A THICKENED STOCHASTIC FIELDS APPROACH FOR TURBULENT COMBUSTION SIMULATION

M. A. Picciani*, E.S. Richardson* and S. Navarro-Martinez**
m.a.picciani@soton.ac.uk
*Faculty of Engineering and the Environment, University of Southampton, Southampton, SO17 1BJ, United Kingdom
**Department of Mechanical Engineering, Imperial College, London, SW7 2AZ, United Kingdom

Abstract

The Stochastic Fields approach is an effective way to implement transported Probability Density Function modelling into Large Eddy Simulation of turbulent combustion. In premixed turbulent combustion however, thin flame-like structures arise in the solution of the Stochastic Fields equations that require grid spacing much finer than the filter scale used for the Large Eddys Simulation. The conventional approach of using grid spacing equal to the filter scale yields substantial numerical error, whereas using grid spacing much finer than the filter length scale is computationally-unaffordable for most industrially-relevant combustion systems. A Partially-Thickened Stochastic Fields approach is developed in this study in order to provide physically accurate and numerically-converged solutions of the Stochastic Fields equations with reduced compute time. The Partially-Thickened Stochastic Fields formulation bridges between the conventional Stochastic Fields and conventional Thickened-Flame approaches depending on the numerical grid spacing utilised, and converges towards Direct Numerical Simulation in the limit of full-resolution. One-dimensional Stochastic Fields simulations of freely-propagating turbulent premixed flames are used in order to obtain criteria for the thickening factor required, as a function of relevant physical and numerical parameters, and to obtain a model for an efficiency function that accounts for the loss of resolved flame surface area caused by applying the thickening transformation to the Stochastic Fields equations. The Thickened Stochastic Fields formulation is tested by performing LES of a laboratory Bunsen flame, demonstrating that the method leads to numerically-converged simulations that agree with results of conventional Stochastic Fields simulations using orders of magnitude more grid points. The present development therefore facilitates the accurate application of the Stochastic Fields approach to industrially-relevant combustion systems.

Introduction

Transported Probability Density Function (PDF) modelling of turbulent combustion is advantageous because the composition PDF provides information needed to evaluate the filtered reaction rates required for Large Eddy Simulation (LES), or the mean reaction rates required for Reynolds-averaged simulations. In particular, the PDF approach is valuable for prediction of combustion processes that are sensitive to turbulence-chemistry interactions, including extinction and ignition, and the formation of various pollutants. The Stochastic Fields approach of Valiño *et al.* [1] has been applied in a number of recent PDF-LES studies because, in contrast with Lagrangian particle PDF formulations, the Stochastic Fields approach guarantees density fields that are continuous in space without the need for special treatment, and it can be solved using the same Eulerian numerical implementation as the LES momentum equations. Stochastic Fields PDF-LES successfully models both non-premixed [2] and premixed combustion [3]. However, in Stochastic Fields simulation of premixed combustion, flame-like structures arise that may be thinner than the LES filter lengthscale [4]. In order to solve the Stochastic Fields equations accurately it is then necessary to have grid spacing finer than the filter lengthscale, substantially adding to the computational time required for the Stochastic Fields simulation. Conversely, following the conventional practice of setting the LES filter lengthscale equal to the numerical grid spacing can lead to substantial numerical error for two reasons [4]. First, numerical diffusion caused by under-resolution changes the local propagation speed of the reaction fronts in the Stochastic Fields solution. Second, wrinkling of the reaction fronts by resolved turbulence is reduced because the numerical diffusion increases the thickness of the fronts.

The Thickened Flame approach [5, 6] has been introduced as a means to ensure accurate numerical resolution of premixed reaction fronts in LES. In the Thickened Flame approach, the governing equations for composition and energy are modified in order to yield thicker reaction fronts that can be resolved accurately on a given numerical grid, and an *efficiency function* model is employed to compensate for the reduction of flame wrinkling that results from the artificial thickening. Importantly, the Thickened Flame approach removes uncharacterised numerical errors that depend both on the numerical grid and numerical methods employed. Instead, the quality of the predictions depends on the accuracy of the efficiency function modelling employed. The efficiency function model should account for effects of un-resolved flame wrinkling on the overall burning rate, but it lacks the more general ability of PDF approaches to describe turbulence-chemistry interactions. The objective of this paper is to set out a new approach for Stochastic Fields-PDF simulation that uses artificial thickening to ensure accurate numerical solution on any given numerical grid. The Thickened Stochastic Fields approach retains at least some of the ability of PDF methods to describe turublence-chemistry interactions and recovers the standard Stochastic Fields formulation when the numerical resolution is sufficient.

Development of the Thickened Stochastic Fields Approach

The Thickened Stochastic Fields approach is best introduced by first reviewing the formulation of the Thickened Flame approach. We consider a scalar transport equation describing reactive flow:

$$\rho\frac{\partial \underline{Y}}{\partial t} = -\rho u_j \frac{\partial \underline{Y}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\rho D \frac{\partial \underline{Y}}{\partial x_j}\right) + \underline{\dot{\omega}}(\underline{Y}), \tag{1}$$

where $\underline{Y}$ is the vector of species mass fractions and enthalpy, u_j is the jth component of the velocity vector, D is the laminar diffusivity (assumed equal for all species), and $\underline{\dot{\omega}}$ is the vector of chemical source terms.

