Abstract

A numerical investigation on the influence of stratification on a turbulent premixed V-shaped flame is conducted. Simulations are carried out using Large Eddy Simulation (LES) with a filtered probability density function (pdf) equation approach for the sub-grid contributions, which is solved using the Eulerian stochastic field method. A reduced version of the GRI 3.0 mechanism with 15 reaction steps involving 19 species is employed to model the chemistry. The configuration being investigated is the Cambridge Stratified Slot Burner (CSSB), of which three conditions: premixed, moderately and highly stratified, with stratification ratios of 1.0, 1.86 and 3.0 respectively, are simulated.

1 Introduction

Lean premixed combustion is widely used in combustion technologies as it can deliver very low emissions at high efficiencies. Lower temperatures and complete combustion result in low emissions of oxides of nitrogen, unburned hydrocarbons and carbon monoxide. However, this mode of combustion is prone to e.g. 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.

The constraints of many practical combustion applications or the design itself e.g. Lean Premixed Prevaporized combustors, lead to an inhomogeneous mixture of fuel and oxidiser resulting in combustion taking place under partially premixed conditions. In general, this mode of combustion can include both premixed and non-premixed modes, while in its basic form it includes only premixed combustion where the equivalence ratio of the mixture exhibits a spatial gradient. The fundamental properties of stratified combustion remain relatively poorly characterised and understood compared to other combustion regimes (Sweeney (2011)).

Previous experimental studies of stratification have been conducted by a number of workers, eg Anselmo-Filho et al (2009), Sweeney et al (2011a). These studies show that stratification can increase the lean flammability limits in comparison to fully premixed combustion. As well as increasing the variation of burning velocity, stratification can also lead to an increase in the flame propagation rate, leading to increased flame wrinkling. In V-flames stratification cause flame thinning, again due to the variation in burning velocity causing stretching and an increase in flame surface density (Anselmo-Filho et al (2009)).

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.

Large Eddy Simulation is a powerful tool for describing the interaction between combustion and turbulence. Combustion occurs mostly at the smallest scales and thus the sub-grid scale combustion model is of central importance in providing an accurate description of turbulence-chemistry interactions. The present work utilises the sub-grid-scale probability density function approach in conjunction with the Eulerian stochastic field solution method. These stochastic fields evolve according to stochastic partial differential equations, which are equivalent to the joint scalar pdf transport equation (Prasad 2011). The method does not involve any assumptions regarding the combustion regime and provides a general description of the flame, thus lending itself very well to partially premixed and stratified combustion. Furthermore it allows for the use of conventional Eulerian CFD solvers. The aim of this work is to investigate the influence of mixture stratification on turbulent premixed V-shaped flames, and validate the Stochastic field method in the premixed stratified combustion context. For the present work the simulations are conducted using the block-structured finite-volume LES code BOFFINLES, which has previously successfully been applied to e.g. Sandia Flame Series (Mustata et al (2006)), spark ignition (Jones et al (2011)) and to an industrial gas-turbine (Bulat et al (2013)).
2 Mathematical Formulation

In the present work a filter with a top-hat shape i.e. implicit, where the filter width \( \Delta \) is related to the local cube root of the grid volume, is used to obtain the filtered transported equations.

Together with Favre filtering, to account for the variation of density as a consequence of combustion, the continuity and Navier-Stokes equations become:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (1)
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial \rho}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (2)
\]

Where the symbols represent their usual quantities.

The transport equation for a scalar can be expressed as:

\[
\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_i \phi_\alpha}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \rho D \frac{\partial \phi_\alpha}{\partial x_j} \right] + \rho \omega_\alpha \left( \phi_\alpha, T \right) - \frac{\partial J_{\alpha sgs}}{\partial x_j} \quad (3)
\]

The there are three unknown term which require closure. \( \omega_\alpha \) is accounted for by introducing a sub-filter stress defined as \( \tau_{ij} = \rho (u_i u_j - u_i u_j) \), which itself is closed using a dynamic version of the Smagorinsky model (Germano et al (1991)). The unknown sub-grid scalar flux \( J_{\alpha sgs} \) in the scalar transport equation is closed using a gradient model following Fick’s law. Lastly a closure for the filtered formation rate is required.

The density-weighted filtered joint pdf for a set of scalars \( \psi \) needed to describe a reaction can be defined as (Jones et al (2002)):

\[
P_{sgs}(\psi; x, t) = \int_{\Omega} \prod_{\alpha=1}^{N_s} \delta(\psi_\alpha - \phi_\alpha(x, t)) G(x - x'; \Delta) d\mathbf{x}' \quad (4)
\]

Where delta is a Dirac delta function.

