum_{n=1}^N dW_i^n \quad (4.3.5)$$

where $b^n dW_i^n = \left(2\bar{\rho} \frac{\mu_{sgs}}{\sigma_{sgs}}\right)^{1/2} \frac{\partial \xi_{\alpha}^n}{\partial x_i} dW_i^n$ is the stochastic term. This is generally true for very large N , however the terms b^n and dW_i^n are not uncorrelated for low values of N , which are typically used for the SFM i.e. $N = 8$ stochastic fields. (The effect of the number stochastic fields was investigated e.g. in the context of (Jones&Navarro-Martinez, 2007) and it was found that 8 fields offered a good compromise between simulation accuracy and computational affordability.) Further to this, it can be seen in Figure 4.2 that if at a given point in the computational domain some of the fields are on the unburned and others on the burned side of the flame, the stochastic terms in the unburned side of a flame will always outweigh, in magnitude, the terms on the

burned side. This necessitates the stochastic terms to be corrected. For this purpose the following correction is introduced in order to ensure the mean contribution is zero:

$$(b^n dW_i^n)_{corrected} = b^n dW_i^n - \langle b dW_i \rangle \quad (4.3.6)$$

The above correction must be applied to every field of each species at every time step. The need for a scaling of the micro-mixing term as well as the above listed modifications to ensure that the large (for low Reynolds numbers), non-vanishing (when $\mu_{sgs} = 0$) stochastic term interacts correctly with the micro-mixing term, raises the question whether the terms can be modified to diminish the need for their strong interaction. It is also questionable that the stochastic terms should be large for low Reynolds numbers, when the pdf being modelled should collapse to a delta-function in the limit of $\mu_{sgs} = 0$. This led to the formulation of the decomposition introduced in Section 3.3.4.

4.4 Digital Inflow Generation

In order to account for turbulence at the inlets to the computational domains without adding the computational expense of simulating a large upstream region of the burner geometries, a digital inflow generation method is employed. A detailed description of the method can be found in (Klein et al., 2003) and (Klein et al., 2006). Essentially a box of turbulence is generated with unit mean and variance using a digital filtering technique. Taylor's Hypothesis is invoked such that the planes formed by the first two dimensions of the box correspond to the computational domains inflow plane, onto which a velocity signal is superimposed. The third dimension can then be interpreted as representing time, $\Delta t = \Delta x_3 / U_3$. Therefore the evolution of the inflow plane can be viewed as the result of convecting the scaled box of turbulence past the inflow plane at the average stream-wise inlet velocity.

The geometry for the swirl burner includes some of the upstream burner geometry in order to allow the flow to develop before the measurement locations. For the V-Flame of the slot burner however, no upstream geometry is included due to lack of sufficient information.

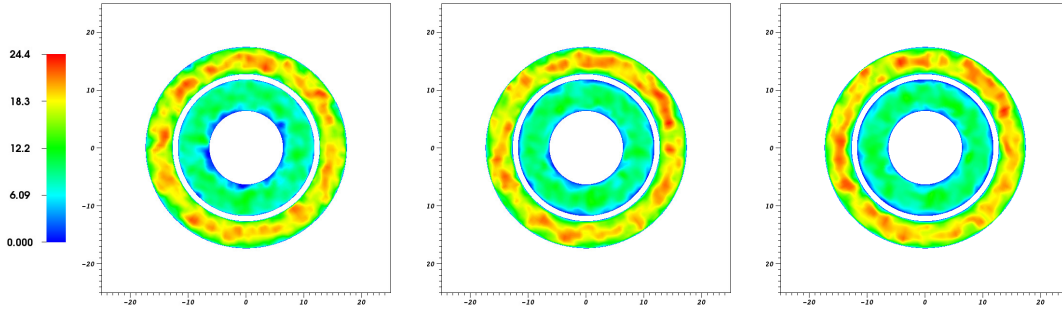


Figure 4.3: Example Inflow Planes for cSwB1

4.5 Asymmetry of swirl burner measurements

Annular bluff bodies can show asymmetric behaviour which can manifest itself in the measurements of the mean profiles of both flow field and scalar fields and is amplified at further downstream locations. This is observed in the experimental measurements of the swirl burner under investigation. Figure 4.4 shows a Favre averaged profile of methane concentration of the fully premixed flame SwB1 at $50mm$ downstream of the burner exit.

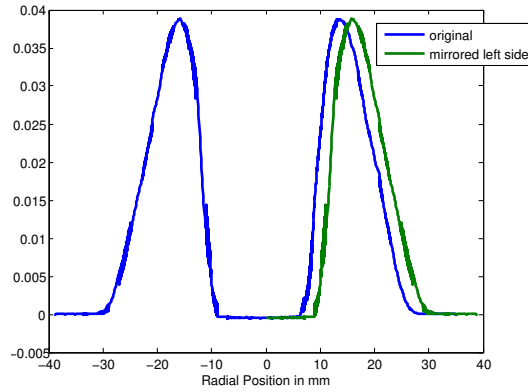


Figure 4.4: Experimentally measured profile of Favre averaged methane concentration for SwB1 at $50mm$ downstream of the burner exit

The left half of the profile has been mirrored across $r = 0mm$, onto the right, to illustrate the difference in distance of the peaks from the burner centreline. In this particular example the difference is approximately $2mm$. In order to compare numerical and experimental results, the experimental profiles, where possible, have been averaged across the measurement profile i.e. shifted to the average position

and then averaged the values.

Similarly, after gathering statistics and time averaging the numerical results over a certain number of time steps, the results are further averaged in the circumferential direction to form the simulation profiles presented in the following chapters. (The V-flame results of the slot burner are averaged in the axial direction of the rod.)

Chapter 5

Simulation of the Cambridge Stratified Slot Burner

A numerical investigation on the influence of stratification on a mildly turbulent premixed V-shaped flame is conducted. The configuration investigated is the Cambridge Stratified Slot Burner, of which three conditions, fully premixed, moderately and highly stratified, with stratification ratios of 1.0, 1.86 and 3.0 respectively, are simulated. Velocity and turbulence intensity for the isothermal case and mean temperature and species concentrations for the premixed, non-stratified case are in good agreement with the experimental data. Moderately good accuracy is also achieved for the moderately and highly stratified cases.

The ability to accurately predict the behaviour of flames under stratified and partially premixed conditions, in particular at high levels of turbulence, is of great importance in the development of lower emissions higher efficiency combustion systems. To achieve this a deeper understanding of the fundamental cases is required, as demonstrated with the laboratory scale, low level turbulence Cambridge Stratified Slot Burner under investigation here. As combustion occurs mostly at the smallest scales the sub-grid scale combustion model is of central importance in providing an accurate description of turbulence-chemistry interactions.

Parts of the results presented in this section have in been previously reported in (Brauner et al., 2014).

5.1 Experimental Details, Setup, Measurement Techniques and Available Data

The Cambridge Stratified Slot Burner studied experimentally by (Anselmo-Filho et al., 2009), (Sweeney et al., 2011a), (Sweeney et al., 2011b). The properties of premixed and stratified lean turbulent V-shaped flames were measured with the aim of investigating in detail the structure of turbulent stratified flames and the influence of various ratios of stratification on premixed combustion.

The slot burner is described as “two-dimensional” and a schematic is shown in Figure 5.1. The burner has six adjacent inflow slots and a turbulence grid at the top of the slots. The two outer slots feed air to shield the flame and prevent entrainment near the measurement locations, whilst the two pairs in the middle feed in methane/air mixtures with variable equivalence ratios. Each of the three pairs of slots has a volumetric air flow rate of 85 l/min and stratification is achieved by splitting a total of 13.1 l/min of methane between the two central slot pairs. The stratification ratio is defined as the ratio of the equivalence ratio of the richer slot pair, $\phi_{E,2}$, to the leaner slot pair, $\phi_{E,1}$. The average equivalence ratio is maintained at 0.77 and 0.73 with and without an acetone tracer. The burner is unconfined and the flame is stabilised on a rod of diameter $d = 1.5\text{mm}$ which is positioned 2mm off the burner centre line and 10mm above the slot exits. The position is chosen such that one of the branches of the V-flame coincides with the mixing layer, indicated by the dot-slash-line in Figure 5.1, of the inlet slot pairs in the region where the measurements are taken.

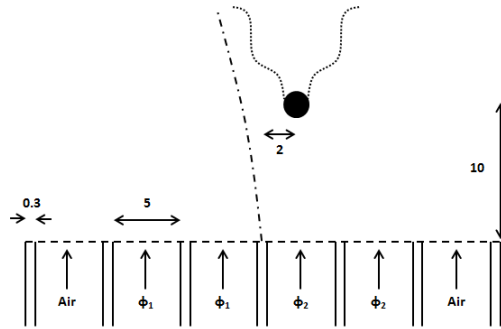


Figure 5.1: Schematic of the Cambridge Stratified Slot Burner geometry.

The turbulence grid used at the inflow is a wire mesh with a 1.02mm square pattern with an open area of approximately 79%. It results in a turbulence intensity of approximately 10% 5mm downstream of the rod and a ratio of u' , the velocity fluctuation, to S_L , the laminar flame speed, of just above unity. The thermal load of the burner is 7.1kW and the estimated values of Damköhler and Karlovitz numbers are $Da = 2.35$ and $Ka = 0.59$. The cold flow conditions of the measurements are summarised in Table 5.1. The flames lie in the corrugated flamelet zone of the Borghi diagram, but with their very low Reynolds numbers lie just adjacent to the laminar flamelet region. The Reynolds number based on the mean inlet velocity and the rod diameter is significantly lower than the quoted Reynolds number. The

Table 5.1: Slot Burner Cold Flow Properties

$\langle u \rangle$ m/s	u' m/s	u'/S_L -	Λ mm	η mm	Re -	Re_Λ -
3.1	0.3	1.3	1.9	0.09	2316	38

measurements were taken using a variety of different techniques: The flame front position was measured using planar laser-induced fluorescence (PLIF) of OH and acetone. Temperatures and concentrations of major species were measured with a combination of Raman scattering, Rayleigh scattering and laser induced fluorescence (LIF) of OH, (Anselmo-Filho et al., 2009). Data for the instantaneous and average flame structure is provided in the form of temperature and equivalence ratio profiles at fixed downstream locations. Profiles of Favre-averages and Favre-averaged rms fluctuations of temperature, species and equivalence ratio are provided at the same locations.

Table 5.2: Slot Burner flame names and stratification-ratios for different operating conditions.

Case	ϕ_2/ϕ_1
fsi	<i>isothermal</i>
fs1	$0.75/0.75 = 1.00$
fs4	$0.98/0.53 = 1.86$
fs6	$1.13/0.38 = 3.00$

5.2 Simulation Set-up

The experiment was conducted for six stratification ratios varying from fully premixed $\phi_2/\phi_1 = 1$ to highly stratified $\phi_2/\phi_1 = 1.16/0.39 \approx 3$. Here the premixed, intermediate $\phi_2/\phi_1 = 1.00/0.54 \approx 1.86$ and highly stratified cases are simulated. The computational domain used extends 45mm beyond the furthest downstream profile measurement location and covers the width of the six slots in the trans-axial direction and 20% of a slot depth in the horizontal direction (Simulation accounting for larger slot depths did not affect the simulation results, and the burner is referred to by (Sweeney et al., 2011a) as "two-dimensional"). A fine mesh of 144x286x24, consisting of about 1M cells divided amongst 48 blocks, is used, resulting in an average mesh spacing of less than 0.3mm in the proximity of the flame in the wake of the rod. The boundaries consist of an inlet, zero-gradient outflow conditions at the outlet, Neumann no-slip and adiabatic conditions at the rod and free slip conditions on all other boundaries.

A digital inflow generator is used to simulate the effect of the turbulence mesh placed over the inlet slots. A augmented reduced mechanism, (Sung et al., 2001) based on the GRI 3.0 mechanism with 15 reaction steps and 19 species is employed for the chemistry. For all cases eight stochastic fields were utilised to represent the sub-grid contributions. A model spark is used to initialise combustion and the simulations are run for one flow-through time after the initial disturbance from the spark has been carried out of the domain, before statistics are gathered.

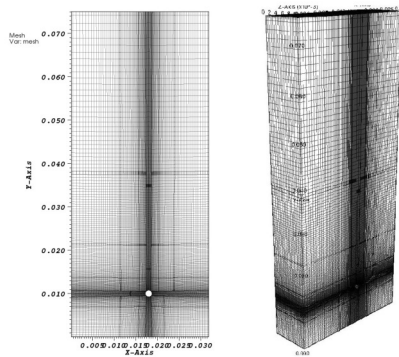


Figure 5.2: Frontal and 3D view of the V-Flame computational domain.