The Thickened Flame Model:

The Thickened Flame equation [5] is obtained by applying the transformation $\mathbf{x}' = F\mathbf{x}$ and $t' = Ft/E$ [5] to Eq. 1,

$$\rho\frac{\partial \underline{Y}}{\partial t'} = -\rho E v_j \frac{\partial \underline{Y}}{\partial x'_j} + \frac{\partial}{\partial x'_j}\left(\rho D E F \frac{\partial \underline{Y}}{\partial x'_j}\right) + \frac{E}{F}\underline{\dot{\omega}}(\underline{Y}). \tag{2}$$

where the convection velocity $\mathbf{v}$ is given by the solution of the similarly-transformed Navier-Stokes equations [7]. In most previous applications of the Thickened Flame approach, following Refs. [5, 6], the thickened scalar transport equation Eq. 2 has been coupled with unthickened LES making the assumption that $E\mathbf{v}$ is equal to the resolved velocity from the LES simulation $\tilde{\mathbf{u}}$. The effect of thickening factor F and efficiency function E can be understood by considering the solution of a steady-state freely-propagating planar premixed flame ($\partial/\partial t' = \partial/\partial t = 0$). The flame thickness given by Eq. 2 is thickened by the factor F and the propagation speed given by $\rho\tilde{u}/\rho_0$, where ρ_0 is the density in the unburned gas, is faster by a factor E compared to flame thickness δ_l and speed S_L given by solution of Eq. 1.

Thickening the species transport equations by factor F with $E = 1$ has the attractive feature that numerical resolution requirements are reduced while laminar flame speeds are unaffected. Turbulent flame speed however depends on the increase in flame surface area caused by wrinkling of the flame front, with the amount of wrinkling depending (at least) on the ratio of turbulent velocity fluctuations to the laminar flame speed u'/S_L and the ratio of the turbulence length scales to the laminar flame thickness, L_T/δ_l. Thickening the flame front to $F\delta_l$ reduces the degree to which the turbulence will wrinkle the flame. The efficiency function E can then be used as a correction factor that increases the local propagation speed in order to compensate for the loss of resolved flame surface area resulting from application of the thickening transformation.

The local propagation speed of the reaction-front resolved by the LES simulation is described as the sub-filter turbulent flame speed $S_{T\Delta}$ [6]. The ratio of the sub-filter turbulent flame speed $S_{T\Delta}$ and the laminar flame speed S_L is assumed to be equal to wrinkling factor Ξ, (equal to the projection of the sub-filter scale flame area in the direction of propagation),

$$\frac{S_{T\Delta}}{S_L} = \frac{A_{sfs}}{\Delta^2} = \Xi_\Delta. \tag{3}$$

Modelling for the sub-filter flame wrinkling in the context of Thickened Flame modelling has been proposed initially by Colin *et al.* [5] and Charlette *et al.* [6] as functions of the non-dimensional sub-filter velocity fluctuations u'/S_L and the non-dimensional filter size Δ_{TF}/δ_l, where $\Delta_{TF} = F\delta_l$ is the effective filter scale in the Thickened Flame model. In general, the effective filter scale Δ_{TF} implied by the Thickened Flame model can be different from the filter length scale Δ used in modelling of the LES momentum or Stochastic Fields equations. Thickening the flame front by factor F reduces the non-dimensional filter size to $\Delta/F\delta_l$, resulting in a reduction in the sub-filter turbulent flame speed by factor $1/E$ as illustrated in Fig. 1. The efficiency function E is defined in Ref. [6] as the ratio of the wrinkling factor in the thickened and unthickened flames,

$$E_{TF} = \frac{\Xi_\Delta\left(u'_{\Delta,TF}/S_L, \Delta_{TF}/\delta_l\right)}{\Xi_\Delta\left(u'_{\Delta,TF}/S_L, \Delta_{TF}/F\delta_l\right)}. \tag{4}$$

The Thickened Stochastic Fields Model:

The unmodified Stochastic Fields equation is given by Valiño *et al.* [8] as,

$$\begin{aligned}\overline{\rho}\mathrm{d}\underline{\zeta}_{(i)} = &-\overline{\rho}\widetilde{u}_j \cdot \frac{\partial \underline{\zeta}_{(i)}}{\partial x_j}\mathrm{d}t + \frac{\partial}{\partial x_j}\left(\overline{\rho}(D + D_T)\frac{\partial \underline{\zeta}_{(i)}}{\partial x_j}\right)\mathrm{d}t + \overline{\rho}\sqrt{2D_T}\frac{\partial \underline{\zeta}_{(i)}}{\partial x_j}dW_{j(i)} \\ &- \frac{\overline{\rho}}{\tau_T}\left(\underline{\zeta}_{(i)} - \widetilde{\underline{\zeta}}\right)\mathrm{d}t + \overline{\rho}\underline{\dot{\omega}}(\underline{\zeta}_{(i)})\mathrm{d}t.\end{aligned} \tag{5}$$

where $\underline{\zeta}_{(i)}(\mathbf{x}, t)$ is the value of the composition vector on the i^{th} field. The terms on the right hand side represent the evolution of the stochastic field composition due to advection by the mean (or resolved) velocity; spatial diffusion by molecular D and turbulent D_T diffusivities;