This pdf describes the behaviour of scalars on the sub filter level by essentially describing the probability of \( \phi = \psi \) arising inside a filter volume, thus providing the information necessary to evaluate the filtered chemical source term. A transport equation describing the evolution of the pdf can be derived from conservation principles and can be expressed as (Jones et al (2011)):

\[
\frac{\partial \rho \tilde{P}_{sgs}(\psi)}{\partial t} + \rho \tilde{u}_j \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_j} = -\frac{\partial}{\partial x_j} \left[ \rho \omega_\alpha(\phi_\alpha, T) \tilde{P}_{sgs}(\psi) \right] - \frac{\partial}{\partial x_j} \left[ \sigma \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_j} \right] \quad (5)
\]

In this formulation the term with the chemical source term does not require closure; however, the last two terms on the r.h.s. do. The first, the sub-grid transport of the pdf, can be closed using a gradient closure similar to the Smagorinsky model. The last term, representing the effect of molecular diffusion on the pdf, cannot be represented due to its one-point nature (Prasad (2011)). It is therefore modelled by decomposing the term and introducing a micro mixing term that represents the sub grid diffusion, which itself is closed using a linear mean square estimation approach. Thus the two modelled terms on the rhs. can be written as:

\[
-\frac{\partial}{\partial x_j} \left[ \left( \frac{\mu}{\sigma} + \frac{\mu_{sgs}}{\sigma_{sgs}} \right) \frac{\partial \tilde{P}_{sgs}(\psi)}{\partial x_j} \right] \quad (6)
\]

\[
- \frac{\rho}{2\tau_{sgs}} \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left( \psi_\alpha - \phi_\alpha(x, t) \right) \tilde{P}_{sgs}(\psi) \quad (7)
\]

The approach used to handle the high dimensionality of the pdf method is the Eularian stochastic field method, where the transport of the pdf is represented by a system of stochastic differential equations that are equivalent to the modelled transport equation (Jones et al (2007)). The Ito formulation of the stochastic integral is used and the equation governing the evolution of the fields can be written as:

\[
d\xi^n_\alpha = -\tilde{u}_i \frac{\partial \xi^n_\alpha}{\partial x_i} dt + \frac{\partial}{\partial x_i} \left[ \Gamma' \frac{\partial \xi^n_\alpha}{\partial x_i} \right] dt + (2\Gamma')^{1/2} \frac{\partial \xi^n_\alpha}{\partial x_i} dW_{ij}^{\gamma} - \frac{1}{2\tau_{sgs}} \left( \xi^n_\alpha - \bar{\xi}_{\alpha} \right) dt + \tilde{\omega}_{ij}^{\gamma} \bar{\xi}_{\alpha} dt \quad (8)
\]

\( \tilde{P}_{sgs} \) is represented by an ensemble of \( N_s \) stochastic fields for each of the \( N \) species included in the reaction mechanism. This stochastic approach has the benefit that computational cost increases linearly with complexity. A more detailed discussion of the method can be found in e.g. Prasad (2011).
3 Flame Configuration

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

The ‘two-dimensional’ slot burner, shown in Figure 1, 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, while 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 pairs of slots in the middle. The stratification ratio is defined as the ratio of the equivalence ratio of the richer slot pair to the leaner slot pair. 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 = 1.5mm which is positioned 2mm off the burner centre line and 10mm above the slots. 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 Figurereffig:graph1, of the inlet slot pairs in the region where the measurements are taken.

![Figure 1: Cambridge Slot Burner Geometry (not to scale)](image)

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 upstream 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 Damköhler and Karlovitz numbers are $Da = 2.35$ and $Ka = 0.59$. The conditions for which measurements are available are summarised in Table 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 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 a fixed downstream locations. Profiles of Favre-averaged and Favre-averaged rms fluctuations of temperature, species and equivalence ratio are provided at the same locations.

### Table 1: Cold Flow Properties

<table>
<thead>
<tr>
<th>$&lt; u &gt;$ (m/s)</th>
<th>$u'/S_L$</th>
<th>$\Lambda$ (mm)</th>
<th>$\eta$ (mm)</th>
<th>Re</th>
<th>Re$_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>0.3</td>
<td>1.3</td>
<td>1.9</td>
<td>0.09</td>
<td>2316</td>
</tr>
</tbody>
</table>

4 Reacting Flow Simulations

The experiment was conducted for six stratification ratios varying from premixed $\phi_2/\phi_1 = 1$ to highly stratified $\phi_2/\phi_1 = 1.16/0.39\approx3$. Here the premixed, intermediate $\phi_2/\phi_1 = 1.00/0.54\approx1.86$ and highly stratified cases are simulated. The computational domain extends 45mm beyond the furthermost 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. A fine mesh of 144x286x24 along the edges, consisting of about 0.9M nodes, divided into 48 blocks is used, resulting in an average mesh spacing of about 0.3mm. The use of an O-Grid around the rod was avoided, as it could be seen to influence the flame angle in the vicinity of the rod. The boundaries consist of an inlet, convective outflow conditions at the outlet, Neumann no-slip and adiabatic conditions at the rod and free slip conditions on all other boundaries.

