Large Eddy Simulation of the Sandia Flame Series (D, E and F) using the Eulerian stochastic field method

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Abstract

Three turbulent piloted methane jet flames with increasing levels of local extinction (Sandia Flames D, E and F) have been computed using Large Eddy Simulation. The smallest unresolved scales of the flow, in which combustion occurs, are represented using the filtered Probability Density Function method where the corresponding evolution equation is solved directly. A dynamic model for the sub-grid stresses together with a simple gradient diffusion approximation for the scalar fluxes is applied in conjunction with the linear mean square estimation closure for *sub-filter scale mixing*. An augmented reduced mechanism (ARM) derived from the full GRI 3.0 mechanism has been incorporated to describe the chemical reaction. The results demonstrate the ability of the method in capturing quantitatively finite rate effects such as extinction and re-ignition in turbulent flames.

Keywords:

Turbulence, Large Eddy Simulation, Joint *pdf*, Stochastic field method, Methane-air flame

1. Introduction

Turbulent combusting flows often exhibit local extinction and re-ignition events. Describing these phenomena is difficult as the expressions describing chemical reaction rates are highly non-linear and because burning occurs mostly in the smallest turbulence scales. In principle a fully resolved Direct

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Numerical Simulation(DNS) would be capable of providing a description of such phenomena though due to the very large computing requirements, especially for high Reynolds number flows, this technique is at present not feasible and is unlikely to become so in the foreseeable future.

A potentially powerful method for describing the interaction between turbulence and combustion is Large Eddy Simulation(LES). In LES the equations of motion are filtered before solution so that the large scale energetic turbulent motions are computed directly while the effects of motions of 'size' smaller than the filter width are modelled. These sub-filter or sub-grid scale (*sgs*) motions have short length and time scales and, at least for the sub-grid fluxes, thus exert a much less influential role and are much easier to model than is the case for the corresponding Reynolds averaged fluxes; simple closure models are usually found to suffice. However, for reacting flows, the filtered chemical source terms, which represent net chemical species formation rates due to chemical reactions, depend strongly on the fluctuations occurring in the smallest, unresolved sub-grid scales and here modelling plays a dominant role. A variety of *sgs* combustion models have been proposed in the past; an overview of recent strategies is provided by [1], [2] and [3].

In LES the one-point joint filtered probability density function (*pdf*) for all of the scalar quantities needed to describe reaction provides a means of predicting the filtered fields of temperature and species mass fraction. This *pdf*, which provides a description of the scalars at a sub-grid scale level, can be obtained from the solution of a modelled form of the equation governing the time evolution of the joint *pdf*. For inert flows models are required to represent sub-grid scale transport of the *pdf* and sub-grid mixing. The chemical source terms appear in closed form in this equation and further modelling for combustion, beyond specification of a chemical reaction mechanism, is not required. The *pdf* equation involves a large number of independent variables and solution is only feasible if stochastic solution methods, where the computational effort grows linearly with the number of scalars, are used. The statistical error associated with stochastic methods decays with $\mathcal{O}(\frac{1}{\sqrt{N}})$ where N is the number of samples, though this has to be offset against their substantially reduced CPU costs.

The most commonly adopted approach to solving the *pdf* evolution equation in turbulent reacting flows in the context of Reynolds averaging (RANS) is the Lagrangian stochastic particle method, where an ensemble of particles are used to represent the joint *pdf*. Initially developed in the 1970s and 1980s, see the seminal work of Pope [4], these methods often included velocity as

a stochastic variable and are therefore *mesh-independent*, which implies that they do not have errors arising from spatial discretisation, though stochastic errors do arise in their place. However the closures and solution techniques involved are complex, especially with respect to the determination of the pressure field [5]. For this reason the recent trend [6, 7, 8, 9] has been to use a Lagrangian solver for the composition joint *pdf* coupled with a standard Eulerian approach for the velocity components. Although Lagrangian approaches have the advantage of not introducing errors associated with the discretisation of spatial gradients, these errors are partially reintroduced by the interpolation required to obtain the statistical moments in physical space. The methods also introduce complex couplings between the Eulerian and Lagrangian solvers, which can be critical in the feedback of chemistry into the flow solver, particularly in the LES context, where the use of some "correction" method is normally needed [10, 1].

Recently, new methods of solving the *pdf* transport equation in a fully Eulerian manner have been developed [11, 12]. These methods are based on stochastic Eulerian fields, which evolve according to stochastic partial differential equations equivalent to the joint *pdf* transport equation. The stochastic field method has close similarities to Spalding's multi-fluid model [13] and to the configuration field methods used in rheology [14, 15]. Similar ideas can also be found in the Ensemble Kalman filtering [16] used in weather predictions and in the simulation of particle transport under stochastic velocity fields in plasma turbulence [17], where the concept of "stochastic field" is used. The method is attractive because the stochastic fields are continuous and differentiable in space and continuous though not differentiable in time. As a consequence, there are no spatially varying sampling errors in the evaluation of statistical moments, which are very easy to compute. The method involves solution of conservation equations in which a stochastic term is included and which consequently can be incorporated into existing CFD codes without undue difficulty, though care has to be taken in the selection of the discretisation scheme used [18]. Examples of recent applications can be found in [19, 20, 21, 22]. Extensions of the method to the joint velocity-scalar *pdf* have also been proposed [23, 24]. In LES the method has been successfully applied to a non-premixed jet flame (Sandia Flame D) [25] and to auto ignition of lifted flames (see [26], [27] and [28]).