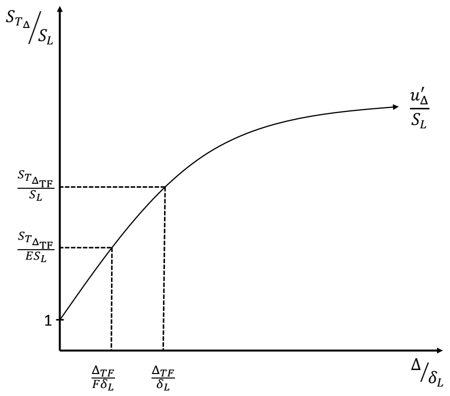

Figure 1: The dependence of wrinkling factor Ξ_Δ on Δ/δ_l and u'_Δ/S_L, indicating the reduction in Ξ_Δ due to thickening by factor F.

unresolved scalar dissipation processes modelled by interaction by exchange with the mean (IEM) [9] with dissipation time scale $\tau_T^{-1} = C_{\phi\Delta}(D + D_T)/\Delta^2$; turbulent advection of fields relative to one another as modelled by a Weiner process where $\mathrm{d}W_{j\,(i)}$ is the component in the j^{th} direction of a normally-distributed Markovian random increment with zero mean and variance equal to the time step dt; and the vector of chemical reaction source terms $\underline{\dot{\omega}}(\underline{\zeta}_{(i)})$.

The Thickened Stochastic Fields equation is obtained by applying to Eq. 5 the same transformation that produces the Thickened Flame model: $\mathbf{x}' = F\mathbf{x}$, $t' = Ft/E$, and, since the Weiner increment vector $\mathbf{dW}$ has dimension $\sqrt{t}$, $\mathbf{dW}' = \sqrt{F/E}\mathbf{dW}$:

$$\begin{aligned}\overline{\rho}\mathrm{d}\underline{\zeta}_{(i)} = &-\overline{\rho}E\widetilde{v}_j\cdot\frac{\partial\underline{\zeta}_{(i)}}{\partial x'_j}\mathrm{d}t' + \frac{\partial}{\partial x'_j}\left(\overline{\rho}(D + D'_T)EF\frac{\partial}{\partial x'_j}\underline{\zeta}_{(i)}\right)\mathrm{d}t' + \overline{\rho}\sqrt{2D'_T EF}\frac{\partial\underline{\zeta}_{(i)}}{\partial x'_j}dW'_{j\,(i)}\\ &-\frac{\overline{\rho}E\left(\underline{\zeta}_{(i)} - \widetilde{\underline{\zeta}}\right)}{F\tau'_T}\mathrm{d}t' + \frac{\overline{\rho}E\underline{\dot{\omega}}(\underline{\zeta}_{(i)})}{F}\mathrm{d}t'. \qquad (6)\end{aligned}$$

In principle the convection velocity $\tilde{\mathbf{v}}$, turbulent diffusivity D'_T and dissipation timescale τ'_T come from solution of similarly-transformed LES momentum equations. However if, following Colin *et al.* [5], the thickened scalar equations are coupled with unthickened LES momentum equations then the velocity $\tilde{\mathbf{u}}$ and turbulent diffusivity D_T from the unthickened LES should be scaled as $\tilde{\mathbf{v}} = \tilde{\mathbf{u}}/E$ and $D'_T = FD_T/E$, where the scaling factors are obtained by dimensional analysis.

The transformation of the Stochastic Fields equation has the effect that the solution for a steady-state planar freely-propagating turbulent flame modelled by Eq. 6 is thickened by factor F and the propagation speed is increased by factor E relative to the solution of Eq. 5. The thickening factor F can therefore be set in order to obtain satisfactory numerical resolution on a particular computational grid. The efficiency function E should then be set in order to account for the reduction in resolved flame surface area that results from thickening of the Stochastic Fields equation.

The Efficiency Function

The specification of the efficiency function for the Thickened Stochastic Fields model relates to the wrinkling of the reaction-fronts in the Stochastic Fields solution, rather than the wrinkling of physical flames considered in the conventional Thickened Flame model. The characteristic thickness δ_{c^*} and propagation speed S_{c^*} of the reaction fronts in the Stochastic Fields solution are in general different from the thickness and speed of the corresponding laminar flame, however the wrinkling dynamics of the reaction-fronts are assumed to be governed by the same function, Ξ_Δ. This assumption is justified because the wrinkling dynamics of reaction fronts in the flamelet regime are dominated by the combination of resolved convection, sub-filter turbulent transport, diffusion and reaction processes in the flamelet regime in both Thickened Flame and Thickened Stochastic Fields simulations. The efficiency function for the Thickened Stochastic Fields model (Eq. 6) is then given by,

$$E_{TSF} = \frac{\Xi_\Delta\left(u'_{\Delta,TSF}/S_{c^*}, \Delta_{TSF}/\delta_{c^*}\right)}{\Xi_\Delta\left(u'_{\Delta,TSF}/S_{c^*}, \Delta_{TSF}/F\delta_{c^*}\right)}, \tag{7}$$

where the effective filter scale of the thickened stochastic fields $\Delta_{TSF} = F\delta_{c^*}$. In general Δ_{TSF} can be different from the filter scale Δ used to evaluate the model for the turbulent diffusivity in Eq. 6.

