RESOLUTION REQUIREMENTS IN STOCHASTIC FIELD SIMULATION OF TURBULENT PREMIXED FLAMES

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Abstract
The spatial resolution requirements of the Stochastic Fields probability density function approach are investigated in the context of turbulent premixed combustion simulation. The Stochastic Fields approach is an attractive way to implement transported Probability Density Function modelling into Large Eddy Simulations of turbulent combustion. In premixed combustion LES, the numerical grid should resolve flame-like structures that arise from solution of the Stochastic Fields equation. Through analysis of Stochastic Fields simulations of a freely-propagating planar turbulent premixed flame, it is shown that the flame-like structures in the Stochastic Fields simulations can be orders of magnitude narrower than the LES filter length scale, implying that the usual practice of setting the LES filter length scale equal to grid spacing leads to severe under-resolution, to numerical thickening of the flame, and to substantial error in the turbulent flame speed. The under-resolution is worst for low Karlovitz number combustion, where the thickness of the Stochastic Fields flame structures is similar to the laminar flame thickness. The effect of resolution on LES predictions is then assessed by performing LES of a laboratory Bunsen flame and comparing the effect of refining the grid spacing and filter length scale independently. The Bunsen flame LES results confirm that setting the LES filter length scale equal to the grid spacing gives substantial numerical error, and that this error affects the Stochastic Fields solution to a greater extent than it affects the flow field solution. The present results have important implications for application of the Stochastic Fields approach to simulation of high-pressure industrial premixed combustion systems where the grid spacing is necessarily much larger than the laminar flame thickness and suggests that some amount of artificial flame thickening might be needed in order to make such simulations numerically accurate.

Introduction
Modelling of chemical reaction terms in turbulent combustion simulations is complicated by the non-linear dependence of reaction rates on fluctuations in composition and temperature. The Probability Density Function (PDF) modelling approach is attractive because, once the joint-scalar PDF for composition and temperature is known, the chemical reaction terms needed for Reynolds-Averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) appear in closed form. In principle, the joint-scalar transported PDF approach is applicable in Reynolds-Averaged Navier Stokes (RANS) and Large-Eddy Simulations (LES) across all modes of turbulent combustion – including the limiting cases of non-premixed and perfectly-premixed combustion – provided that turbulent transport and micro-mixing effects are modelled adequately and that the PDF equation is solved accurately. The present study investigates the use of the Stochastic Fields approach [1] for modelling the joint-scalar PDF evolution, and considers the requirements for obtaining numerically accurate solutions in the

challenging case of turbulent premixed combustion.

The Stochastic Fields formulation has been developed rigorously through independent contributions by Valino [1, 2] and Sabel'nikov [3]. The one-point probability density function of composition throughout a spatial solution domain is modelled by an ensemble of composition fields that span the spatial domain. Each of the composition fields evolves according to a stochastic differential equation given in modelled form by Valiño [2] as,

$$\overline{\rho}\mathrm{d}\underline{\zeta}_{(i)} = -\overline{\rho}\widetilde{\mathbf{u}}\cdot\nabla\underline{\zeta}_{(i)}\mathrm{d}t + \nabla\left(\overline{\rho}(D+D_T)\nabla\underline{\zeta}_{(i)}\right)\mathrm{d}t + \overline{\rho}\sqrt{2D_T}\nabla\underline{\zeta}_{(i)}d\mathbf{W}_{(i)} - \frac{\overline{\rho}}{\tau_T}\left(\underline{\zeta}_{(i)} - \widetilde{\underline{\zeta}}\right)\mathrm{d}t + \overline{\rho}\underline{\dot{\omega}}(\underline{\zeta}_{(i)})\mathrm{d}t. \tag{1}$$

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; unresolved scalar dissipation processes modelled by interaction by exchange with the mean (IEM) [4] with dissipation time scale τ_T; turbulent advection of fields relative to one another as modelled by a Weiner process where dW is 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 $\underline{\dot{\omega}}(\underline{\zeta}_{(i)})$.