The aim of the present paper is to demonstrate the capability of the filtered probability density function/stochastic field method in simulating flames with finite rate chemistry effects. The Sandia Flame series (D, E and

F) have been chosen for this purpose. They represent an ideal target, as they encompass a range of turbulent burning regimes from a simple diffusion flame (Flame D) to partially premixed flames with strong extinction and re-ignition (Flames E and F) in essentially the same geometric configuration.

2. Mathematical Formulation

The Continuity and Navier-Stokes equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \rho g_i \quad (2)$$

where μ is the viscosity, g_i is the gravitational acceleration vector and where the isotropic part of the stress has been adsorbed into the pressure.

The conservation of mass for the chemical species α is:

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_j Y_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\rho D_\alpha \frac{\partial Y_\alpha}{\partial x_j} \right] + \rho \dot{\omega}_\alpha(\underline{Y}, T)^1. \quad (3)$$

where Y_α is the mass fraction of species α . Fick's law has been used and Soret effects (diffusion of species due to temperature gradients) have been neglected. It is conventional in turbulent combustion [29] to assume equal diffusivities for all species, $D_\alpha = D$, which can be related to the viscosity through the Schmidt number $\sigma = \frac{\mu}{\rho D}$, which in gases is often assumed to be constant with a value $\sigma \approx 0.7$.

The energy equation can be written in terms of the total enthalpy:

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\frac{\mu}{\sigma} \frac{\partial h}{\partial x_j} \right] + \dot{q}_R + \frac{\partial p}{\partial t} + \tau_{ij} \frac{\partial u_i}{\partial x_j}, \quad (4)$$

where $h = \sum_\alpha Y_\alpha h_\alpha(T) + u_i u_i / 2$ includes the enthalpies of formation and where the thermal and mass diffusivities have been assumed to be identical, *i.e.* unity Lewis number [30]. At low Mach numbers acoustic interactions and viscous heating can be neglected. Furthermore if the thermodynamic pressure can be assumed constant then the mass and energy conservation

¹no summation is implied by repeated Greek subscripts

equations, (3) and (4), can be rewritten in terms of a general reactive scalar ϕ_α , $\alpha = 1, N_s$ where N_s is the number of scalars required to describe the system, *i.e.* the number of species plus enthalpy.

$$\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_j \phi_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_j} \right] + \rho \dot{\omega}_\alpha(\underline{\phi}), \quad (5)$$

For the non-radiative and constant pressure flows consider in the present work the source term for enthalpy is identically zero.

2.1. The Filtered Navier-Stokes Equations

In LES a spatial filter is applied to the equations of motion: the spatial filter of a function $f = f(\mathbf{x}, t)$ is defined as its convolution with a filter function, G , according to:

$$\bar{f}(\mathbf{x}, t) = \int_{\Omega} G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) f(\mathbf{x}', t) d\mathbf{x}' \quad (6)$$

where the filter function must be positive definite in order to maintain filtered values of scalars such as mass fraction within bound values and to preserve the nature of the chemical sources terms (a filter that changes sign may change consumption terms to formation terms). The integration is defined over the entire flow domain Ω and the condition that the filter kernel G should be positive definite implies that it has the properties of a *pdf*.

The filter function has a characteristic width Δ which, in general, may vary with the position. The filtering operation (6) commutes with spatial differentiation if the filter width varies smoothly with position. In the present work a box or 'top hat' filter defined by:

$$\begin{aligned} G(\mathbf{x} - \mathbf{x}') &= \frac{1}{\Delta^3} \quad \text{for } |\mathbf{x} - \mathbf{x}'| < \frac{\Delta}{2} \\ &= 0 \quad \text{otherwise} \end{aligned}$$

is used. The density variations in the unresolved scales that arise in combusting flows can be treated through the use of density weighted, or Favre, filtering, defined by $\tilde{f}(\mathbf{x}, t) = \overline{\rho f} / \bar{\rho}$. Application of the density weighted filtering operation to the equations of motion results in:

Continuity

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0, \quad (7)$$

Momentum

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (2\mu \bar{e}_{ij}) - \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} \quad (8)$$

where $\bar{e}_{ij}$ is the resolved rate of strain tensor. The deviatoric part of the sub-grid scale stress tensor $\tau_{ij}^{sgs} = \bar{\rho} (\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j)$ is determined with the Smagorinsky model [31] :

$$\tau_{ij}^{sgs} - \frac{\delta_{ij}}{3} \tau_{kk}^{sgs} = 2\mu_{sgs} \left(\tilde{e}_{ij} - \tilde{e}_{kk} \frac{\delta_{ij}}{3} \right)$$

with

$$\mu_{sgs} = \bar{\rho} (C_S \Delta)^2 ||\tilde{e}_{ij}||$$

where $||\tilde{e}_{ij}|| \equiv \sqrt{2\tilde{e}_{ij}\tilde{e}_{ij}}$ is the Frobenius norm of the resolved rate of strain tensor, $\tilde{e}_{ij} = 0.5 \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$. The filter width is taken as the cube root of the local grid cell volume and the parameter C_S is obtained through the dynamic procedure of Piomelli and Liu [32]. As with the viscous stress the isotropic part of the sub-grid stress is adsorbed into the pressure.

Scalar Equation

$$\frac{\partial \bar{\rho} \tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\bar{\rho} D \frac{\partial \tilde{\phi}_\alpha}{\partial x_j} \right] + \overline{\rho \dot{\omega}_\alpha(\underline{\phi})} - \frac{\partial J_{sgs}}{\partial x_j}, \quad (9)$$

where two terms need to be modelled; the transport due to sub-grid fluctuations, $J_{sgs} = \bar{\rho} (\widetilde{u_j \phi_\alpha} - \tilde{u}_j \tilde{\phi}_\alpha)$, and the filtered net formation rate $\overline{\rho \dot{\omega}_\alpha(\underline{\phi})}$.

2.2. Filtered Probability Density Function

Using the filtering operation, equation (6) and following Gao and O'Brien [33] a density weighted sub-grid (or filtered) *pdf* for the N_s scalar quantities needed to describe reaction (the number of species considered plus enthalpy) can be defined:

$$P_{sgs}(\underline{\psi}; \mathbf{x}, t) = \int_{\Omega} \mathcal{F}(\underline{\psi}; \mathbf{x}', t) G(\mathbf{x} - \mathbf{x}', \Delta) d\mathbf{x}'. \quad (10)$$

where $\mathcal{F}(\underline{\psi}; \mathbf{x}, t) = \prod_{\alpha=1}^{N_s} \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}, t))$ is a fine-grained *pdf* and $\underline{\psi}$ represents the phase or sample space of the scalar quantities $\underline{\phi}$. With the filter

defined by equation (6), P_{sgs} describes the probability of $\phi = \psi$ arising within the filter volume. An exact evolution equation for this quantity can then be derived, *e.g.* [33, 34, 35], from the appropriate conservation equations by standard methods. The result is:

$$\begin{aligned} \bar{\rho} \frac{\partial \tilde{P}_{sgs}(\underline{\psi})}{\partial t} + \bar{\rho} \tilde{u}_j \frac{\partial \tilde{P}_{sgs}(\underline{\psi})}{\partial x_j} &+ \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left[\bar{\rho} \dot{\omega}_\alpha(\underline{\psi}) \tilde{P}_{sgs}(\underline{\psi}) \right] = \\ &- \frac{\partial}{\partial x_j} \left[\overline{\rho(\underline{\psi}) \mathcal{F}(\underline{\psi}) u_j} - \bar{\rho} \tilde{u}_j \tilde{P}_{sgs} \right] \\ &- \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\overline{\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \mathcal{F}(\underline{\psi})} \right) \end{aligned} \quad (11)$$

where equal diffusivities have been assumed and the spatial and temporal dependency of the *pdf* have been dropped for compactness.

The first term on the right of equation (11) is approximated by a simple gradient closure directly analogous to the Smagorinsky model:

$$\overline{\rho(\underline{\psi}) \mathcal{F}(\underline{\psi}) u_j} - \bar{\rho} \tilde{u}_j \tilde{P}_{sgs} = - \frac{\mu_{sgs}}{\sigma_{sgs}} \frac{\partial \tilde{P}_{sgs}}{\partial x_j} \quad (12)$$

where σ_{sgs} is a constant turbulent Prandtl/Schmidt number assigned the value 0.7, [3], [25], [36]. The second term on the right of equation (11) can also be written;

$$\begin{aligned} &- \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left(\overline{\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \mathcal{F}(\underline{\psi})} \right) = \frac{\partial}{\partial x_i} \left[\frac{\mu}{\sigma} \frac{\partial P_{sgs}(\underline{\psi})}{\partial x_i} \right] \\ &- \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left\{ \left(\overline{\frac{\mu}{\sigma} \frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \bigg|_{\phi = \underline{\psi}}} \right) P_{sgs}(\underline{\psi}) \right\} \end{aligned} \quad (13)$$