Previous studies have developed models for the function Ξ_Δ on the basis of theory and empirical information from direct numerical simulations and laboratory measurements of flame response [5, 6]. The purpose of the TSF approach however is to provide simulation results that maintain the same flame propagation speeds as the underlying Stochastic Fields modelling when the computational grid spacing is increased. The modelling for Ξ_Δ should not seek to improve the agreement between the Stochastic Fields model and DNS or experiment, rather it should fit to predictions of the underlying unthickened Stochastic Fields model. Improving the physical accuracy of the underlying Stochastic Fields modelling is outside the scope of the present study. The functional dependence of the wrinkling factor on the filter-scale turbulence properties $\Xi_\Delta(u'_\Delta/S_L, \Delta/\delta_l)$ is therefore obtained from Stochastic Fields simulations across a range of conditions. The set up of inexpensive one-dimensional Stochastic Fields simulations in order to obtain data for δ_{c^*}/δ_l and S_{c^*}/S_L is presented in the next Section.

Determination of Wrinkling Factor from 1D Stochastic Fields simultions

The dependence of the sub-filter scale turbulent flame speed and reaction-front thickness on filter-scale turbulence properties is evaluated in a one-dimensional Stochastic Fields simulation of a freely-propagating planar turbulent flame. The one-dimensional approach neglects the effects that curvature and bulk strain have on the local propagation of reaction-fronts in Stochastic Fields LES of premixed combustion, but has the advantage that the simulations are computationally inexpensive compared to three-dimensional LES and still represent the transport processes normal to the resolved reaction front that dominate the dynamics of the resolved reaction front.

The filter-scale turbulence properties are specified by the filter lengthscale Δ and the corresponding sub-filter scale velocity fluctuation u'_Δ. The turbulent diffusivity required in Eq. 5 is modelled as $D_T = C_{\mu\Delta} u'_\Delta \Delta$, with $C_{\mu\Delta} = 0.09$. The turbulent mixing frequency is modelled by $\tau_T^{-1} = C_{\phi\Delta}(D + D_T)/\Delta^2$, with model coefficient $C_{\phi\Delta}$ scaled with $1/Re_\Delta = S_l\delta_{th}/(u'_\Delta\Delta)$ [10].

The consumption speed of the reaction front on the individual stochastic fields is evaluated by integrating the fuel consumption rate through the flame and, due to the stochastic nature of the consumption speed given by Eq. 5, averaging over time. In this statistically-stationary case, the overall consumption speed of the ensemble average of the stochastic fields is neces-

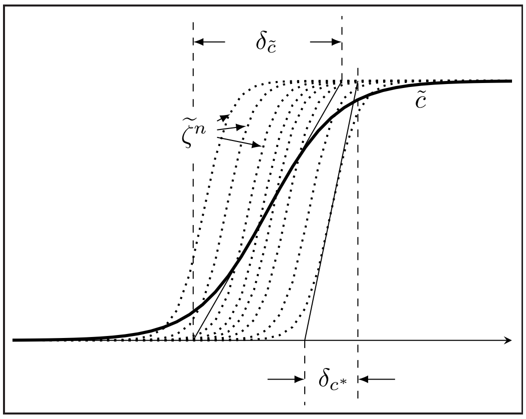

Figure 2: A schematic diagram showing the thickness (δ_{c^*}) of the individual stochastic fields progress variable profiles (dashed lines) and the thickness ($\delta_{\tilde{c}}$) of the resolved flame progress variable profile (solid line).

sarily equal to the averaged consumption speed of the individual stochastic fields ($S_{c^*} = S_{T\Delta}$). The thicknesses of individual stochastic fields are evaluated as $\delta_{c^*} = 1/|\nabla\zeta_{c(i)}|_{\max}$, as illustrated in Fig. 2, and time-averaged.