5.3 Results

The velocity of the generated inflow conditions is estimated using the single experimental profile available at $y=15\text{mm}$ above the turbulence grid over $x=0$ to 16mm relative to the burner centre line. The turbulence intensity is estimated using a length scale of 1.9mm , corresponding to the estimated integral length scale. These measurements were taken without the rod in place and only for the stream-wise velocity and corresponding turbulence intensity. The plots in Figure 5.3 show the mean velocity and turbulence intensity profiles respectively. Using the generated inflow data, the simulated mean velocity is in very good agreement with the velocity profile of the measurement. Away from the centre plane ($x=0\text{mm}$) the turbulence intensity profiles are also in good agreement, while at the centre plane there are discrepancies. The one available measured profile cover only half of the burner width, thus to generate inflow data for both halves without additional information, it was assumed that the measured profiles are symmetrical. This is likely a significant cause of differences, along with the lack of additional flow field information.

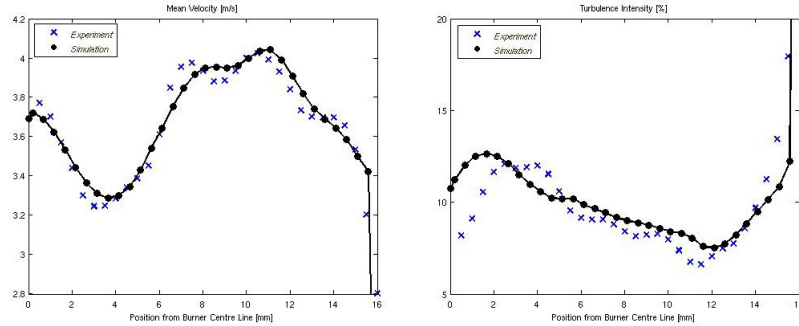


Figure 5.3: Mean velocity and turbulence intensity in stream-wise direction.

Profile measurements of temperature and species concentrations are provided at two downstream locations, $y=25\text{mm}$ and $y=30\text{mm}$. The profiles have a length of 7mm with positions $x=-5$ to 2mm and $x=-6.5$ to 0.5mm relative to the burner centre line, at the respective y -values for the premixed case. The stratified cases are measured at $x=-7.5$ to -0.5mm and $x=-9.5$ to -2.5mm at the same y -values. In comparing simulation results with experimental data the flame angle and burning velocity are crucial in achieving good agreement of profiles.

Sample instantaneous and mean images of methane concentration are shown in

Figure 5.4 and Figure 5.5 on the mid-plane of the simulations computational domain. The flame fronts are mildly turbulent and show wrinkling of ‘size’ of the order of the integral length scale. The flame is stabilised on the rod and the co-flow air shields the premixed region.

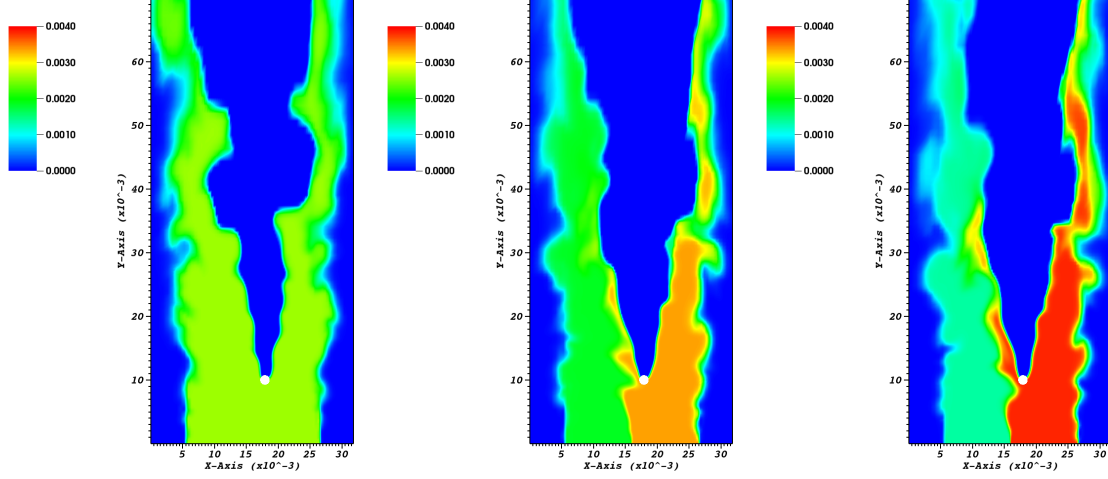


Figure 5.4: Three instantaneous snapshots of fs1, fs4 and fs6.

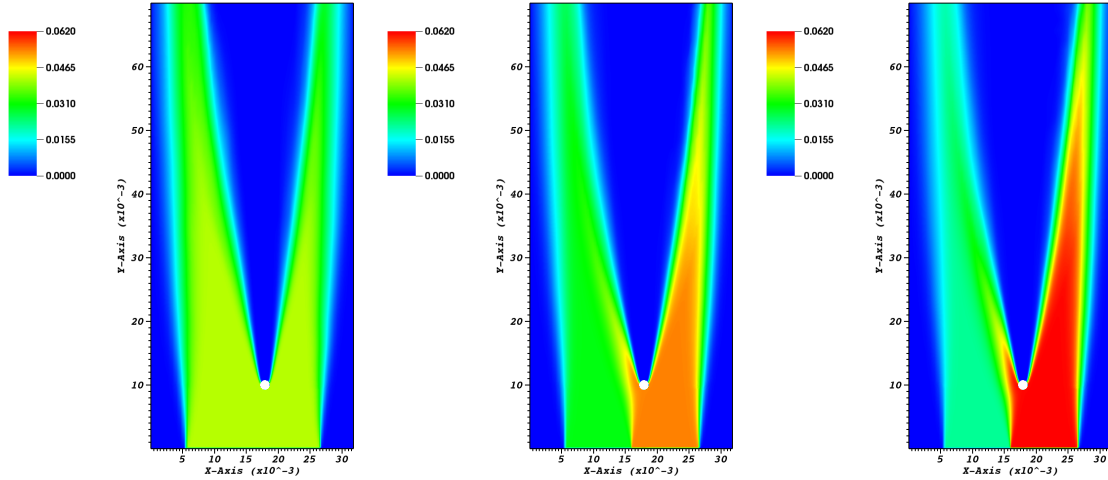


Figure 5.5: Three time averaged snapshots of fs1, fs4 and fs6.

The fuel/air mixture is assumed to be homogeneous leaving each slot, downstream of which in the stratified cases the interaction/mixing between streams of different methane concentrations can be seen. In the vicinity and downstream of the rod the interaction of the mixing layer with the left flame branch near the locations at which profile measurement are take can be observed. For the stratified cases 3 burning zones are captured, roughly separated by the measurement locations. This

can be seen clearly in the second and in particular third images of Figures 5.4 and 5.5. First, between the rod and the lower location, due to the rod being off centre, premixed combustion occurs at the higher equivalence ratio of the slot pairs. In the second region the flame interacts with the stratified mixing layer and back supported burning from high towards low equivalence ratios takes place. High temperatures and increased presence of radicals behind the flame can result in higher burning velocities supporting combustion into the lean mixture. Further downstream the flame interacts predominantly with the leaner mixture of the slot pairs, which for the highly stratified case is below the lean flammability limit.

Figures 5.6 through 5.8 compare profiles from the simulation results with experimental data for mean temperature and mean values of the major species concentrations of the three flames at both scalar measurement locations.

Effect of changes to SFM implementation on V-Flame

Figure 5.6 includes additionally to the final simulation results profiles from simulations performed prior to the incorporation of the changes to the formulation of the SFM (Chapter 3) and the code implementation in BOFFIN-LES (Chapter 4). These early results were computed using the same mesh and computational domain, as well as the same boundary conditions and are indicated by the dashed (magenta) lines. It can be seen clearly that the flame position differs strongly from the experimental data due to the flame spreading rate being significantly over-predicted. This was attributed to the non-vanishing stochastic term and its possible non-zero mean. The final updated results are indicated by the solid (black) lines.

For the premixed flame, Figure 5.6 the flame spreading rate and flame ‘thickness’ are well reproduced by the simulations and the peak, gradient and locations of the profiles of temperature, CH_4 , O_2 and CO_2 are in good agreement with the measurements. The simulated levels of CO and H_2 are somewhat lower than the measured values although it is to be noted that the concentrations are small. The simulated and measured profiles for the moderately stratified flame at $y = 25\text{mm}$, 5.7 are in good agreement. In contrast to the premixed case this case the levels of

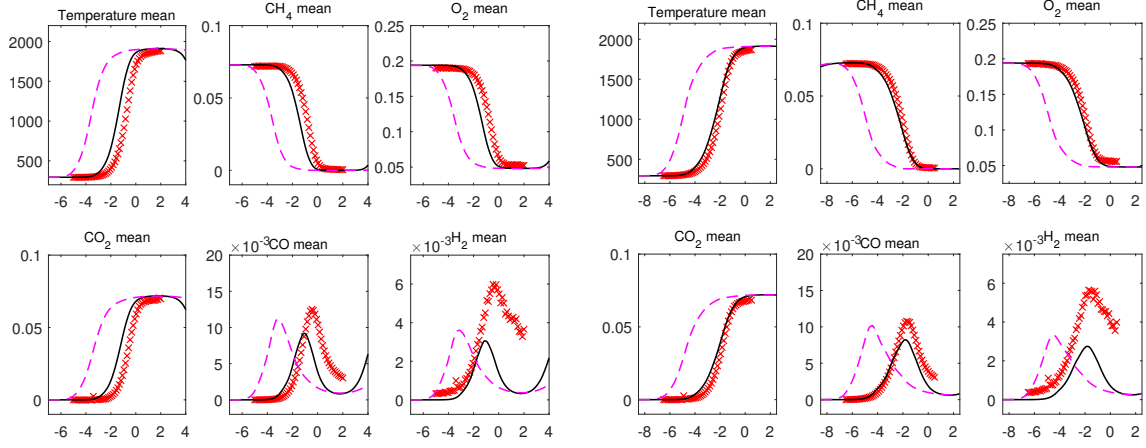


Figure 5.6: Mean profiles of temperature and major species for the premixed flame fs1 at $y=25$ (left) and $y=30\text{mm}$ (right). The dashed lines represent simulation results prior to the implementation of changes introduced in Chapters 3 and 4

CO and H_2 are also reproduced well. The magnitudes of the species concentrations and temperature are also accurately reproduced at $y = 30\text{mm}$, Figure 5.7, although here the simulated flame spreading rate (burning velocity) is somewhat too low with the result that the profiles are ‘shifted’ compared with the measurements. This indicates, that the first region i.e. fully premixed, is captured well, however for this low turbulence/Reynolds number burner, the effects of stratification further downstream might not be captured as well. The under estimation of the flame spreading rate is more evident in the case of the highly stratified flame, Figure 5.8 where the simulated profiles are all shifted compared with the measurements at both measurement locations. This is possibly due to the stronger mixing at higher stratification ratio with steep gradients across the mixing layer between the slots. This appears not to be captured well by the simulations and effectively moves the second observed region lower and closer to the lower measurement location.

In all cases, the effect of differential diffusion could account for some of the differences in flame locations. The increased diffusion of radicals of lighter species such as H_2 from the richer towards the leaner equivalence ratio could increase the burning velocity. For the moderately and highly stratified cases this could also lead to improved results due to back-support further propagating the flame into the leaner mixture.

The profile shapes, in terms of width, gradient and magnitude are well reproduced

by the computations. In spite of the discrepancies in the predicted burning velocities it appears that the methodology is capable of reproducing flame structure and producing relatively good results for the species concentrations and also the flame brush thickness, which is reflected in the temperature profiles.