The final term in equation (13) comprises the filtered conditional ‘scalar dissipation rates’, represents *sub-grid scale mixing* and describes the effect of molecular diffusion on $\tilde{P}_{sgs}(\underline{\psi})$. There are several models available for this term although none of them is entirely satisfactory (see [7] and references therein for reviews). In the present work the Linear Mean Square estimation (LMSE) closure [37, 38, 39], although originally formulated for the complete molecular diffusion term, is adopted. The model was also proposed independently in stirred reactor studies where it is known as Interaction by Exchange

with the Mean (IEM), [40]. The LMSE closure has been used previously in the LES studies of Mustata *et al.* [25] and Jones and Navarro-Martinez [26, 28, 41]. Thus the final term in equation (13) is replaced by:

$$\frac{1}{\tau_{sgs}} \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_{\alpha}} \left[\left(\psi_{\alpha} - \tilde{\phi}_{\alpha}(\mathbf{x}, t) \right) \bar{\rho} \tilde{P}_{sgs}(\underline{\psi}) \right] \quad (14)$$

where the *sub-grid mixing* time scale τ_{sgs} is assumed to be, [42], given by:

$$\frac{1}{\tau_{sgs}} = C_d \frac{\mu + \mu_{sgs}}{\bar{\rho} \Delta^2} \quad (15)$$

with the *sub-grid scale mixing* constant $C_d = 2$.

As is well known, [39] the LMSE closure preserves the shape of the *pdf* and, for example, in the absence of other influences an initially segregated mixture, i.e. a *pdf* comprising two delta functions, would remain segregated. However in the present application such a *pdf* has to be viewed as pathological and is inconsistent with LES concepts. In LES the energetic motions are resolved and the representation of *sub-grid scale mixing* provided by the LMSE model may be adequate in many practical situations. Some support for this view is provided in [43]. The LMSE model is also known to perform well for continuous *pdf*'s and to be consistent with the Gaussian *pdf*'s that often arise in passive scalar mixing problems. In addition there is no evidence that any alternative proposals would perform better in LES and the computation cost would be substantially larger.

It is often suggested that the scalar dissipation rates alone, e.g. the mixture fraction variance decay rate, might provide a more accurate means of determining a *sgs* mixing time scale. However this is not the case in the present situation. The mixture fraction dissipation rate has dimensions of time^{-1} only because mixture fraction itself is dimensionless. However mixture fraction is normalised with the conditions in one of the inflow streams so that its value there is unity. This normalisation is both arbitrary and *non local*. For example in the Sandia flames presently considered the mixture fraction is conventionally defined to be unity in the inflowing central jet which comprises 25 % methane and 75 % air, but it could equally well be defined to correspond to the methane mass fraction at the jet inlet. i.e. to have the value 0.25 in the inflowing jet. The corresponding dissipation rates would then differ by a factor of 16. The clear implication of this is that the scalar dissipation rates do not correspond to any *local physically meaningful turbulence time scale*.

Their use in the present context is thus inappropriate. This is in contrast to laminar flows in cases where a mixing layer is bounded by two streams in which the mixture fraction is 0 and 1 such as occurs in opposed jet flows. In these circumstances the quantity

$$\frac{\nu/\sigma}{(\xi_{+\infty} - \xi_{-\infty})^2} \left(\frac{\partial \xi}{\partial x_2} \right)^2$$

with $\xi_{+\infty} = 1$ and $\xi_{-\infty} = 0$ and where x_2 is the normal distance does provide a measure of the rate of mixing. The quantity $(\xi_{+\infty} - \xi_{-\infty}) \left| \frac{\partial \xi}{\partial x_2} \right|_{\xi=0.5}^{-1}$ also provides a measure of the thickness of the mixing layer, akin to the vorticity thickness. However in a turbulent flow it is unlikely, except perhaps very close to the inlet, that scalar mixing will occur only at the ‘interface’ between stream 1 fluid and stream 2 fluid: if this were to be the case then at high turbulence Reynolds numbers the mixture fraction pdf would comprise two delta functions. This should not be taken to imply that the scalar dissipation rate is irrelevant in combustion. In the flamelet regime reaction will occur in the mixing layer at the ‘interface’ between stream 1 fluid and stream 2 fluid and in these circumstances the scalar dissipation rate can provide some measure of the rate of flame stretch. Also in both unsteady flamelet formulations and in Conditional Moment Closures the scalar dissipation rate (or the conditional form thereof) appears as a multiplier of a term involving the second derivative with respect to the mixture fraction sample space. The complete term is thus independent of the normalisation and the use of scalar dissipation rates appears entirely proper. The important point is that the scalar dissipation rate itself is not a *physically meaningful turbulence mixing time scale*.

A local *sgs* time scale representative of mixture fraction, (ξ) fluctuations can be obtained from:

$$\tau_s = \frac{\overline{\xi^2} - \bar{\xi}^2}{\chi_\xi}$$

where χ is the scalar (mixture fraction) dissipation rate. However this time scale is comparable with the time scale given by equation (15), indeed the constant C_d represents the ratio of the mechanical and scalar *sgs* turbulence time scales.