S_{c^*}/S_L and δ_{c^*}/δ_l are evaluated by one-dimensional Stochastic Fields simulations for a range of range of u'_Δ/S_L and Δ/δ_l. The numerical methods and thermo-chemical models employed are described in the subsequent section. 512 Stochastic Fields are used for the one-dimensional simulations, with uniform computational grid spacing selected to ensure at least 20 points within the reactiom fronts in each case. The data are modelled by power-law functions of u'_Δ/S_L and Δ/δ_l in the general form employed by Charlette *et al.* [6],

$$f_i(u'_\Delta/S_L, \Delta/\delta_l) = \left(1 + A_i \left(\frac{u'_\Delta}{\Delta}\right)^{a_i} \left(\frac{\Delta}{\delta_L}\right)^{b_i}\right)^{\beta_i}. \tag{8}$$

The range of u'_Δ/S_L and Δ/δ_l used to fit the coefficients in Eqs. 8 corresponds to the ranges of Karlovitz number Ka $\in (0.5 - 50)$ and filter lengthscale ratios $\Delta/\delta_l \in (1 - 50)$ that are representative of practical LES simulations of premixed combustion in internal combustion engines and gas turbines. A least squares fit to the data yields $[A, a, b, \beta] = [1.117, 0.7498, 1.424, 0.4766]$ for S_{c^*}/S_L and $[A, a, b, \beta] = [0.5339, 0.4083, 0.8394, 0.8264]$ for δ_{c^*}/δ_l. The curve-fits give excellent agreement across the relevant parameter space, as shown in Fig. 3.

Last, with the addition of a model for the dependence of the sub-filter scale turbulence velocity fluctuation u'_Δ on the filter length scale, and with knowledge of the laminar flame speed and thickness, the Thickened Stochastic Fields Efficiency Function E_{TSF} can be evaluated through the following steps:

1. Evaluate u'_Δ for the Stochastic Fields filter scale Δ;
2. Evaluate δ_{c^*}/δ_l and S_{c^*}/S_L corresponding to u'_Δ/S_L and Δ/δ_l using Eq. 8;
3. Evaluate $F = n\Delta_x/\delta_{c^*}$ and $\Delta_{TSF} = n\Delta_x$, where n is the minimum number (e.g. 7) of grid spacings Δ_x required within the reaction-front thickness δ_{c^*};
4. Calculate $u'_{\Delta,TSF}$ for the effective Thickened Stochastic Fields filter scale Δ_{TSF};

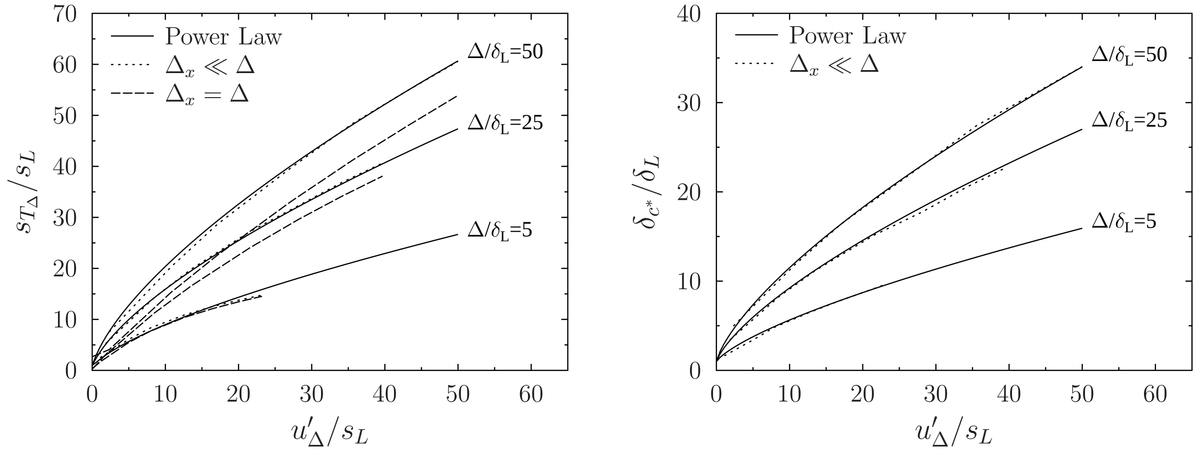

Figure 3: Wrinkling factor S_{T_Δ}/S_L (left) and non-dimensional reaction front thickness δ_{c^*}/δ_l (right) versus sub-filter turbulence intensity u'_Δ/S_L for well-resolved Stochastic Fields ($\Delta_x \ll \Delta$), Stochastic Fields simulation with $\Delta_x = \Delta$, and the curve fit to the well resolved data given by Eq. 8.

5. Evaluate Eq. 7 for E_{TSF} using the power law curve fit Eq. 8 for the wrinkling factors.

Turbulent premixed Bunsen flame LES

The F3 turbulent premixed Bunsen flame described by Chen *et al.* [11] is simulated using Stochastic Fields-LES, Thickened Stochastic Fields-LES and the Artificially-Thickened Flame LES approach of Charlette *et al.* [6]. The flame is characterised by Karlovitz numbers of order unity, indicating that combustion takes place across the flamelet and thin reaction zone regimes, and therefore is challenging for PDF methods. The flame has simple boundary conditions and has served as the basis for numerous investigations of pdf modelling for turbulent premixed combustion [12–15, 3].