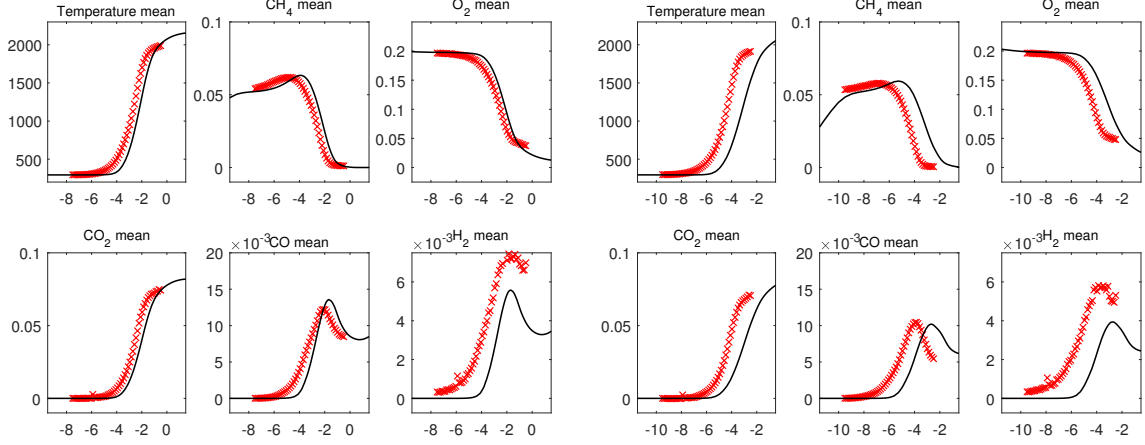


Figure 5.7: Mean profiles of temperature and major species for the moderately stratified fs4 flame at y=25 (left) and y=30mm (right)

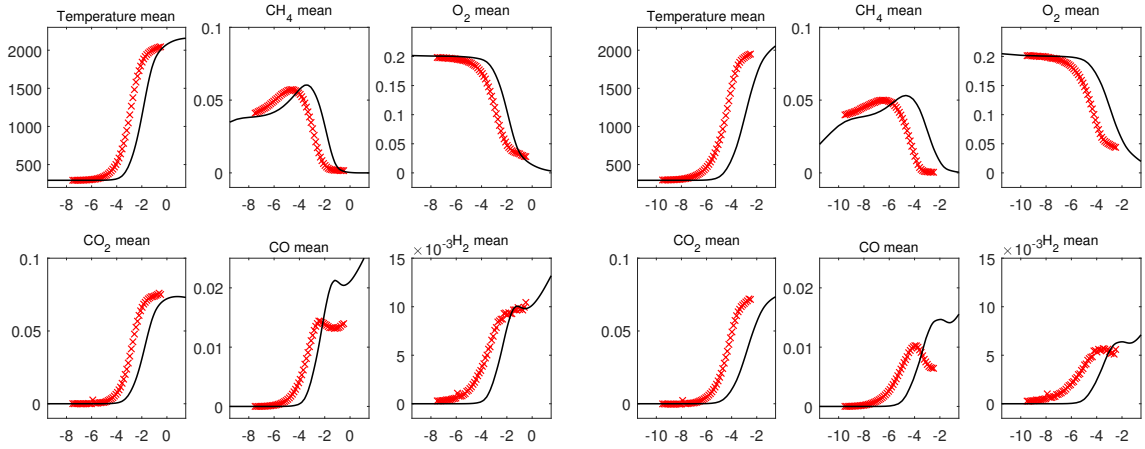


Figure 5.8: Mean profiles of temperature and major species for the highly stratified flame fs6 at y=25 (left) and y=30mm (right)

5.4 Conclusion

The LES-PDF method with the stochastic field solution method with a reduced yet still detailed chemical reaction mechanism has been applied to the premixed, moderately and highly stratified flames of the Cambridge Stratified Slot Burner.

Velocity and turbulence intensity measurements have been reproduced well. In all three cases the flame structure is reproduced with good accuracy although discrepancies between the measured and simulated flame spreading rate become apparent with increased levels of stratification. Possible reasons include the uncertainty in the applicability of the Smagorinsky model at low Reynolds numbers, particularly in regard to its use in the pdf equation, temperature boundary conditions for the rod and the ‘molecular’ diffusion models currently used in the formulation. The results suggest, that the assumption of $Le = 1$, normally made for turbulent higher Reynolds number flows is not appropriate for this test case. The modifications to the SFM however produce significantly improved results over the original formulation (Figure 4.1). To further improve, in future work a comparison to simulations using full species transport properties with a Hirschfelder and Curtiss approximation will be undertaken. The Cambridge Stratified Slot Burner is likely not well suited to LES, however it does provide a good test case to investigate and improve the limit behaviour of LES models, which can be important in particular in premixed burners with flame holders.

Chapter 6

Simulation of the Cambridge Stratified Swirl Burner

In order to further develop combustion systems it is important to investigate the fundamental properties of stratified combustion, in e.g. simpler test cases such as the stratified V-Flame in the previous chapter, and gain the ability to accurately predict the behaviour of flames under these conditions. However, typical gas turbine combustion chambers for example feature complex geometries with a range of turbulent flows and physical conditions and generally use swirl as a means of improving mixing, as well as stabilising and shortening the flames.

In this chapter a more complex, higher Reynolds number burner configuration is investigated, namely the Cambridge Stratified Swirl Burner. Simulations are performed for 9 operating conditions, 3 isothermal and 6 burning, with varying degrees of swirl and mixture stratification. Some results have previously been reported in (Brauner et al., 2016).

6.1 Experimental Details, Setup, Measurement Techniques and Available Data

The Cambridge Stratified Swirl Burner provides a flame series that allows for the numerical investigation of flames operating at laboratory conditions closer to those of an industrial configuration, while still providing detailed experimental data to

validate models against.

The experiments were conducted by and finding reported in (Barlow et al., 2012), Sweeney et al. (2012a), Sweeney et al. (2012b), (Zhou et al., 2013), (Zhou, 2014). The burner consists of a central bluff body surrounded by two concentric annular channels and a co-flow assembly to prevent entrainment of ambient air near the measurement locations. A schematic of the burner is show in Figure 6.1, including the approximate location of the flame brush indicated by the dashed lines. Each annulus supplies a stream of premixed methane/air mixture, the equivalence ratios of which can be varied. The average equivalence ratio is maintained at $\phi_{avg} = 0.75$. The outer annulus can additionally introduce swirl with different swirl to flow ratios (SFR). The SFR is defined as the ratio of flow rate passing through the swirler passage to the axial flow rate. The flow in the outer annulus has a mean velocity of $U_o = 18.7m/s$, in the inner annulus of $U_i = 8.7m/s$ and the co-flow air of $U_{co} = 0.4m/s$. The Reynolds numbers based on these velocities and the annuli exits are $Re_o = 11500$ and $Re_i = 5960$ for the outer and inner annuli respectively. The burner is unconfined and the flame is stabilised at the central bluff body. The Damköhler number is estimated to be between 0.89 and 1.24 and the Karlowitz number between 93 and 215. Under these conditions the flame falls into the thin reaction zone regime. The configurations investigated in the work presented here are the non-swirling and highly swirling, premixed moderately and highly stratified cases, the operating conditions of which are summarised in Table 6.1.

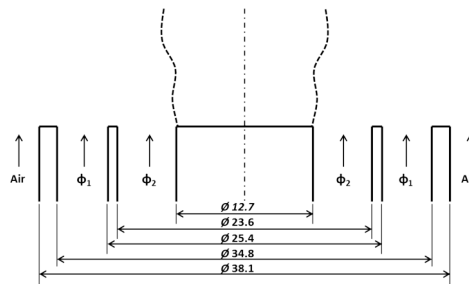


Figure 6.1: Schematic of the Cambridge Stratified Swirl Burner geometry.

Extensive velocity, temperature and mass fraction measurements are available at increments of $10mm$ above the burner exit. Velocity measurements were taken with laser Doppler anemometry (LDA) as well as particle image velocimetry (PIV), while

Table 6.1: Swirl Burner flame names, stratification-ratios and swirl-flow-ratios for different operating conditions.

Case	$\phi_{inner}/\phi_{outer}$	SFR
cSwB1	<i>isothermal</i>	0.00
cSwB2	<i>isothermal</i>	0.25
cSwB3	<i>isothermal</i>	0.33
SwB1	$0.750/0.750 = 1.0$	0.00
SwB3	$0.750/0.750 = 1.0$	0.33
SwB5	$1.000/0.500 = 2.0$	0.00
SwB7	$1.000/0.500 = 2.0$	0.33
SwB9	$1.125/0.375 = 3.0$	0.00
SwB11	$1.125/0.375 = 3.0$	0.33

Rayleigh and Raman scattering line measurements were taken for the temperature and major species respectively. Flows involving an annular bluff body are sensitive to the alignment of the ducts and even minor deviations can result in asymmetric flow behaviour. This is reflected in the measurements profiles and was also reported by (Nambully et al., 2014a).

6.2 Simulation Set-up

The burner was investigated using three meshes: small and coarse, large and intermediate, and large and fine.

The smallest and coarsest computational domain begins directly at the bluff-body and extends 150mm downstream of the bluff body and 100mm in the radial direction. The intermediate and fine domains used include 25mm of the annuli upstream of the bluff body in order to better capture the flow conditions at the burner exit. Furthermore, they extend 300mm downstream of the bluff body in the axial direction and 200mm in the radial direction. The mesh used, slices of which are shown in Figure 6.2, consists of approximately four million nodes divided into 163 blocks, resulting in an average mesh spacing of about 0.3mm in the vicinity of the bluff body. The finest mesh consists of eleven million nodes divided into 610 blocks, with mesh growth in the streamwise direction only beginning downstream of the measurement locations. This results in a mesh spacing of about 0.25mm in the streamwise direction at all measurement locations. Due to the computational expense of the

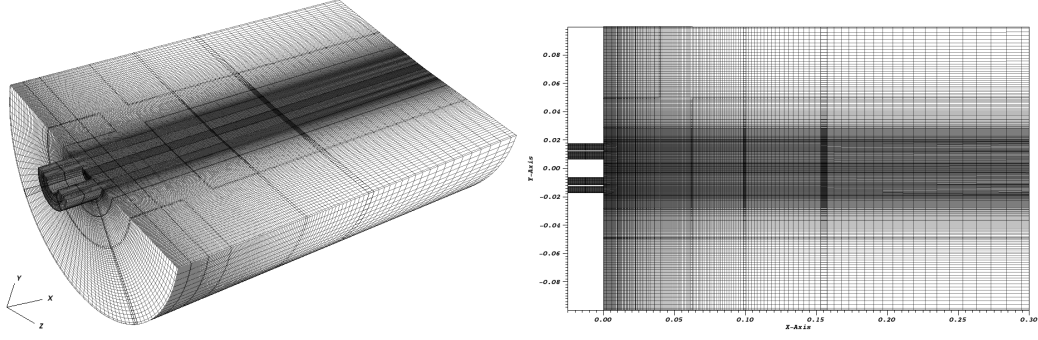


Figure 6.2: Slices through the computational mesh.

fine mesh, it has only been used for two of the burning cases: SwB5 and SwB7. The boundaries consist of two annuli inlets, one large co-flow inlet, zero-gradient outflow conditions, adiabatic and Neumann no-slip conditions with a wall function at the bluff body and annuli walls and free slip conditions on all other boundaries. To characterise the inflow conditions a digital inflow generator is used to model the effect of the turbulence at the burner exit. Experimental velocity measurements at $2mm$ above the bluff body are imposed on the generated turbulence and applied to the domain inlets. The species concentrations at the inlets are assumed to be homogeneous. A detailed augmented reduced version of the GRI 3.0 mechanism with 15 reaction steps and 19 species is employed for the chemistry. For the burning cases eight stochastic fields are utilised to represent the sub-grid contributions. The simulations are initialised with a single field and a spark model is used to initialise combustion. Followed by this, the simulations are allowed to settle before switching to 8 stochastic field and eventually gathering statistics over the duration of at least 2 full domain flow through times based on the inlet velocity of the inner annulus.

6.3 Simulation Results

Results for the mean and fluctuating velocities of both the isothermal and burning cases as well as temperature and major species for the burning cases are presented at three measurement locations downstream of the bluff body: 10, 30 and 50 mm. The isothermal results also include a comparison of data at 2mm downstream of the bluff body.