![Figure 2: Mesh cross section at mid-plane and computational domain](image)

A digital inflow generator is used to model the ef-
fect of the turbulence mesh placed over the inlet slots. A detailed description of the method can be found in Klein et al (2006). The ARM reduced GRI 3.0 mechanism with 15 reaction steps and 19 species is employed for the chemistry. For the premixed case eight stochastic fields were utilised to represent the sub-grid contributions. For the stratified cases only a single field has been used. A model spark is used to initialise combustion and the simulations are allowed to settle before statistics are gathered.

5 Results and Discussion

The velocity and turbulence intensity of the generated inflow conditions are estimated using the single experimental profile available at y=15mm above the turbulence grid over x=0 to 16mm relative to the burner centre line. These measurements were taken without the rod in place. Figures 3 shows the mean velocity and turbulence intensity profiles respectively. The generated inflow data closely matches the velocity profile at the measurement location. The velocity fluctuations agree with the experimental data away from the centre line; this is likely due to the incorporation of both the effect of the sheets metal separating the slots as well as the effect of turbulence grid in the inflow data generation process.

Profile measurements of scalars quantities are provided at two downstream locations, y=25mm and y=30mm. The profiles have a length of 7mm with positions x=-2 to 5mm and x=-0.5 to 6.5mm relative to the burner centre line, at the respective y-values for the premixed case. The stratified cases are measured at x=-0.5 to 7.5mm and x=2.5 to 9.5mm at the same y-values. Therefore flame angle and burning velocity are crucial in comparing data.

Sample instantaneous and mean images of methane concentration are shown in Figures 4, 5 and 6 on the mid-plane of the computational domain. The flame fronts are turbulent and show wrinkling of ‘size’ of the order of the integral length scale. The flame stabilised on the rod and the co-flow air is shielding the premixed region.

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 mixing layers interaction with the left flame branch near the locations at which scalar profile measurement are taken can be 
observed. For the stratified cases 3 burning zones are captured, roughly separated by the scalar measurement locations. This can be seen clearly in 5 and in particular 6. 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 interact with the stratified mixing layer and back supported burning from high towards low equivalence ratios takes place. High temperatures and increased presence of radicals 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 7, 8 and 9 compare profiles from the simulation results against experimental data for temperature and mean values of major species concentrations of the three flames at both scalar measurement locations. The applied methodology provides good results for the species concentrations and also the flame brush thickness, which here is reflected by the gradients of the curves. Noticeable differences can only be seen in the profile locations, otherwise trends and magnitudes are captured well. It must be noted, that all profiles presented here have been shifted in order to accommodate a the difference in flame angle. -2.5mm for the premixed case with 8 stochastic fields i.e. the flame angle is over predicted, and 1mm for the stratified cases using only one field i.e. the flame angle is under predicted. One of the major issues encountered in this test case is the reproduction of the flame angle. A number of investigations have been conducted, however the flame angle in the vicinity of the rod remains approx. 13° as opposed to 4° suggested by the experimental data for the premixed flame. Using a single field for the premixed case produced results in good agreement with the experimental data, however the flame spreading rate is under predicted of the stratified cases, were sub-grid fluctuations and micro-mixing play a larger role.

6 Future Work
Issues that need to be addressed are:

- Effect of the dynamic Smagorinsky model on a turbulent but low Reynolds number flow
- Wall treatment in the vicinity of the rod
- Wall temperature effects, lifted flame
- Accurately capturing the effect of the turbulence grid of the inflow slots using inlet velocity generation
- Use of full transport properties of the species.

- Influence of stochastic fields on low Reynolds number flows with low sub-grid scale fluctuations and micro-mixing

7 Conclusions
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 flames of the Cambridge Stratified Slot Burner. Velocity and turbulence intensity measurements have been reproduced and the combustion results are promising for the species concentrations and temperature. However, the over-prediction of flame angle is an issue that needs to be addressed before detailed simulations of the stratified cases can be conducted.

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Figure 8: Mean profiles of temperature and major species at $y=25\text{mm}$ and $y=30\text{mm}$ for the moderately stratified flame.

Figure 9: Mean profiles of temperature and major species at $y=25\text{mm}$ and $y=30\text{mm}$ for the highly stratified flame.
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