A 12 mm diameter nozzle delivers a turbulent jet of stoichiometric methane-air with bulk velocity 30 ms^{-1}. The flame is stabilised by a ring of stoichiometric methane-air pilot flames surrounding the nozzle with 68 mm outer diameter and bulk velocity 1.32 ms^{-1}. Further downstream the flame entrains air from a quiescent laboratory environment. Profiles of mean and rms velocity fluctuations are reported in [11]. Due to heat exchange between the pilot flames, the jet of reactants, the burner and the environment, the pilot flame temperature has been estimated in previous LES studies [3] as 1785 K, the reactant jet temperature as 300 K, and the temperature and pressure of the surrounding air as 300 K and 1 atm.

The spatially-filtered continuity and momentum equations [3] are closed with the constant-coefficient Smagorinsky model for the sub-filter scale turbulent stresses [16], with Smagorinsky constant equal to 0.09. The turbulent diffusivity required in Eq. 5 is modelled assuming turbulent Schmidt number equal to 0.7 and the dissipation timescale is modelled by $\tau_T^{-1} = C_{\phi\Delta}(D + D_T)/\Delta^2$, with model coefficient C_ϕ once again scaled as proposed in [10].

The Thickened Stochastic Fields approach is implemented as described in the previous section, with the sub-filter scale root mean square velocity modelled by,

$$u'_\Delta = c_2 \Delta^3 |\nabla \times (\nabla^2(\tilde{\mathbf{u}}))|. \tag{9}$$

where $\tilde{\mathbf{u}}$ is the resolved velocity corresponding to filter scale Δ and $c_2 = 2.0$ is a model constant [5].

Thermo-chemical models: The premixed combustion kinetics are modelled using a one-step reaction model for methane-air flames,

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O. \tag{10}$$

The fuel reaction rate is modelled by the Arrhenius law,

$$\dot{\omega}_{CH_4} = A \cdot \left(\frac{\rho Y_{CH_4}}{M_{CH_4}}\right)^{n_{CH_4}} \left(\frac{\rho Y_{O_2}}{M_{O_2}}\right)^{n_{O_2}} \exp\left(-\frac{E_a}{RT}\right), \tag{11}$$

where T, Y_{CH_4}, Y_{O_2}, M_{CH_4}, M_{O_2} and R denote temperature, fuel and oxygen mass fractions, corresponding molar weights and the universal gas constant, respectively. The pre-exponential factor, the activation energy and the model exponents are $A = 1.1 \times 10^{10}$ (cgs), $E_a = 20,000$ cal/mol, $n_{CH_4} = 1.0$ and $n_{O_2} = 0.5$. The use of such simple chemical modelling is justified by the focus of the present study on evaluation of the numerical resolution requirements of the Stochastic Fields approach, rather than assessing the physical accuracy of the Stochastic Fields approach per se.

Temperature dependent properties are modelled with NASA polynomials and, due to the use of equal diffusivities in the Stochastic Fields formulation, the Schmidt and Prandtl numbers are both set equal to 0.7, while the mixture kinematic viscosity is modelled with Wilkes law. These values lead to a laminar flame speed $S_L = 0.38$ ms^{-1}, a thermal thickness of 0.646 mm and a burnt gas adiabatic temperature $T_b = 2328$ K in atmospheric stoichiometric conditions.

Numerical implementation: The Stochastic Fields equation is implemented within the block-structured BOFFIN computational fluid dynamics code [17, 3]. The code is a second order accurate finite volume method based on fully implicit low-Mach-number formulation using a staggered storage arrangement. The Weiner process is approximated by time-step increments $dt^{1/2}\eta_i^n$ where η_i^n is a $\{-1, 1\}$ dichotomic random vector [18]. The chemical source terms are solved using a Newton method-based stiff solver.

The turbulent Bunsen flame is simulated on a computational grids characterised by 1.0 mm grid spacing at the inlet. The grids are Cartesian, with a uniform region of grid around the inlet with transverse extent equal to twice the nozzle diameter. The axial grid spacing increases linearly in the axial direction. Sixteen stochastic fields are used in the three-dimensional simulations. The computational timestep for the simulation was $4.6\mu s$. The turbulent inflow is modelled with the digital filter based method of Klein *et al.* using the mean and rms velocity profiles from [11]. The number of grid points within the reaction front thickness as 7 for the Thickened Stochastic Fields.

Flame Sensor: Artificial thickening of the scalar equations is typically necessary only in regions of the flow containing thin reaction fronts. Thickening in regions where it is not required leads to an unnecessary loss of simulation fidelity, for example by over-predicting the rate of fuel-air premixing in partially-premixed combustion systems. To overcome this, Durand *et al.* [19] introduced dynamic thickening by a flame sensor Ω to remove the effects of thickening away from reaction fronts. The original flame sensor given by Durand *et al.* [19] is adapted with a tanh function in order to give more uniform thickening through the flame [20]:

$$\Omega = \tanh\left(16\beta\left(c\left(1-c\right)\right)^2\right), \tag{12}$$

where c is a relevant progress variable and factor β adjusts how quickly the sensor approaches unity for $c > 0$. Taking β equal to 5 ensures uniform thickening of the reaction zone in the present simulations. The flame sensor $\Omega > 0$ indicates the presence of a flame front and $\Omega = 0$ its absence. The thickening factor is then rewritten as

$$F = 1 + (F_0 - 1)\Omega, \tag{13}$$

where F_0 is the thickening factor determined as a function of the grid spacing and the desired number of grid points within the reaction front.