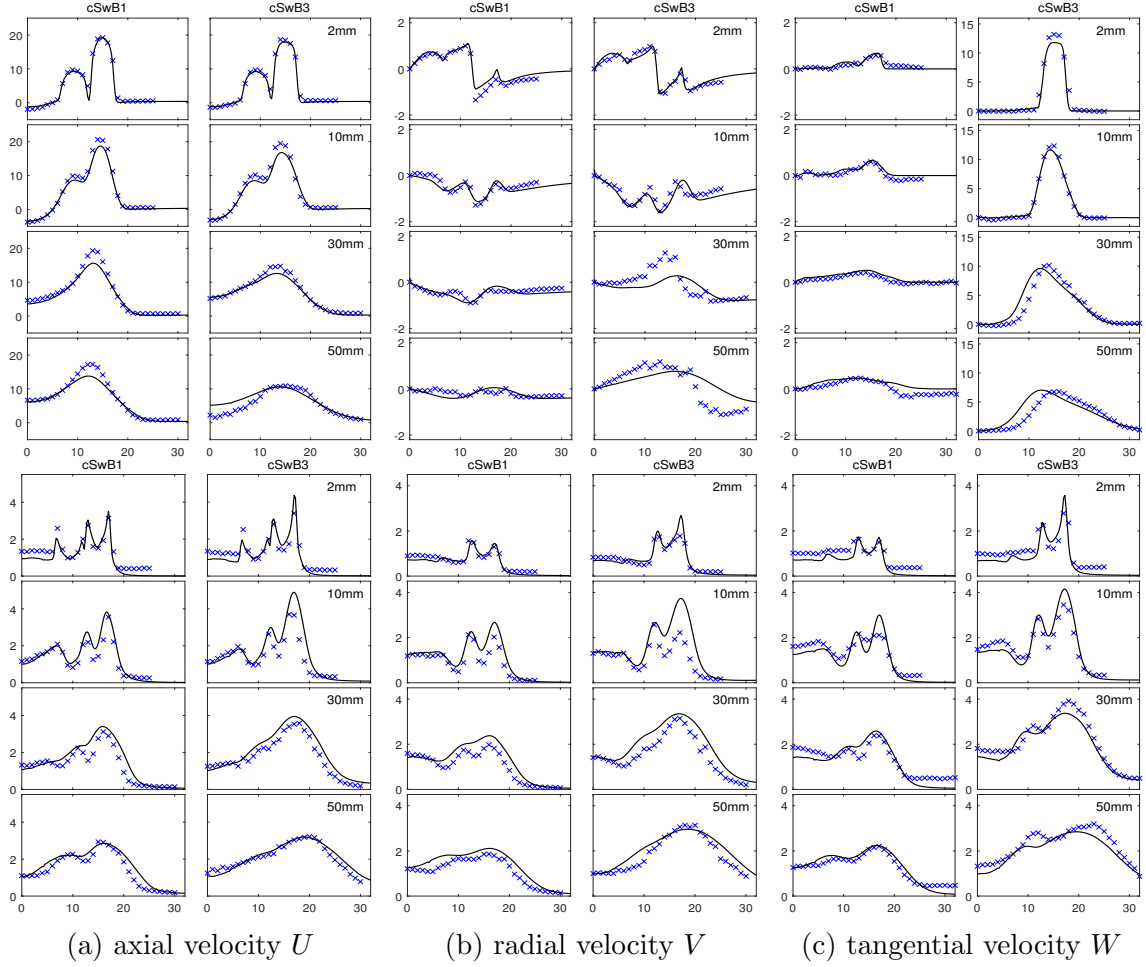


Figure 6.3: Comparison of axial (U) (first two columns), radial (V) (middle two columns) and tangential (W) (last two columns) mean and rms velocities for the isothermal, non-swirling case, cSwB1, and highly swirling case with $SFR = 0.33$, cSwB3.

6.3.1 Isothermal Flow Field Results

Figure 6.3 compare simulation results (solid line) to experimental data (crosses) for all mean and fluctuating velocity components of the isothermal non-swirling, cSwB1, and highly swirling, cSwB3, cases.

For both cases the axial velocity is in very good agreement at the first measurement location. However, the peak velocities are slightly under-predicted as the distance from the burner exit increases. A small under prediction of the peak swirl velocity is observed for cSwB3 in Figure 6.3 (right most column), as well as a shift of the profiles towards the centreline as the distance from the burner increases. This is likely due to loss of angular momentum by inclusion of part of the annuli geometry,

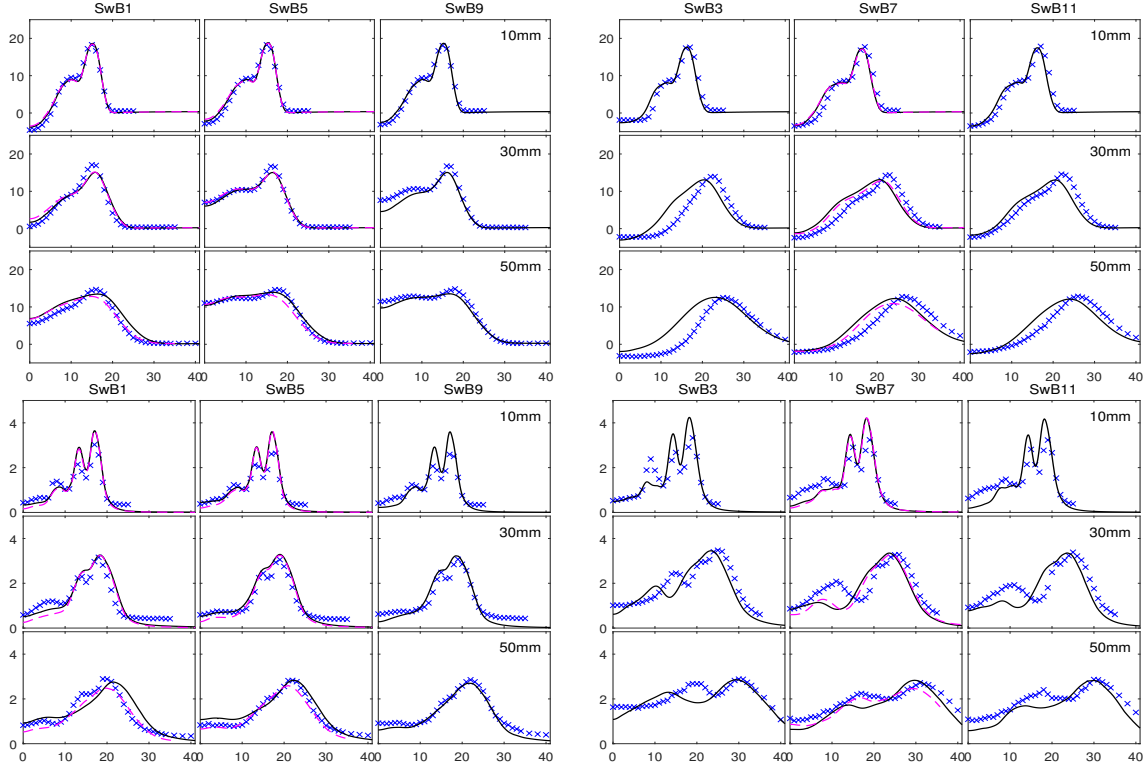


Figure 6.4: Comparison of axial (U) mean and rms velocities for all burning cases

which is not accounted for when using the measurement profile at 2mm to generate the turbulent inlet conditions. The radial shift may indicate that the computational domain could be too small to capture the extent of the isothermal swirling flow. Overall, without any adjustments, the results show good agreement for both cases and serve to support the choice of inflow conditions.

6.3.2 Reacting Flow Field Results

Figures 6.4 through 6.6 show mean and fluctuating velocities for the six burning cases SwB1, SwB3, SwB5, SwB7, SwB9, SwB11. The non-swirling configurations are shown on the left and the swirling ones on the right side of the page.

For the three non-swirling cases, SwB1, SwB5 and SwB9 the axial velocities are reproduced well, including the recirculation zone in the wake of the bluff body. The radial velocities (V) are slightly over-predicted at the furthest downstream location, which is reflected in the scalar results, shifting them away from the centreline. This is possibly due to the growth of the mesh spacing as the distance from the burner

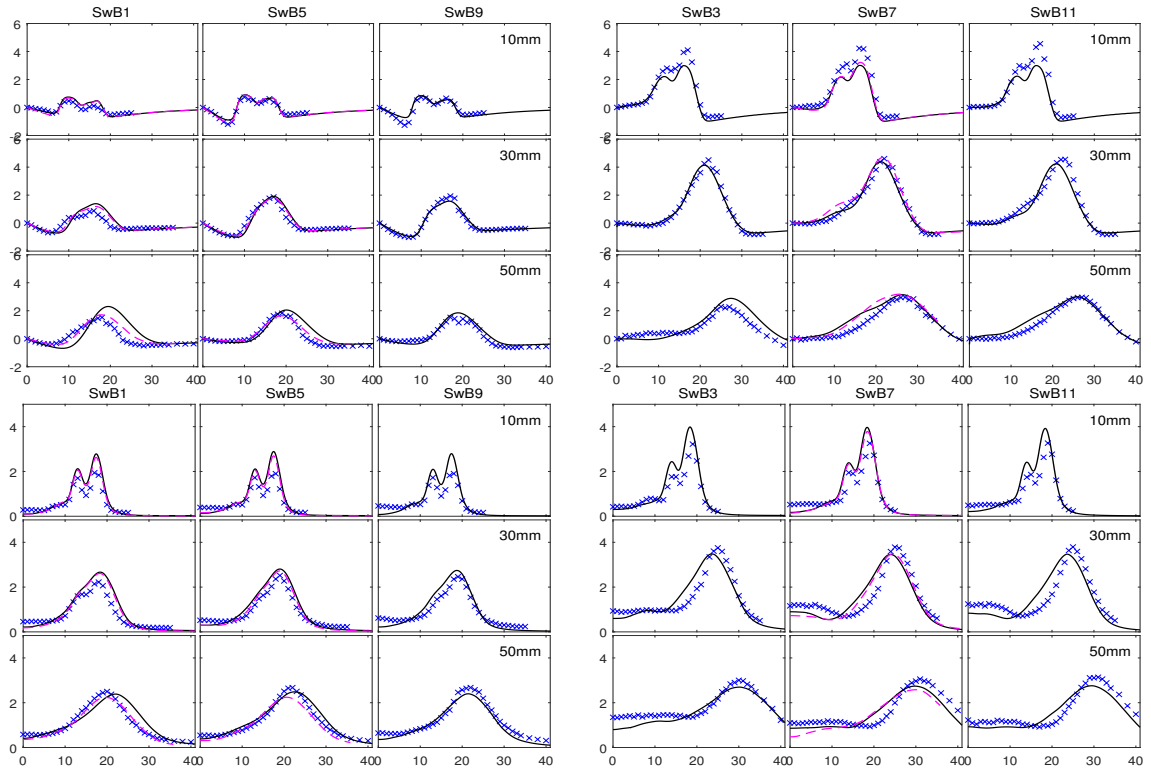


Figure 6.5: Comparison of radial (V) mean and rms velocities for all burning cases

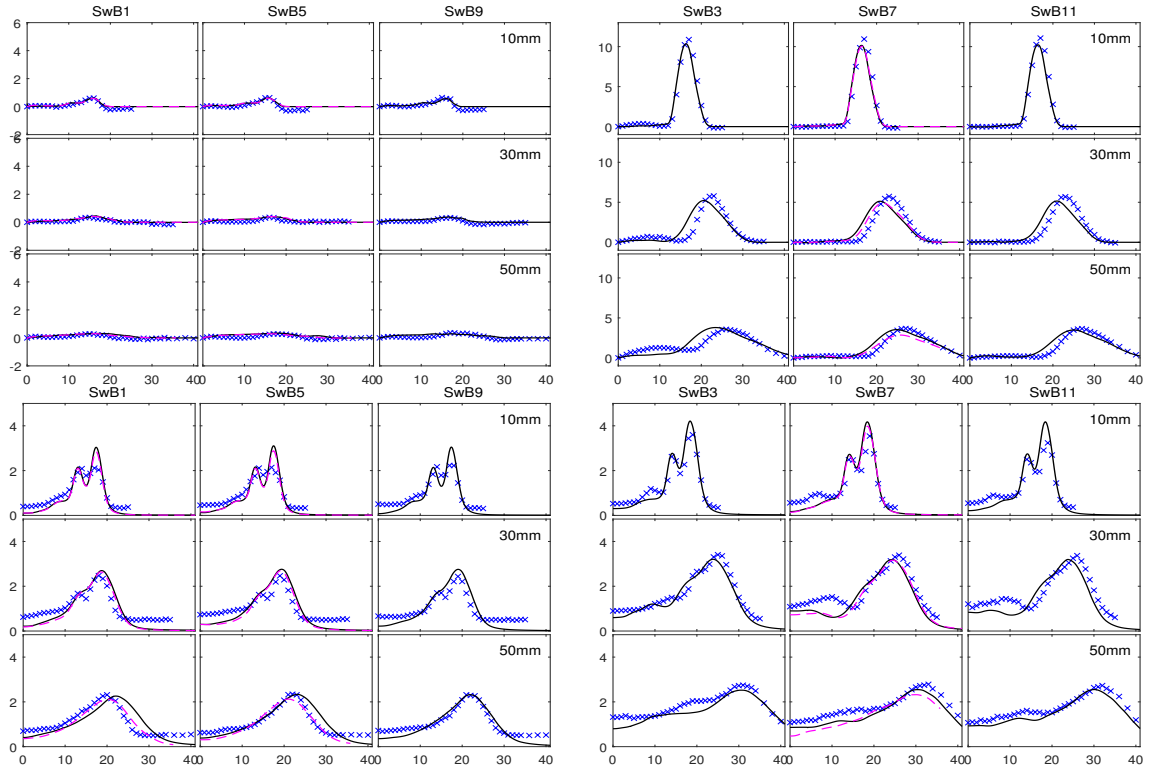


Figure 6.6: Comparison of tangential (W) mean and rms velocities for all burning cases

exit increases. The otherwise good results are improved for the radial velocity on the finer mesh indicated by the dashed (magenta) lines. For the swirling cases, SwB3, SwB7 and SwB11 the peak swirl/tangential velocities (W) are slightly under predicted, likely due to the above mentioned choice of inlet conditions and inclusion of part of the burner geometry. The axial velocities (U) in the burned mixture behind the flame front are over predicted at further downstream locations, in particular for the premixed case SwB3. This is however not reflected in the results for species concentrations. The cause of this is likely the omission of heat loss to the burner and thus over-prediction of temperature resulting in lower density. The use of the finer mesh for SwB7 again results in slightly better agreement with the experimental data. Agreement might further be improved through use of a larger computational domain in both diameter and length to better capture the extent of the recirculating and swirling regions. Overall however, trends and magnitudes are captured well and good agreement with the experimental data is achieved for both mean and fluctuating velocities. The discrepancies will be discussed further in relation to the temperature and species results.