Finally it is to be noted that all of the moments arising from solution of the closed form of equation (11) are smooth on a scale of $\mathcal{O}(\Delta)$.

2.3. Stochastic Field Method

Equation (11), with the closure approximations (12) and (14) incorporated, is solved using the Eulerian stochastic field method. $\tilde{P}_{sgs}(\underline{\psi})$ is represented by an ensemble of N stochastic fields for each of the N_s scalars, namely $\xi_\alpha^n(\mathbf{x}, t)$ for $1 \leq n \leq N$, $1 \leq \alpha \leq N_s$. Two formulations of the method can be devised depending on whether an Ito or Stratonovich interpretation of the stochastic integral is adopted; for a description of these alternatives see [11] and [12]. In the present work the Ito formulation is adopted and the stochastic fields thus evolve according to:

$$\begin{aligned} \bar{\rho} d\xi_\alpha^n = & - \bar{\rho} \tilde{u}_i \frac{\partial \xi_\alpha^n}{\partial x_i} dt + \frac{\partial}{\partial x_i} \left[\Gamma \frac{\partial \xi_\alpha^n}{\partial x_i} \right] dt + \bar{\rho} \sqrt{\frac{2\Gamma}{\bar{\rho}}} \frac{\partial \xi_\alpha^n}{\partial x_j} dW_i^n \\ & - \frac{\bar{\rho}}{2\tau_{sgs}} \left(\xi_\alpha^n - \tilde{\phi}_\alpha \right) dt + \bar{\rho} \omega_\alpha^n(\xi_\alpha^n) dt \end{aligned} \quad (16)$$

where $\Gamma = \frac{\mu}{\sigma} + \frac{\mu_{sgs}}{\sigma_{sgs}}$ represents the total diffusion coefficient and dW_i^n represent increments of a vector Wiener process, different for each field but independent of the spatial location $\mathbf{x}$. This stochastic term has no influence on the first moments (or filtered values) of ξ_α^n . 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 (16) 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, [44] 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 (11). 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 (16) are not to be mistaken with any particular realization of the real field, but rather form an equivalent stochastic system (both sets have the same one-point *pdf*, [45]) 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 (11) 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 were obtained from:

$$\tilde{\phi}_\alpha = \frac{1}{N} \sum_{n=1}^N \xi_\alpha^n \quad (17)$$

3. Simulation Parameters

3.1. Experimental setup

The chosen test cases for the present paper are the well documented Sandia piloted jet Flames D, E and F, [46], which exhibit increasing levels of extinction, with Flame F reportedly being close to blow-off. These flames have been the subject of experimental studies by Schneider *et al*, [47], who performed LDV velocity measurements and Frank and Barlow, [48] who measured the temperature and the concentrations of chemical species. The fuel (25 % methane diluted in 75 % air by volume) is injected through a central jet of diameter of 7.2 mm with bulk velocities of 49.9, 74.4 and 99.2 m/s corresponding to Flames D, E and F respectively. For all three flames the surrounding annular pilot comprises a mixture of C₂H₂, H₂, air, CO₂ and N₂ with an equivalence ratio of 0.77 with the same nominal enthalpy and equilibrium composition as methane/air at the given equivalence ratio. The bulk velocities are 11.4 (D), 17.1 (E) and 22.8 m/s (F) respectively. The temperatures of the jet and pilot are 290 K and 1880 K for flames D and E while the pilot temperature of Flame F is said to be slightly lower, though there are uncertainties about the exact value. A temperature of 1860 K, previously used by Xu and Pope [49] has been adopted for Flame F in this work. The stoichiometric mixture fraction of these flames, based on a mixture fraction of unity in the fuel jet, is 0.351. A more detailed summary of the experimental configuration and measurement techniques can be obtained from [48].

The Sandia Flames, predominantly Flame D, have been a target for many simulations in the past, for examples of non-stochastic approaches see [36], [50], [3] and [51]. Transported *pdf* simulations in a RANS context have been performed by Xu and Pope [49], Tang *et al* [52] and Lindstedt *et al* ([9] and [53]). Computations with LES combined with the sub-grid *pdf* equation have been performed by Sheikhi *et al*, [54] for Flame D and by Raman and Pitsch [55] for Flames D and E using a Lagrangian particle scheme while Mustata *et al*, [25] applied the Eulerian stochastic field method in conjunction with a four-step global reaction mechanism to Flame D. To date, however there appear to have been no published LES of the complete series, particularly of Flame F.