The flame sensor can also be applied in the Thickened Stochastic Fields approach however use of the filtered progress variable in Eq. 12 may under-thicken the stochastic fields that are at the front or rear of the flame brush, where the filtered progress variable is close to zero or unity. Instead, acceptable results can be obtained by evaluating the flame sensor for every stochastic field and, since all fields must have the same thickening factor, taking the maximum value of $\Omega_{(i)}$ across all fields.

Results and Discussion

In the present LES with Karlovitz number in the range 1-10 [11] and 1 mm filter scale, the power law model for the thickness of the Stochastic Fields reaction fronts (Eq. 8) indicates that the Stochastic Fields reaction front thicknesses are between 2-4 times the laminar flame thickness ($\delta_L = 0.65$ mm). The requirement of 7 grid points within the reaction front implies that a fully-resolved Stochastic Fields simulation would require a grid spacing around 0.25 mm, which is one quarter of the filter scale in this case. A grid spacing of 0.25 mm implies 4^3 times more grid points than when following the convention of using a grid spacing equal to the filter scale. The disparity between the filter scale and the grid spacing required for full-resolution stochastic fields simulation is even greater in LES of industrial burners (for example with $\Delta/\delta_L \approx 50$ and millions of filter volumes in the simuation domain), to the extent that fully-resolved Stochastic Fields simulations of many practical combustion systems is not feasible computationally (since the number of control volumes would need to be orders of magnitude greater than the number of filter volumes). In order to obtain correct grid-independent results it is necessary either to reduce the number of filter volumes in the simulation domain, or to follow a different approach, such as the Thickened Stochastic Fields methodology developed here.

It is desirable that the thickening factor for the Thickened Stochastic Fields approach should be substantially-less than the thickening factor for the conventional Thickened Flame approach. When the flame is thickened its interactions with the turbulent flow are modified, and the Damköhler number (Da= $L_T s_L/u'\delta_L$) and Karlovitz number (Ka= $(u'^3\delta_L/S_L^3 L_t)^{1/2}$) change by E/F and $(F/E^3)^{1/2}$ respectively. In the present LES the Stochastic Fields reaction front thicknesses are predicted to be 2-4 times the laminar flame thickness – implying that the thickening factor for the Thickened Stochastic Fields should be between 2-4 times lower than in the equivalent Thickened Flame simulation. The thickening factor used in the Thickened Stochastic Fields calculation is generally around 3, compared with a thickening factor of 12 required for a conventional Thickened Flame simulation. Figure 3 shows that the difference in thickening factors grows as the ratio Δ/δ_L and Karlovitz number increase. Consequently the thickening factor for Thickened Stochastic Fields in a LES of an industrial gas turbine burner with Karlovitz number equal to 10 and $\Delta/\delta_L \approx 50$ would a factor of around 20 smaller than in the corresponding Thickened Flame calculation. (in these estimates the sub-filter turbulence intensity u'_Δ has been related to the Karlovitz number by an inertial range scaling of u' [6]). The large difference in thickening factor shows that the Damköhler and Karlovitz numbers are much less affected by thickening than in the conventional Thickened Flame approach.

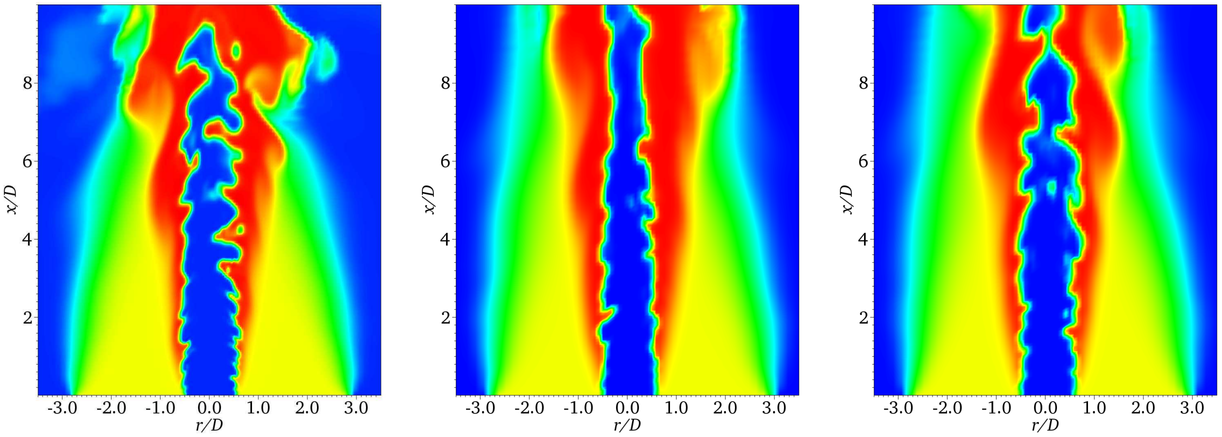

Figure 4: Instantaneous temperature contours of an individual stochastic field from the Bunsen flame LES: Stochastic Fields with $\Delta_x = 0.5$ mm $\Delta = 1.0$ mm; Stochastic Fields with $\Delta_x = \Delta = 1.0$ mm; Thickened Stochastic Fields with $\Delta_x = \Delta = 1.0$ mm.