In the region behind the bluff body the flow is well resolved with instantaneous ratios of turbulent to molecular viscosity μ_{sgs}/μ , of less than 1 for the isothermal cases. For the burning cases there is even lower sub-grid viscosity contribution in the wake of the bluff body due to re-laminarisation caused by the increase in molecular viscosity and decrease in density of the hot reaction products. Figure 6.7 compares time-averaged progress variable, right (blue), to the ratio of sub-grid viscosity to molecular viscosity, left (red), for the burning case SwB1. The dashed horizontal line indicates a ratio of $\mu_{sgs}/\mu = 1$ and $c \approx 0.18$. It can be seen that at each measurement location $\mu_{sgs}/\mu > 1$ only occurs in regions of zero or initially rising progress variable values.

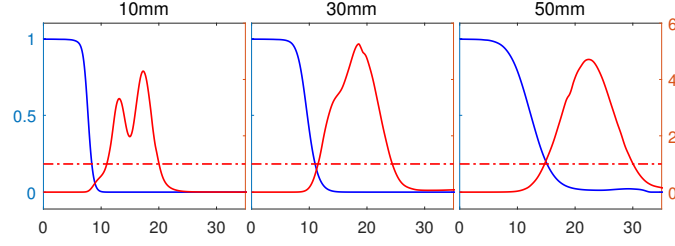
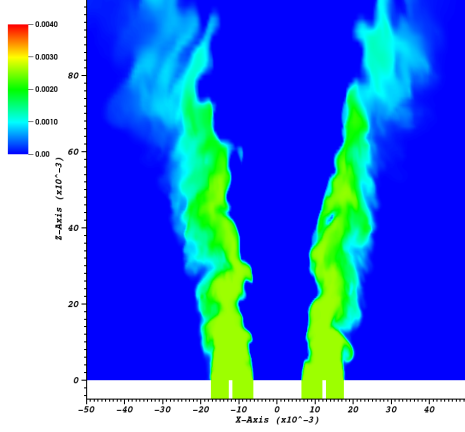


Figure 6.7: Time-averaged comparison of a progress variable (left/blue) to the ratio of sub-grid viscosity to molecular viscosity (right/red) of the flame SwB1 at three measurement locations. Dashed line indicates $\mu_{sgs}/\mu = 1.0$.

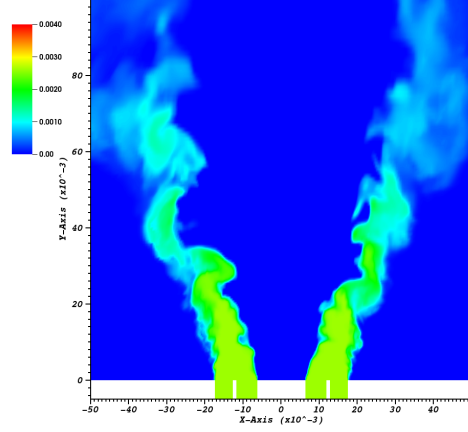
The stochastic field method relies on the turbulent viscosity for both the stochastic and the micro-mixing terms and in well resolved or laminar regions with diminishing sub-grid viscosity needs to recover the laminar flame propagation characteristics. In the original formulation of the SFM the stochastic term did not vanish as the viscosity ratio approached zero and furthermore depends on the species gradient, which is steep across premixed flames. To ensure the correct behaviour it relied solely on the scaling of the micro-mixing term, similar to that proposed by (Prasad, 2011) used at low viscosity ratios.

6.3.3 Reacting Species and Temperature Results

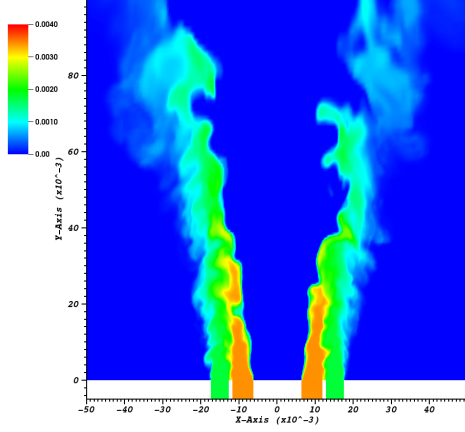
Figures 6.8 and 6.9 show sample simulation results of instantaneous snapshots of methane concentration and time-averaged mean shots. The images are taken from a plane in which the burner centre line lies. The top left image shows the premixed, non-swirling case, SwB1. The effect of swirl can be seen in the images to the right and the effect of increasing stratification in the images below. The fuel/air mixtures entering the domain are assumed to be homogeneous and downstream of the burner exit mixing of the outer annulus stream with the co-flow can be seen for all cases and mixing of the inner and outer annuli streams for the stratified cases. Combustion first takes place at the equivalence ratio of the inner (lower velocity, richer) stream, before the flame interacts with the shear layer and stratified mixture formed by the equivalence ratio and velocity gradients of the annuli streams. In this region, starting at around 30mm, “back- supported” burning from high towards low equivalence ratios takes place. High temperatures and increased presence of



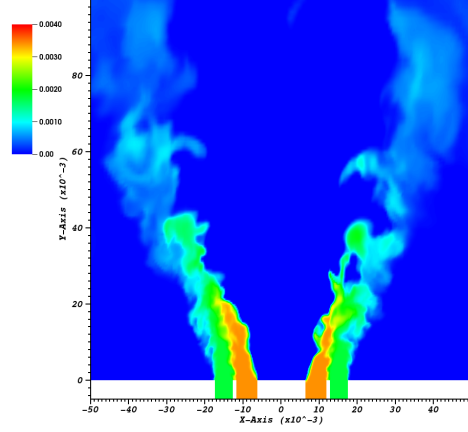
(a) SwB1



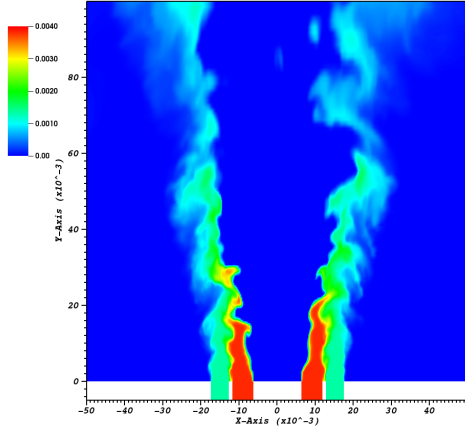
(b) SwB3



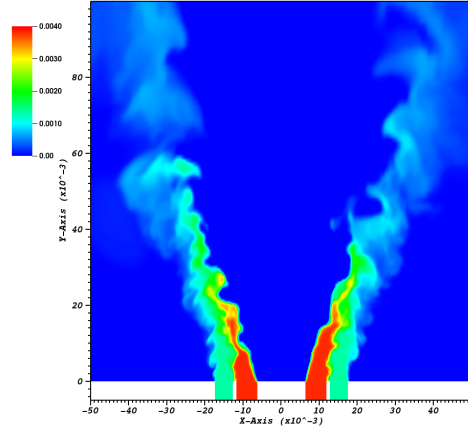
(c) SwB5



(d) SwB7

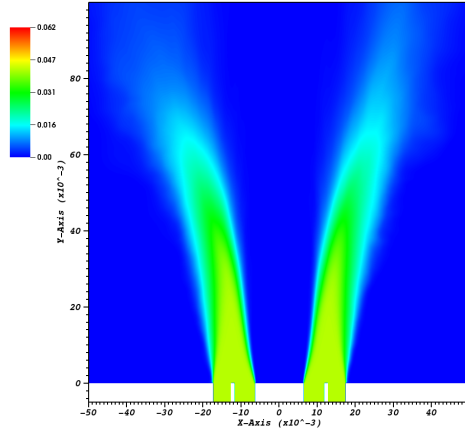


(e) SwB9

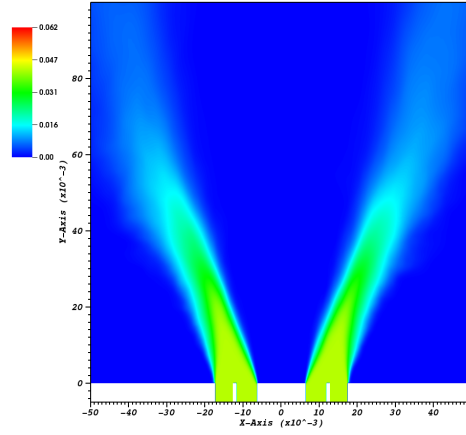


(f) SwB11

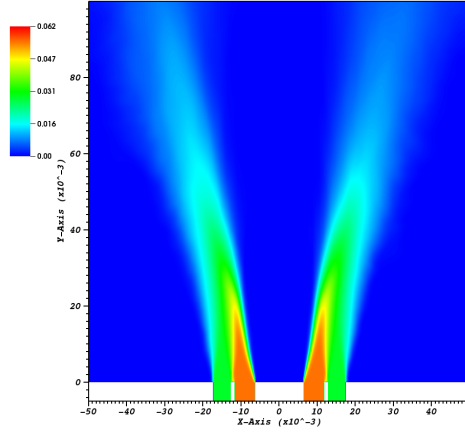
Figure 6.8: Instantaneous snapshots of methane concentration of the six burning cases. Left: non-swirling, right: swirling with swirl-flow-ratio = 0.33. Top row: premixed. Middle row: moderately stratified with ratio = $1.0/0.5 = 2$. Bottom row: highly stratified with ratio = $1.125/0.375 = 3$.