Following successful validation of the Stochastic Fields approach in a range of non-premixed combustion scenarios including Refs. [5–7], a smaller number of Stochastic Fields simulations of premixed combustion have been reported [8–10]. The degree of predictive accuracy shown in the case of premixed combustion is encouraging because the sub-models employed, such as the interaction by exchange with the mean (IEM) micro-mixing model [4], are essentially unchanged from those employed in previous non-premixed modelling efforts. Stochastic Fields is an attractive way to implement transported probability density function (PDF) modelling for turbulent reacting flows for two main reasons: It guarantees a density field that is continuous and differentiable in space, and it can exploit similar Eulerian solution methods and domain decomposition schemes implemented for the momentum equations.

Given the possible advantages of the Stochastic Fields equations in terms of the physical description of premixed combustion applications, the objective of this study is to investigate the numerical requirements for spatial resolution of the Stochastic Fields equations in turbulent premixed combustion applications. In the following section, resolution requirements are discussed in the context of premixed combustion, then the resolution requirements are investigated numerically in the subsequent sections, first in a simplified one-dimensional test problem, and then in respect of LES of a piloted stoichiometric Bunsen flame experiment by Chen *et al.* [11].

Numerical resolution of the Stochastic Fields equation in premixed combustion

Spatial resolution requirements of the Stochastic Fields equations in premixed combustion LES have not been discussed in the academic literature on Stochastic Fields. In a turbulent premixed flame, each Stochastic Field contains a reaction front that "resembles" premixed flames. Strictly, the reaction fronts in the Stochastic Fields are not required to correspond to actual flame fronts in a physical flow, and therefore we use the term "reaction front" to avoid confusion. In turbulent premixed combustion the averaged thickness of the reaction-diffusion front in individual Stochastic Fields is necessarily less than the thickness of the ensemble average of all the stochastic fields. The combined effects of an exchange with the mean micro-mixing model and an eddy-diffusivity model for the unresolved turbulent transport thicken the individual Stochastic Fields relative to the average thickness of the instantaneous flame fronts that would be expected in the actual turbulent flame. In LES, the average thickness of the individual Stochastic Field reaction fronts is expected to depend on the effective filter length scale and combustion regime. In general, we expect the thermal thickness of the Stochastic Fields reaction fronts to be between the thermal thickness of an unstrained laminar premixed flame and the thermal thickness of the ensemble-averaged (RANS) or resolved (LES) temperature field.

Karlovitz numbers much greater than unity (i.e. broken reaction zones) have the effect of thickening instantaneous flame fronts [12], and therefore also thicken the Stochastic Field reaction fronts, reducing resolution requirements. Conversely, the most stringent resolution requirements are expected for low Karlovitz number flames that characterise combustion in the flamelet regime. Flamelet-type combustion is prevalent in most important premixed combustion applications including spark-ignition engines and industrial gas turbines. However, it is not evident from a priori analysis of Eq. (1) whether a given grid spacing will be sufficient to resolve the individual Stochastic Fields, and resolution requirements need to be investigated numerically.

The grid spacing required in order to numerically resolve a reaction-diffusion front varies depending on the numerical discretisation employed, the details of the chemistry and transport models employed, and the numerical accuracy desired. For high-accuracy simulation of premixed combustion with a detailed chemistry model, more than twenty points may be required within each reaction-diffusion front. Whereas five points with a reaction diffusion front may be taken as an absolute minimum requirement for less accurate engineering simulations with simple (e.g. single-step) chemistry models [13]. Low-order numerical methods and TVD schemes used for some LES of turbulent reacting flows can remain stable even when the governing equations are under resolved, providing numerical diffusion that spreads the reaction fronts across multiple grid points.