3.2. Chemical reaction kinetics

An accurate description of chemical reaction is clearly needed if local extinction and reignition phenomena are to be reproduced accurately. Unfortunately full and detailed elementary reaction mechanism for methane-air combustion inevitably involve a large number of species and reactions, which renders them unusable in LES computations. The use of reduced chemical reaction mechanisms is essential in order to maintain computational costs at manageable levels. In the present work the augmented reduced mechanism (ARM) of Sung *et al* [56] for methane combustion is used. This comprises fifteen reactions and nineteen species derived from the GRI 3.0 mechanism using quasi-steady state assumptions for minor intermediates. The reduced mechanism includes species such as HO_2 , H_2O_2 , CH_2O that are key to correctly predicting ignition delay.

3.3. Numerics

For the simulation, an in-house block-structured, parallel, boundary conforming coordinate LES code, BOFFIN-LES [57] has been used. The code is parallelised using the MPI message passing routines. It comprises a second-order-accurate finite volume method, based on an implicit low-Mach-number formulation using a co-located storage arrangement. For the momentum equation convection terms an energy-conserving discretisation scheme is used and all other spatial derivatives, with exception of the convective terms of the scalar equations, are approximated by standard second-order central differences. As is common practice [58, 59], a total variation diminishing (TVD) scheme [60] is used for the scalars to avoid unphysical overshoots and second law violations. The stochastic field equations are solved using the weak first order temporal approximation described in [25, 26]. The spatial discretisation of the stochastic term in the field equations was accomplished using a central difference approximation and the application of the TVD scheme was found to be unnecessary; bound violations did not arise. An approximate factorisation scheme was applied to handle chemical reaction and the resulting rate equations were integrated using a Newton method based stiff ODE solver. To avoid performance loss due to load balancing, the integration work was additionally parallelised.

The solution domain extends 20 jet diameters in the radial direction and 50 diameters in the downstream direction. The mesh used comprised $81 \times 81 \times 160$ nodes in the x -, y - and z -directions respectively. Grid clustering was applied to resolve the strong gradients that arise near the inlet. Free slip

conditions have been employed for all lateral boundaries and a convective outflow condition has been applied at the outflow plane. Following [25] and [26] eight stochastic fields have been used to characterize the influence of the sub-grid fluctuations. The simulations were performed on a CRAY XT4 (AMD 2.6 GHz dual core Opteron processor) on 512 CPU's, with about 1.5 days required for one simulation run.

4. Simulation of the Sandia Flames

4.1. Results

In this part of the paper, simulation results for Flames D, E and F are presented and discussed. All statistical quantities were collected, typically, for a period of 15-20 flow through times, based on the jet bulk velocity, after the initial flow was allowed to reach a statistically steady state. For most radial profiles and scatter plots, three axial positions have been chosen in order to focus on zones with extinction, $z/D = 7.5$; re-ignition, $z/D = 15$ and with diffusion flame like behaviour, $z/d = 30$.

Snapshots of the temperature fields for all three flames are shown in Figures 1(a) to 1(c). The black lines in these plots indicate isolines of the stoichiometric mixture fraction. Flame D shows almost no extinction whereas Flame E and Flame F exhibit extinction pockets along the isoline of stoichiometric mixture fraction with the latter case exhibiting a greater degree of extinction. These pockets typically extend over a few cells and re-ignite further downstream. The increase of extinction from Flame D to Flame F can be seen more clearly in the instantaneous scatter plots, Figures (2) to (4), where the temperatures arising in the stochastic fields are plotted against their corresponding mixture fraction values and compared to the measurements. The maximum temperatures that occur close to the stoichiometric mixture fraction are slightly over predicted for all three flames. Strong scattering in the temperature-mixture fraction plots are evident in the simulations of Flames E and F at $z/D = 7.5$ and $z/D = 15$ whereas Flame D exhibits diffusion flame characteristics. The results of the simulations are in good overall agreement with measurements except at the furthestmost downstream position for Flame F, where little scatter is evident in the simulated results.

Radial profiles of the time-mean and *rms* of the axial velocity of all three flames are shown in Figures 5(a) to 5(c). The profiles at 15 D only are shown for Flame E, as there are no measurements available for the other two locations. Both mean and *rms* velocity fluctuations are in good agreement

with measurements, though the spreading of the velocity at $z/D = 7.5$ is slightly under predicted. In Figures 6(a) to 6(c) radial profiles of the mean mixture fraction and temperature are shown. For all three flames, the mixture fraction on the centreline is somewhat over predicted at $z/D = 15$ and $z/D = 30$ though in other respects the agreement with measurements is excellent. The discrepancies in the mean mixture fraction profiles at and in the vicinity of the centreline are closely similar to those observed by Raman and Pitsch [55] in their LES/FDF of Flames D and E and in the RANS/*pdf* computations of Cao and Pope, [61] of Flames D, E and F. The temperature profiles for Flame D are in excellent agreement with the experimental data. For Flame E, the maximum temperatures at $z/D = 7.5$ and $z/D = 15$ are over predicted by around 200 K but otherwise the agreement with measurements is also good. The maximum temperatures for Flame F are over predicted by a greater margin than is the case for Flame E. However the basic characteristics of re-ignition have been captured, with the temperature at $z/D = 30$ being higher than at $z/D = 15$.