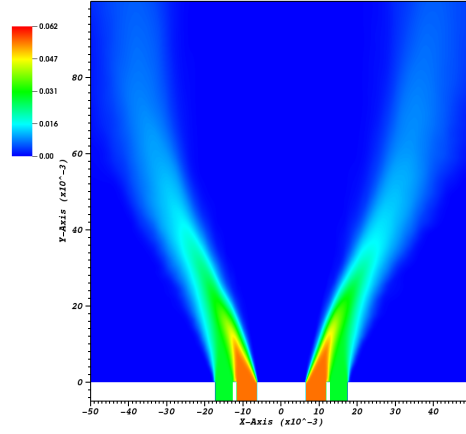
(a) SwB1



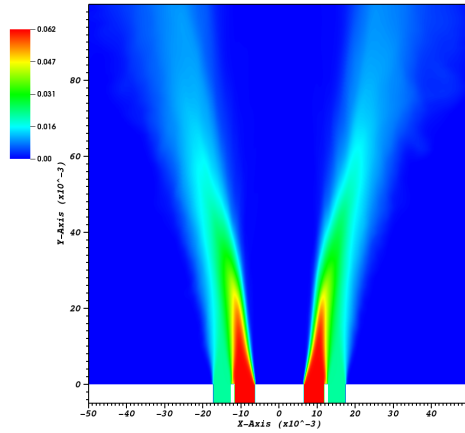
(b) SwB3



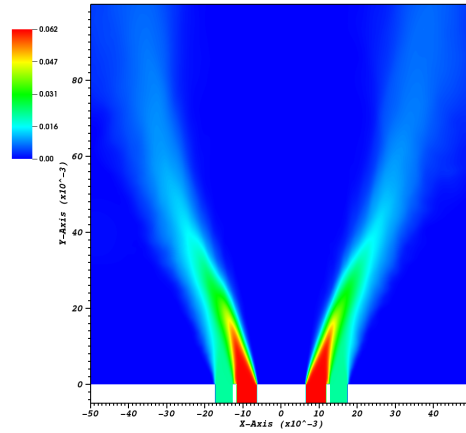
(c) SwB5



(d) SwB7



(e) SwB9



(f) SwB11

Figure 6.9: Time-averaged shots of methane concentration of the six burning cases. Left: non-swirling, right: swirling with swirl-flow-ratio = 0.33. Top row: premixed. Middle row: moderately stratified with ratio = $1.0/0.5 = 2$. Bottom row: highly stratified with ratio = $1.125/0.375 = 3$.

radicals and higher levels of turbulence from the outer annulus stream result in higher burning velocities supporting combustion into the lean mixture. Further downstream the flame interacts predominantly with the leaner mixture.

Figure 6.10 compares the mean and rms of temperature values for all burning cases. Dashed (magenta) lines are included wherever simulation results on the finest grid are available. For the non-swirling cases agreement with the experimental results is good at the lower measurement location, while the spreading is over-predicted at the downstream locations, mirroring the velocity results. For the swirling cases the spread is predicted well, however the temperature of the hot products close to the burner centre line is over predicted at all locations, which is reflected in the higher axial velocities. The bluff body surface temperature and potential heat loss to the bluff body as well as radiative heat transfer have not been included in the present simulations and may explain the higher temperatures. A lower bluff body surface temperature should have the effect of lifting the entire flame slightly further away from the bluff body, potentially resulting in better agreement with experimental data at all measurement locations. Radiative heat transfer could have a small influence on areas of the flow further away from the burner.

Figures 6.11 to 6.14 compare mean and rms values of CH_4 , O_2 , CO_2 , and CO for all cases. The experimental profiles were measured across half of the burner at $30mm$ and across the entire burner at the $10mm$ and $50mm$ measurement locations. The observations made for temperature are also reflected in the species concentrations. Agreement with the experimental data is improved when comparisons are made with both sides of the measurements profile taken across the entire burner, thus accounting better for the asymmetry of the data.

Figure 6.11 shows that for the non-swirling flames the flame spread, i.e. the consumption of CH_4 , is still overestimated. Agreement with the experimental data is improved on the finer grid. For the swirling flames the flame spread is predicted very well, with only the peak value being under-predicted. Agreement is however not improved on the finer grid. Other species follow the general trend of outward shifted profiles for the non-swirling flames, but good agreement of profiles for the swirling flames, with slight improvements on the finer computational grid.

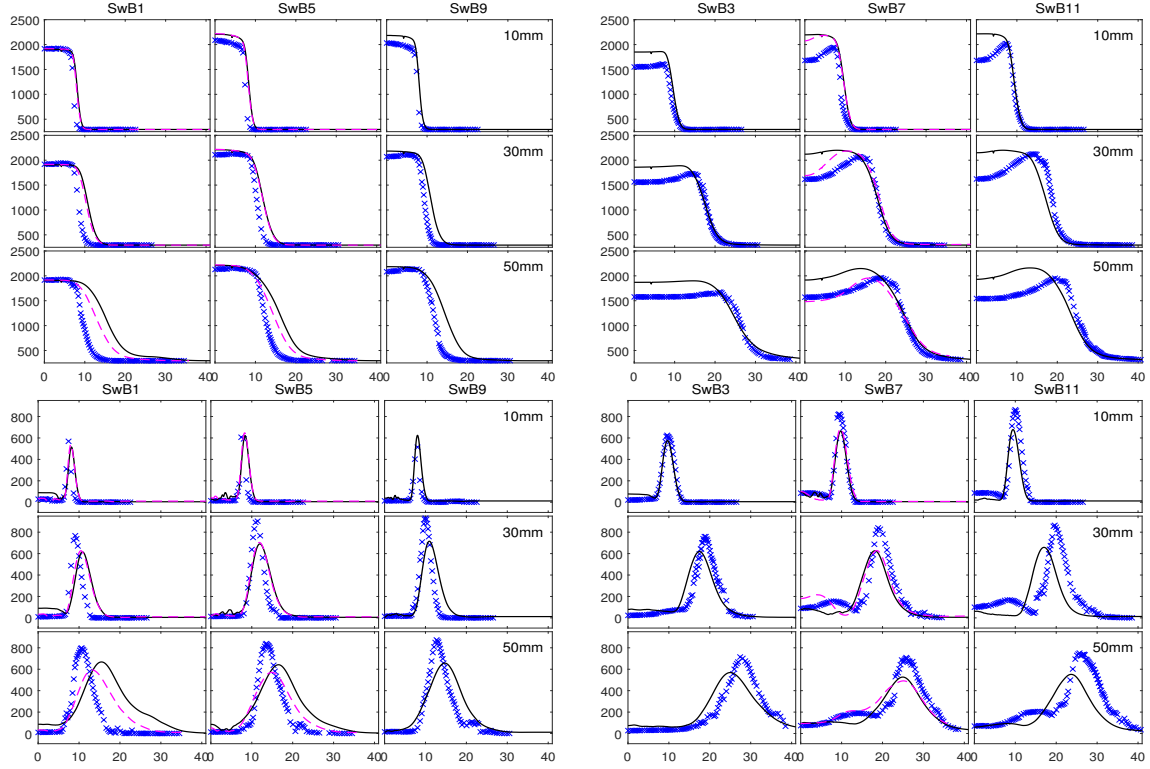


Figure 6.10: Comparison of mean and rms temperature (T) for all burning cases at 10, 30 and 50 mm

For all swirling flames it can be observed that the concentration of O_2 is lower and of CO_2 is higher than expected in the recirculation zone. This is not observed for the non-swirling cases. On the finer computational grid the profiles return to the curves of the experimental data at the two furthest downstream measurement locations, however not for the location closest to the burner exit. The observations for O_2 and CO_2 are likely a result of the lower computed peak value of CH_4 , i.e. faster consumption, and the negative axial velocities near the burner centre line at all measurement locations (Figure 6.4). It is however also possible that not the finer grid, but longer simulation times improve agreement with the experimental data near the burner centre line. The negative axial velocities at the core of the swirling flow field are significantly lower in magnitude than those of the hot reaction products, making it computationally expensive to compute for the length of time required for the flow field to become statistically stationary. This was thought to have been afforded, however SwB7 on the fine grid was computed for longer, with improved results and longer integration times might therefore also improve results

for the other swirling flames.

For the non-swirling flames it can be observed that the concentrations of CO is under estimated in the recirculation zone. In (Barlow et al., 2012) it is reported that accumulation of e.g. CO is observed near the bluff body in the recirculation zone due to differential diffusion: faster diffusing species of the products and intermediates reach the flame quicker and are consumed, slower diffusing species are trapped or carried away without interaction with the flame. This has not accounted for in the simulations and should improve the agreement with experimental data.

6.4 Conclusion

The LES-pdf method with the stochastic field solution method with a reduced yet still detailed chemistry scheme has been applied to the premixed, moderately and highly stratified, non-swirling and swirling flames of the Cambridge Stratified Swirl Burner. A modified version of the pdf-equation is used to ensure that the method is consistent with the limiting case of negligible sgs-variations, an essential feature if measurements in low Reynolds number laboratory flames are to be reproduced. The simulated velocity fields and profiles are in very good agreement with measured data for the isothermal and burning cases both with and without swirl. For the flames the overall agreement with measured profiles of temperature and O_2 , CO , CO_2 and CH_4 mass fractions is good with maximum values being well reproduced by the non-swirling simulations and profile locations by the swirling simulations. There are some local discrepancies in the central regions of the swirling flames, which, it is suggested, arise because of domain size and length of time simulated. The flames studied all have moderate Reynolds numbers and so the inclusion of more accurate transport properties accounting for differential diffusion effects may alleviate this and further improve the results.

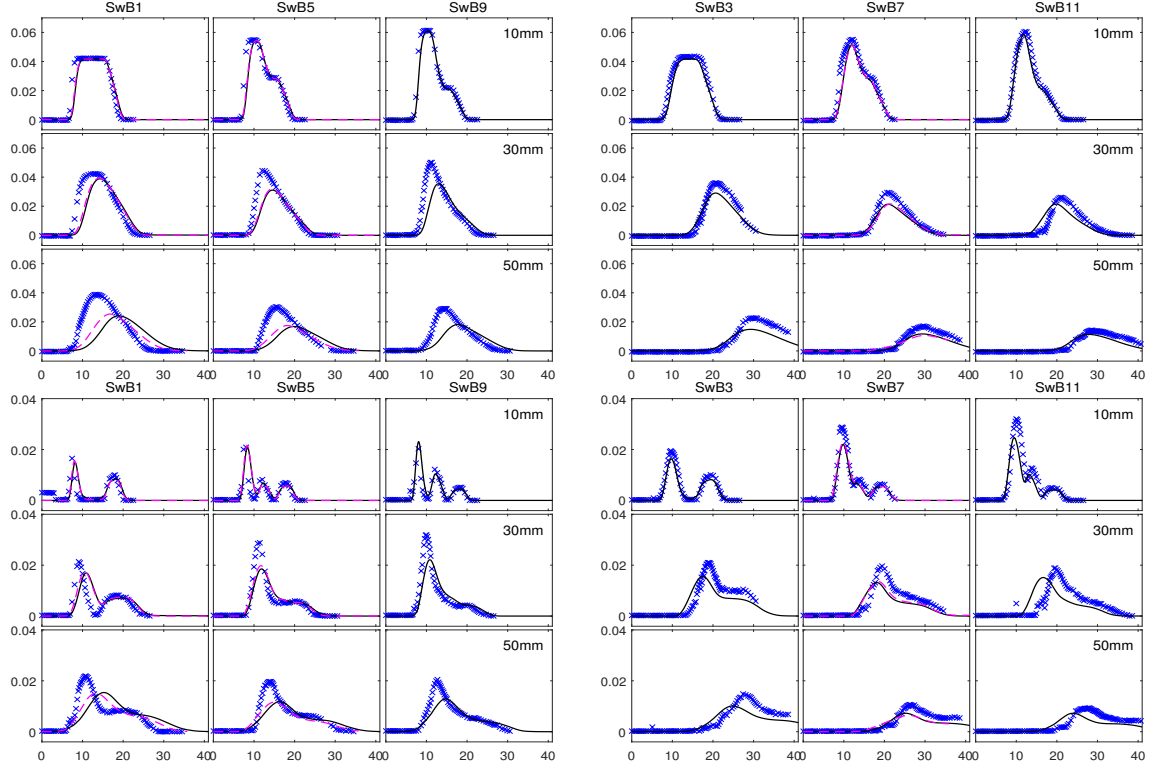


Figure 6.11: Comparison of mean and rms methane (CH_4) for all burning cases at 10, 30 and 50 mm