Contour maps of instantaneous temperature stochastic fields are shown for three simulations of the premixed Bunsen flame with filter length scale of 1 mm. The first simulation solves the Stochastic Fields equation with $\Delta_x = 0.5$ mm, the second solves the Stochastic Fields equation with $\Delta_x = 1.0$ mm, and the third is a Thickened Stochastic Fields simulation with $\Delta_x = 1.0$ mm. Since the grid spacing required for well-resolved Stochastic Fields simulation has been estimated as 0.25 mm in this case, both of the first two simulations are expected to be affected by numerical diffusion. Comparison of the instantaneous temperature fields shows that the average thickness of the stochastic fields is less (equal to 4.6 mm averaged over the flame surface) in the simulation with $\Delta_x = 0.5$ mm, compared with the other two cases (7.5 mm for Stochastic Fields with $\Delta_x = 1.0$ mm and 8.6 mm for the Thickened Stochastic Fields). The Thickened Stochastic Fields equation yields flame thicknesses close to the intended 7 grid spacings, indicating that the Thickened Stochastic Fields simulation is numerically accurate. In contrast, the results of the Stochastic Fields simulation are highly-sensitive to the grid spacing.

The radial profiles of the predicted mean methane mass fraction and axial velocity are shown for the three simulations in Fig. 5. The differences in the modelling and numerical solution do not strongly affect the velocity field, however the solution of the reactive scalars is more sensitive. The use of the Thickened Stochastic Fields approach has the effect of moving the predictions towards those given by Stochastic Fields simulations with greater resolution.

Conclusions

A Thickened Stochastic Fields approach is proposed that seeks to ensure adequate numerical resolution of the Stochastic Fields equation in premixed turbulent combustion. The approach correctly reduces to either conventional Stochastic Fields, Thickened Flame models, or Direct Numerical Simulation depending on the numerical resolution provided and the filter scale selected. The key features of the new approach are that the numerical resolution can be adjusted in order to manage computational cost without affecting the overall turbulent flame speed; and the numerical implementation is a trivial modification of the conventional Stochastic Fields implementation.

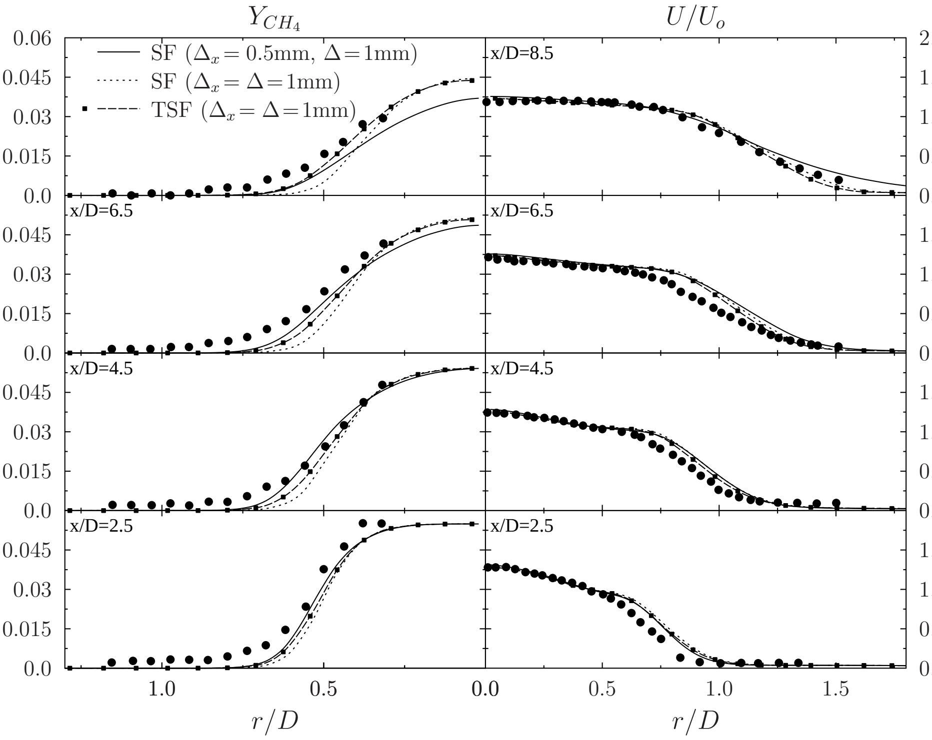

Figure 5: Radial distributions of the time-averaged methane mass fraction $\langle\widetilde{Y_{CH_4}}\rangle$ and the normalised mean axial velocity at various axial locations for the three simulations from Fig. 4.

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