The radial profiles of the time averaged mean species mass fractions and *rms* fluctuations for all three flames are shown in Figures 7 to 12, with the species plotted being CO, CO₂, O₂, H₂O, CH₄ and H₂. For Flames D, E and F the agreement with the measured profiles is good though the maximum mean values of H₂ and to a lesser extent CO mass fraction are over predicted near the nozzle with the effect being somewhat more pronounced for Flame F. The *rms* mass fraction fluctuations are remarkably accurately reproduced in all three cases.

The conditional means of temperature and the mass fractions of CH₄, H₂O, CO₂, CO and H₂ are plotted as a function of mixture fraction in Figure 13 for Flame F. Profiles are shown at the two axial locations $z/D = 7.5$ and $z/D = 15$ where local extinction is evident. At $z/D = 7.5$ the temperatures in the main extinction zone (close to stoichiometric) and the corresponding levels of H₂O, CO, and H₂ are over predicted whereas the composition and temperatures on the lean and rich sides of stoichiometric are reasonably well reproduced. In contrast at $z/D = 15$, only the lean side is captured well and the extinction region and the fuel rich region are over predicted. The over prediction shown in the radial profiles of CO and H₂ is also emphasised here. The results presented here for Flame F are closely similar to those obtained by Xu and Pope [49] both when plotted in physical space as well as in mixture fraction space. This may be related to the fact very similar reduced mechanisms were used in both cases - ARM derived from GRI-mech.

Figure 14 shows the history of the temperature at a fixed point ($r/D=1.11$, $z/D=15$, a point where the flame is reportedly close to blow-off) for a fixed time interval is shown. The filter width at this point is 1.2 mm . The filtered temperature and the rms of the sub-grid temperature fluctuations are plotted together with the simulated and measured time-averaged temperatures. The unlabeled lines represent the individual stochastic fields. The mean temperature is about 400 K higher than the experimental data, whereas the resolved scale temperature *rms* is well reproduced. The reason for this is uncertain though it has to be acknowledged that Flame F is very close to blow-off and it represents a severe test of all aspects of the simulation.

4.2. Statistical convergence

Prior to further parametric studies, the instantaneous statistical errors arising from with the stochastic field method are examined. As mentioned in the introduction of the paper, the statistical error decays at a rate of $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$. While a full and detailed investigation of the possible stochastic errors is beyond the scope of the present paper some indications of the accuracy of solution is provided by an examination of the (instantaneous) filtered mixture fraction field. The filtered form of the mixture fraction equation was solved in addition to the stochastic field equations and, though redundant, it provides a means of monitoring any stochastic mass conservation errors that arise throughout the simulations. The mean mixture fraction field at any instant of time can also be constructed from the stochastic fields using Equation 17. Radial profiles of filtered mixture fraction obtained by the two methods are shown in Figure 15 for Flame F at three time instances and three axial positions. The differences between the two sets of profiles are negligible, suggesting that statistical convergence, at least of the mean fields, has been achieved. Furthermore, profiles of rms sub-grid temperature fluctuations also shown at the same locations and times, Figure 16, indicate that sub-grid fluctuations cannot be ignored. The values reach maximum values around the inner and outer shear layers, regions of reaction as well as extinction and re-ignition.

4.3. Influence of the sub-grid mixing

The *rms* sub-grid temperature fluctuation as seen in Figure 14 has a value of about 230 K in average and can reach values of close to 500 K, which is about 30% of the predicted mean temperature. It is of interest at

this point to examine the influence of the sub-grid contribution. Apart from the choice of the number of stochastic fields, the only model parameter that directly influences the sub-grid contribution is the *sub-grid scale* constant C_d . It has previously been demonstrated, [25, 28] that eight and sixteen fields produce near identical results for Flame D, albeit with a different reaction mechanism and in LES studies of auto-ignition phenomena. In RANS based Lagrangian particle methods micro-mixing plays a central role, as the change in composition space occurs solely through the influences of chemical reaction and micro-mixing. In previous works (see [62], [9] and [49]), the results achieved have been shown to be very sensitive to the value of this constant. To investigate whether this is the case for LES the value of C_d was increased by 50 %, i.e. $C_d = 3.0$ and the corresponding results are shown in Figures 17(a) and 17(b). The radial temperature profiles and the conditional mean temperatures then obtained are very closely similar to those obtained with $C_d = 2$. This suggests strongly that the *sub-grid scale* constant C_d does not have the same significance in LES as it does RANS based transported *pdf* methods, at least not for in the present case.