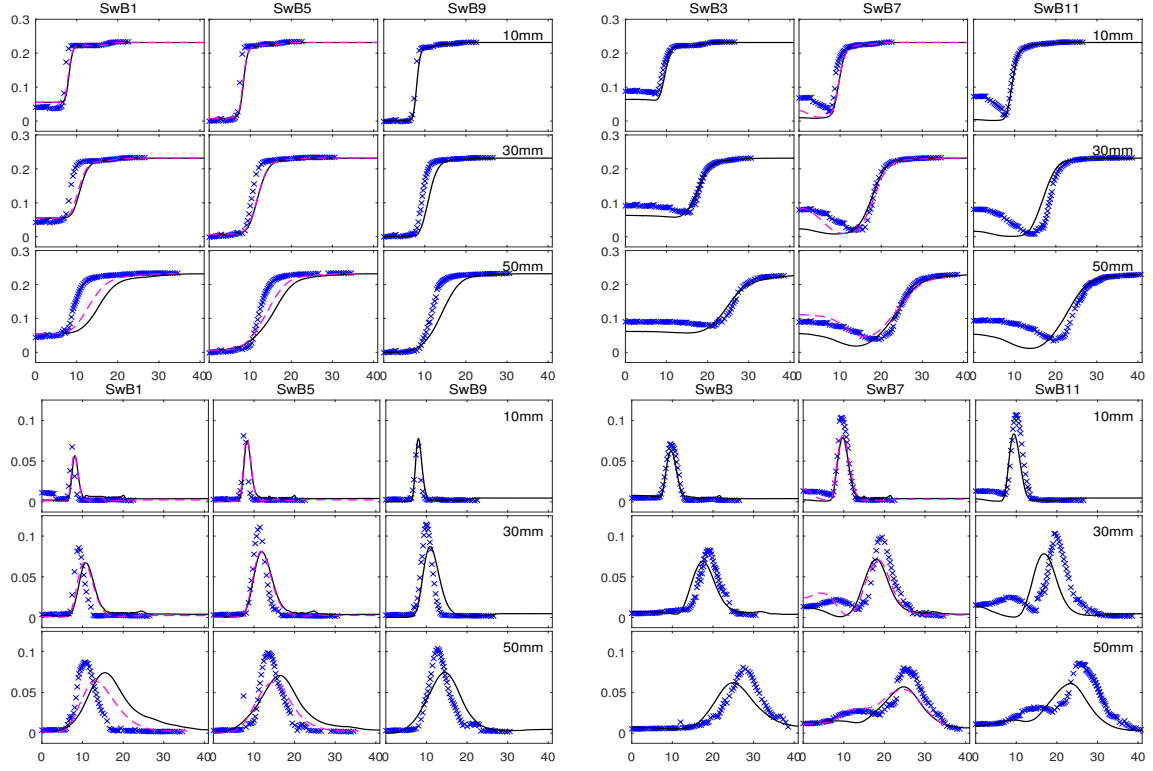


Figure 6.12: Comparison of mean and rms oxygen (O_2) for all burning cases at 10, 30 and 50 mm

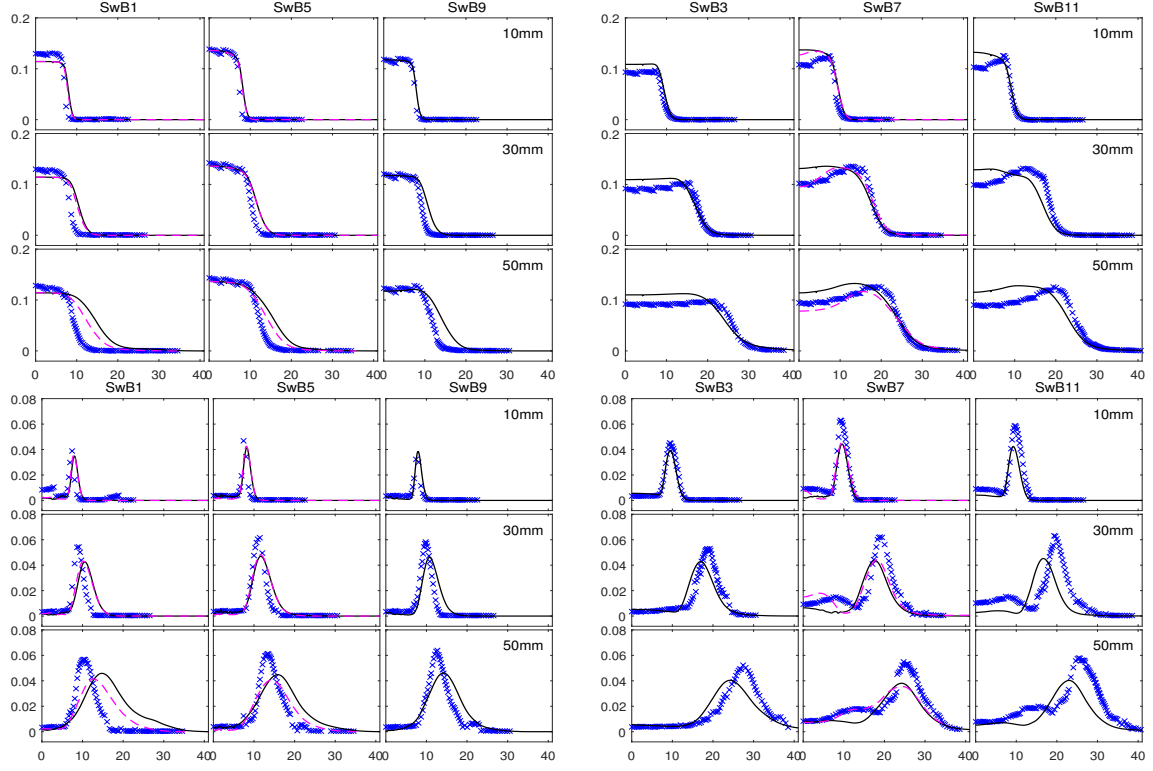


Figure 6.13: Comparison of mean and rms carbon dioxide (CO_2) for all burning cases at 10, 30 and 50 mm

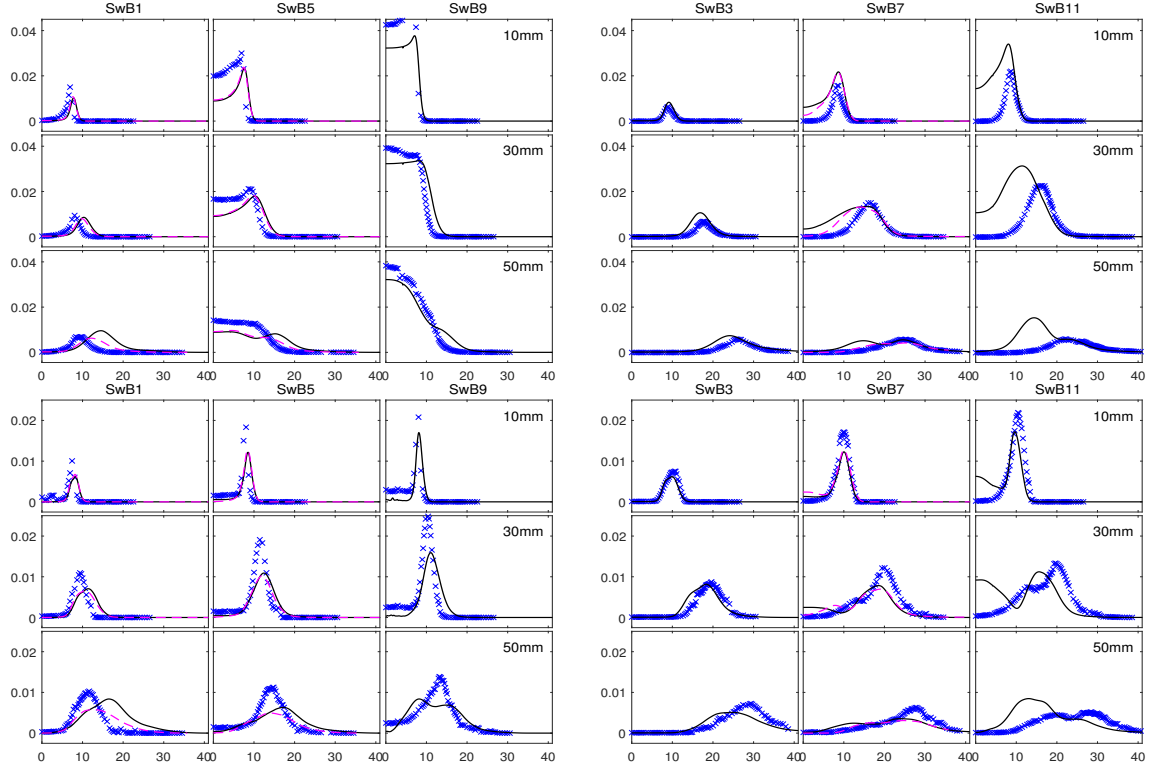


Figure 6.14: Comparison of mean and rms carbon monoxide (CO) for all burning cases at 10, 30 and 50 mm

Chapter 7

Conclusion

The transported pdf method in conjunction with the Eulerian stochastic field method has been applied to two premixed and stratified burner configurations with different levels of turbulence and flow complexity as well as stratification ratios and burning regimes. Base on the results of initial studies a reformulation of the PDF equation and adjustments to the stochastic field solution algorithm to ensure correct behaviour in the absence of turbulence were proposed and implemented. The modifications were applied to simulations of both burner configurations and found to improve the predictive capabilities of the method. All cases used the augmented reduced mechanism based on GRI 3.0 and 8 stochastic fields were used to characterise the effect of the sub-grid contributions.

The first test case was the Cambridge Stratified Slot Burner, investigated for 3 different stratification ratios. Difficulties with the original formulation of the SFM in predicting the quasi-laminar / low turbulence flames of this burner manifested themselves through large over-predictions of burning velocity and thus flame spread/angle. This prompted the investigation of the stochastic and micro-mixing terms and their implementations. The modifications to the SFM produce significantly improved results over the original formulation and good agreement with the experimental data. Findings from these simulations suggest, that the assumption of $Le = 1$, normally made for turbulent higher Reynolds number flows is not appropriate for this test case and could account for some of the observed discrepancies.

The second test case was the Cambridge Stratified Swirl Burner, investigated for 3

different stratification ratios and 2 different swirl-to-flow ratios. The experimental data was processed to account for its asymmetry. The simulated velocity fields and profiles are in very good agreement with measured data for the isothermal and burning cases both with and without swirl. For the flames the overall agreement with measured profiles of major species mass fractions and temperature is good. Some local discrepancies in the central regions of the two swirling flames are still observed. The flames studied have moderate Reynolds numbers and the inclusion of more accurate transport properties accounting for differential diffusion effects may alleviate some of the discrepancies and further improve the results. Further, the bluff body was assumed adiabatic and applying temperature boundaries accounting for heat loss to the burner could change the relaminarisation dynamics in the wake of the bluff body and improve results in its vicinity. For the swirling cases longer simulation integration times should also result in improved agreement with experimental data. The Eulerian Stochastic Field Method has proven to be a powerful tool and has previously been applied to and validated against a variety of different burner configurations and flame types under turbulent conditions. The methods behaviour in laminar and well resolved flow regions has now also been investigated and subsequently has been successfully applied for the first time to burners exhibiting pre-mixed stratified combustion. To further improve the methods capabilities, in future work a comparison to simulations using both heat loss boundary conditions and full species transport properties with a Hirschfelder and Curtiss approximation to account for differential diffusion effects will be undertaken. Additionally, it is of interest to extend the capabilities to compressible flows including spray in order to investigate thermo-acoustic interactions, such as combustion instabilities and noise in laboratory scale burners and full scale combustion chambers.

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Appendix A

Appendix

A.1 Enthalpy Equation

The flux vector q_i of the enthalpy equation 2.1.5 can be rearranged and under the assumption that $Le = 1$, can be significantly reduced in complexity. This is sometimes referred to as the Shvab-Zeldovich form. Expressing Equation 2.1.4 in terms of individual species, the enthalpy is:

$$h_\alpha = \int_{T_o}^T c_{P,\alpha} dT + \Delta h_\alpha^o \quad \text{and thus} \quad h = \sum_{\alpha=1}^{N_s} h_\alpha(T) Y_\alpha \quad (\text{A.1.1})$$

Starting from the spatial derivative of h , where $h = h(T, Y_\alpha)$ and applying the chain rule:

$$\frac{\partial h}{\partial x_i} = \frac{\partial h}{\partial T} \frac{\partial T}{\partial x_i} + \frac{\partial h}{\partial Y_\alpha} \frac{\partial Y_\alpha}{\partial x_i} \quad (\text{A.1.2})$$

For the first term on the rhs, from 2.1.5:

$$\frac{\partial h}{\partial T} = c_P \quad (\text{A.1.3})$$

For the second term on the rhs, from A.1.1 and the product rule:

$$\frac{\partial h}{\partial Y_\alpha} = \frac{\partial}{\partial Y_\alpha} \left(\sum_{\alpha=1}^{N_s} h_\alpha(T) Y_\alpha \right) = \sum_{\alpha=1}^{N_s} \left(Y_\alpha \frac{\partial h_\alpha(T)}{\partial Y_\alpha} + \frac{\partial Y_\alpha}{\partial Y_\alpha} h_\alpha(T) \right) = \sum_{\alpha=1}^{N_s} h_\alpha(T) \quad (\text{A.1.4})$$

Thus Equation A.1.2 becomes:

$$\frac{\partial h}{\partial x_i} = c_P \frac{\partial T}{\partial x_i} + \sum_{\alpha=1}^{N_s} h_\alpha \frac{\partial Y_\alpha}{\partial x_i} \quad (\text{A.1.5})$$

With the relationship $c_P = Pr\lambda/\mu$ this can be rearranged as:

$$\lambda \frac{\partial T}{\partial x_i} = \frac{\mu}{Pr} \left(\frac{\partial h}{\partial x_i} - \sum_{\alpha=1}^{N_s} h_\alpha \frac{\partial Y_\alpha}{\partial x_i} \right) \quad (\text{A.1.6})$$

Using Fick's law for diffusion fluxes and the definition of the Schmidt number $Sc = \mu/\rho D$, q_i (Equation 2.1.6) becomes:

$$\begin{aligned} q_i &= -\frac{\mu}{Pr} \frac{\partial h}{\partial x_i} + \frac{\mu}{Pr} \sum_{\alpha=1}^{N_s} h_\alpha \frac{\partial Y_\alpha}{\partial x_i} - \rho D \sum_{\alpha=1}^{N_s} h_\alpha \frac{\partial Y_\alpha}{\partial x_i} \\ &= -\frac{\mu}{Pr} \frac{\partial h}{\partial x_i} + \left(\frac{\mu}{Pr} - \frac{\mu}{Sc} \right) \sum_{\alpha=1}^{N_s} h_\alpha \frac{\partial Y_\alpha}{\partial x_i} \end{aligned} \quad (\text{A.1.7})$$

Under the assumption that $Le = 1$ only the first term on the rhs of Equation A.1.7 remains.

A.2 Adiabatic Flame Temperature Polynomial

The following polynomial is used in post-processing to compute the adiabatic flame temperature required by the progress variable over the interval $\phi_E = [0.35, 1.16]$:

$$\begin{aligned} T_a(\phi_E) &= 25352\phi_E^6 - 115733\phi_E^5 + 209879\phi_E^4 \\ &\quad - 194616\phi_E^3 + 96941\phi_E^2 - 22554\phi_E + 2952.1 \end{aligned} \quad (\text{A.2.1})$$

The interval $\phi_E = [0.0, 0.35[$ is extended linearly:

$$T_a(\phi_E) = 2514\phi_E + 295 \quad (\text{A.2.2})$$

A.3 Fine Grained pdf

The first derivative of a simple δ -function $\mathcal{P}(\psi) = \delta(\psi - \phi(t))$, similar to the marginal fine grained pdf, but here without the dependence on $\mathbf{x}$, is obtained using the Chain Rule is:

$$\begin{aligned} \frac{\partial}{\partial t} (\delta(\psi - \phi(t))) &= \delta' \frac{\partial(\psi - \phi(t))}{\partial t} \\ &= \frac{\partial \mathcal{P}}{\partial \psi} \times (-) \frac{\partial \phi}{\partial t} \\ &= - \frac{\partial \mathcal{P}}{\partial \psi} \frac{\partial \phi}{\partial t} \end{aligned} \tag{A.3.1}$$

Similarly, and using the above result, the second derivative of a simple δ -function $\mathcal{P}(\psi) = \delta(\psi - \phi(x))$ is obtained following:

$$\begin{aligned} \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} (\delta(\psi - \phi(x))) \right) &= \frac{\partial}{\partial x} \left(- \frac{\partial \mathcal{P}}{\partial \psi} \frac{\partial \phi}{\partial x} \right) \\ &= \frac{\partial}{\partial \psi} \left(\frac{\partial}{\partial x} \left(- \mathcal{P} \frac{\partial \phi}{\partial x} \right) \right) \\ &= \frac{\partial}{\partial \psi} \left(- \frac{\partial \mathcal{P}}{\partial x} \frac{\partial \phi}{\partial x} - \mathcal{P} \frac{\partial^2 \phi}{\partial x^2} \right) \\ &= \frac{\partial}{\partial \psi} \left(\frac{\partial \mathcal{P}}{\partial \psi} \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} - \mathcal{P} \frac{\partial^2 \phi}{\partial x^2} \right) \\ &= \frac{\partial^2}{\partial \psi^2} \left(\mathcal{P} \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial \psi} \left(\mathcal{P} \frac{\partial^2 \phi}{\partial x^2} \right) \end{aligned} \tag{A.3.2}$$

The first derivative of the joint fine grained pdf in 3.2.10 makes use of the properties of the δ -function as follows:

$$\begin{aligned}
\frac{\partial \mathcal{F}}{\partial t} &= \frac{\partial}{\partial t} \left(\prod_{\alpha=1}^N \delta(\psi_{\alpha} - \phi_{\alpha}(\mathbf{x}, t)) \right) \\
&= \sum_{\alpha=1}^N \frac{\partial}{\partial t} (\delta(\psi_{\alpha} - \phi_{\alpha}(\mathbf{x}, t))) \prod_{\substack{\beta=1 \\ \beta \neq \alpha}}^N \delta(\psi_{\beta} - \phi_{\beta}(\mathbf{x}, t)) \\
&= \sum_{\alpha=1}^N -\frac{\partial \mathcal{F}_{\alpha}}{\partial \psi_{\alpha}} \frac{\partial \phi_{\alpha}}{\partial t} \prod_{\substack{\beta=1 \\ \beta \neq \alpha}}^N \delta(\psi_{\beta} - \phi_{\beta}(\mathbf{x}, t)) \quad \text{note: } \mathcal{F}_{\alpha} \\
&= \sum_{\alpha=1}^N -\frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \frac{\partial \phi_{\alpha}}{\partial t}
\end{aligned} \tag{A.3.3}$$

Similarly for spatial derivatives:

$$\frac{\partial \mathcal{F}}{\partial x_i} = - \sum_{\alpha=1}^N \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \frac{\partial \phi_{\alpha}}{\partial x_i} \tag{A.3.4}$$

A.4 Fine Grained pdf transport equation

The first term on the right hand side of Equation 3.2.12 can be decomposed by recognising that it resembles a term of the rearranged product rule $f \cdot g' = (f \cdot g)' - f' \cdot g$, where the $'$ indicates $\frac{\partial}{\partial x_i}$.

$$- \sum_{\alpha=1}^{N_s} \frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \left(\frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \right) \right) = - \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial x_i} \left(\frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \left(\frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \right) \right) + \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial x_i} \left(\frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \right) \left(\frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \right) \tag{A.4.1}$$

Inserting the Equation A.3.4 into the first term on the rhs. it simplifies to:

$$- \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial x_i} \left(\frac{\partial \mathcal{F}}{\partial \psi_{\alpha}} \left(\frac{\mu}{\sigma} \frac{\partial \phi_{\alpha}}{\partial x_i} \right) \right) = \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial \mathcal{F}}{\partial x_i} \right) \tag{A.4.2}$$

Assuming for the second term that symmetry of second derivatives holds for $\mathcal{F}$ and using A.3.4:

$$\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial x_i} \left(\frac{\partial \mathcal{F}}{\partial \psi_\alpha} \right) \left(\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \right) = \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\partial \mathcal{F}}{\partial x_i} \right) \left(\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \right) \quad (\text{A.4.3})$$

$$= \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(- \sum_{\beta=1}^N \frac{\partial \mathcal{F}}{\partial \psi_\beta} \frac{\partial \phi_\beta}{\partial x_i} \right) \left(\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \right) \quad (\text{A.4.4})$$

$$= - \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\mathcal{F} \frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \right) \quad (\text{A.4.5})$$

A.5 Stochastic fields equation from sub-grid pdf equation

Inserting the stochastic fields definition of the pdf

$$\tilde{P}_{sgs} = \frac{1}{N} \sum_{n=1}^N \prod_{\alpha=1}^{N_s} \delta(\psi_\alpha - \xi_\alpha^n(\mathbf{x}, t)) = \frac{1}{N} \sum_{n=1}^N \delta(\boldsymbol{\psi} - \boldsymbol{\xi}^n(\mathbf{x}, t)) = \frac{1}{N} \sum_{n=1}^N \delta_\xi^n \quad (\text{A.5.1})$$

into the sub-grid pdf transport equation term by term results in the following:

Unsteady Term

$$\bar{\rho} \frac{\partial \tilde{P}_{sgs}}{\partial t} = \frac{1}{N} \sum_{n=1}^N \frac{\partial}{\partial t} \bar{\rho} \delta_\xi^n \quad (\text{A.5.2})$$

Advection Term

$$\begin{aligned} \tilde{\rho} u_i \frac{\partial \tilde{P}_{sgs}}{\partial x_i} &= \frac{1}{N} \sum_{n=1}^N \tilde{\rho} u_i \frac{\partial \delta(\boldsymbol{\psi} - \boldsymbol{\xi}^n(\mathbf{x}, t))}{\partial x_i} \\ &= \frac{1}{N} \sum_{n=1}^N \left(\tilde{\rho} u_i \times (-) \sum_{\alpha=1}^N \frac{\partial \delta_\xi^n}{\partial \psi_\alpha} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \\ &= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\delta_\xi^n \left(\tilde{\rho} u_i \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \right) \right) \end{aligned} \quad (\text{A.5.3})$$

Diffusion Term

Recalling the equations from the previous appendices

$$\begin{aligned}
\frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \tilde{P}_{sgs}}{\partial x_i} \right) &= \frac{1}{N} \sum_{n=1}^N \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \delta(\boldsymbol{\psi} - \boldsymbol{\xi}^n(\mathbf{x}, t))}{\partial x_i} \right) \\
&= \frac{1}{N} \sum_{n=1}^N \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \times (-) \sum_{\alpha=1}^N \frac{\partial \delta_\xi^n}{\partial \psi_\alpha} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \\
&= \frac{1}{N} \sum_{n=1}^N \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \times (-) \delta_\xi^n \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \right) \\
&= \frac{1}{N} \sum_{n=1}^N \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\partial (-) \delta_\xi^n}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) - \delta_\xi^n \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \right) \\
&= \frac{1}{N} \sum_{n=1}^N \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\sum_{\beta=1}^N \frac{\partial \delta_\xi^n}{\partial \psi_\beta} \frac{\partial \xi_\beta^n}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) - \delta_\xi^n \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \right) \\
&= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \sum_{\beta=1}^N \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\delta_\xi^n \frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \frac{\partial \xi_\beta^n}{\partial x_i} \right) - \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\delta_\xi^n \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{\sigma_T} \frac{\partial \xi_\alpha^n}{\partial x_i} \right) \right) \right)
\end{aligned} \tag{A.5.4}$$

Molecular Diffusion/Mixing Term

$$\sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\tilde{P}_{sgs} \frac{\mu}{\sigma} \frac{\partial \xi_\alpha^n}{\partial x_i} \frac{\partial \xi_\beta^n}{\partial x_i} \right) = \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\delta_\xi^n \frac{\mu}{\sigma} \frac{\partial \xi_\alpha^n}{\partial x_i} \frac{\partial \xi_\beta^n}{\partial x_i} \right) \right) \tag{A.5.5}$$

Micro-Mixing Term

Making use of the sifting property of δ_ξ^n , ξ_α^n is sifted out of ψ_α , while for every other $\beta \neq \alpha$ in $\boldsymbol{\psi}$, $\int \delta(x) dx = 1$.

$$\begin{aligned}
\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\bar{\rho} C_d}{2\tau_{sgs}} (\psi_\alpha - \tilde{\phi}_\alpha) \tilde{P}_{sgs} \right) &= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\bar{\rho} C_d}{2\tau_{sgs}} (\psi_\alpha - \tilde{\phi}_\alpha) \right) \delta(\boldsymbol{\psi} - \boldsymbol{\xi}^n(\mathbf{x}, t)) \right) \\
&= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\frac{\bar{\rho} C_d}{2\tau_{sgs}} (\xi_\alpha^n - \tilde{\phi}_\alpha) \right) \right)
\end{aligned} \tag{A.5.6}$$

Reaction Rate Term

$$\begin{aligned}
\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} \left(\bar{\rho} \dot{\omega}_{\alpha}^n(\boldsymbol{\psi}) \tilde{P}_{sgs} \right) &= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} (\bar{\rho} \dot{\omega}_{\alpha}^n(\boldsymbol{\psi})) \delta(\boldsymbol{\psi} - \boldsymbol{\xi}^n(\boldsymbol{x}, t)) \right) \\
&= \frac{1}{N} \sum_{n=1}^N \left(\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} (\bar{\rho} \dot{\omega}_{\alpha}^n(\boldsymbol{\xi}^n)) \right) \tag{A.5.7}
\end{aligned}$$