4.4. Influence of the pilot inlet temperature

With Flame F being very close to a blow off, it is of interest to see how the simulation reacts to changes in the inflow boundary conditions, in particular to the pilot inlet temperature. For this the experiments indicate a measurement error of ± 50 K with a nominal temperature of 1860 K, so that the lower limit is 1810 K. Here the temperature is reduced by a further 30 K to 1780 K. The resulting radial profiles of temperature and the conditional temperatures at $z/D = 7.5$ and 15 are shown in Figures 18(a) and 18(b). The maximum temperatures arising from the reduced pilot temperature are about 100K lower than those obtained with the nominal temperature, with the ‘thickness’ of the radial profiles being unaffected. The conditional mean profile shown in Figure 18(b) displays a corresponding fall in temperature around and on the rich side of stoichiometric conditions whereas the lean side remains unaffected. The impact of the temperature variation at the inlet can be directly related to the sensitivity to the chemical reaction mechanism.

5. Conclusions

The Sandia Flames D, E and F have been simulated with the LES-*sgs* probability density function evolution equation method in conjunction with

the Eulerian stochastic field solution technique. Eight stochastic fields were utilized to characterize the influence of the sub-grid fluctuations. An augmented reduced mechanism derived from the full GRI 3.0 mechanism involving 19 species and 15 reaction steps has been employed to describe the chemical reactions. The increased levels of local extinction arising from the increased jet velocities of Flames D to F were reproduced by the simulations. The profiles of mean mixture fraction, temperature and mass fractions of CO, CO₂, O₂, H₂O, CH₄ and H₂ were shown to be in very good agreement with measurements for Flames D and E. The discrepancies that appear locally in H₂ and to a lesser extent CO can probably be related to limitations in the reduced reaction mechanism used in the simulations. The results presented represent a significant improvement over those obtained previously for Flame D using a global 4-step mechanism.

The simulations of Flame F, which is close to blow-out, were in qualitative agreement with measurements; local extinction and re-ignition was reproduced. However the degree of extinction of Flame F was under-predicted. Conditional means showed an over prediction in temperatures around and on the rich side stoichiometric conditions, whereas the lean side was well reproduced. The similarity of the results for Flame F to those obtained earlier by Xu and Pope, [49] using a RANS based transported *pdf* method with a very similar reduced reaction mechanism (ARM derived from GRI-mech) suggests strongly that chemical kinetics plays a dominant role in Flame F.

An increase of the *sub-grid scale mixing* constant resulted in negligible changes in the mean temperatures suggesting that the sensitivity to the *sub-grid scale mixing* model may be somewhat less in the LES-*pdf* formulation than is the case in RANS based transported *pdf* methods, at least for the given flame configurations. An examination of the influence of a reduction in the temperature of the inflowing pilot gas for Flame F showed a corresponding fall in mean temperatures throughout the flame, consistent with a sensitivity to the chemical mechanism.

Overall the LES-*sgs pdf* equation method has been shown to be capable of simulating local extinction and re-ignition phenomena to a good accuracy. The results were obtained without any adjustment or calibration of the model constants and this makes it very attractive method for application to complex combustion problems.

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Figure 1: Snapshots of the temperature fields for Flame D (a), E(b) and F(c). The black lines indicate iso-contours of the stoichiometric mixture fraction.

Figure 2: Instantaneous scatter plots of temperature versus mixture fraction for Flame D.

Figure 3: Instantaneous scatter plots of temperature versus mixture fraction for Flame E.

Figure 4: Instantaneous scatter plots of temperature versus mixture fraction for Flame F.

Figure 5: Radial profiles of mean and *rms* axial velocity at three axial locations for Flames D(a), E(b) and F(c).

Figure 6: Radial profiles of temperature and mixture fraction at three axial locations.

Figure 7: Radial profiles of mean and *rms* CO mass fraction.

Figure 8: Radial profiles of mean and *rms* CO₂ mass fraction at three axial locations.

Figure 9: Radial profiles of mean and *rms* O_2 mass fraction at three axial locations.

Figure 10: Radial profiles of mean and *rms* H_2O mass fraction at three axial locations.

(a) Flame D

(b) Flame E

(c) Flame F

Figure 11: Radial profiles of mean and *rms* CH_4 mass fraction at three axial locations.

Figure 12: Radial profiles of mean and *rms* H_2 mass fraction at three axial locations.

Figure 13: Conditional means of temperature, CH_4 , H_2O , CO_2 , CO and H_2 for Flame F.

Figure 14: Time history at a fixed point for temperature. The unlabeled lines represent the individual stochastic fields. The filtered cell value along with the *rms* sub-grid temperatures is further plotted. The horizontal lines represent the simulated and measured time-averaged temperatures.

Figure 15: Mixture fraction computed from the stochastic fields and transported for three time instances at three axial positions

Figure 16: Sub-grid temperature for three time instances at three axial positions

Figure 17: Mean temperature (a) and conditional mean temperature(b) for Flame F for two different values of *sgs mixing* constant.

Figure 18: Mean temperature (a) and conditional mean temperature(b) for Flame F for two different pilot inlet temperatures.