In implicitly-filtered LES, the effective filter length scale used in modelling for the unclosed sub-filter scale terms usually depends on the grid spacing. Previous Stochastic Fields LES studies [5–10] have all set the filter length scale equal to the grid spacing (or the cube root of the cell volume). When the filter length scale depends on the grid spacing, the effects of numerical resolution errors cannot be distinguished from scale-dependence of the sub-grid modelling. Vreman *et al.* [14] investigated the effects of numerical error in non-reacting LES by changing the filter scale independently from the grid spacing. For a fixed filter scale they found significant differences in LES predictions between simulations with the grid spacing equal to either the filter scale or one half of the filter scale. They did not proceed to refine the grid to the extent that grid-independence of the predictions was demonstrated, presumably due to the computational expense of further refining the three-dimensional grid. The approach of refining the numerical resolution while keeping the filter lengthscale unchanged is also appropriate for assessment of numerical error and resolution requirements in the Stochastic Fields equations and this approach is employed in this study. Due to the computational expense of highly-resolved three-dimensional Stochastic Fields simulations, the numerical resolution requirements are assessed across a wide range of combustion regimes using in a simplified one-dimensional test case relating to freely-propagating turbulent flames, before verifying the conclusions from the one-dimensional study in a three-dimensional LES of a turbulent premixed Bunsen flame [11].

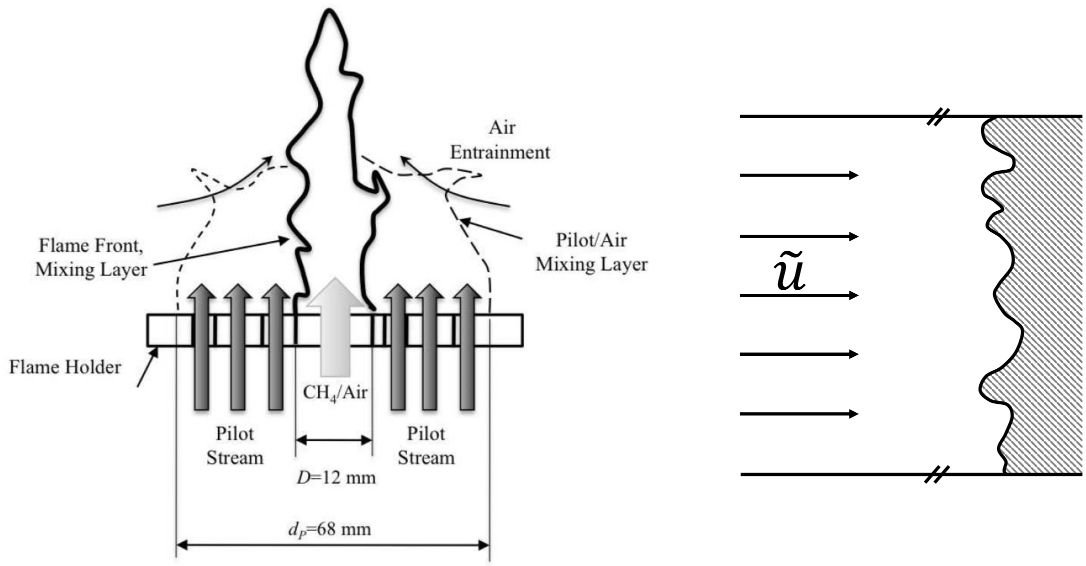

Figure 1: Schematic diagrams of the turbulent premixed Bunsen flame case (left) and of the freely-propagating planar turbulent premixed flame test case (right).

Formulation

The statistically-stationary freely-propagating planar turbulent premixed flame test case and the turbulent premixed Bunsen flame of Chen *et al.* [11] are illustrated schematically in Fig. 1.

Freely-propagating turbulent flame RANS: The planar turbulent premixed flame is statistically homogeneous parallel to the flame and it is investigated initially using a one-dimensional Reynolds Averaged Stochastic Fields simulation. The turbulence is assumed to be uniform throughout the flame and specified by setting the ratio of the rms velocity fluctuation to the laminar flame speed u'/S_L and the ratio of the integral length scale of the turbulence normalised to the thermal thickness of the laminar flame, L_T/δ_{th}. The turbulent diffusivity and mixing time scale required in Eq. (1) are then modelled by the following relations:

$$D_T = C_\mu u' L_T, \tag{2}$$

and

$$\tau_T = \frac{C_\phi L_T}{2u'}. \tag{3}$$

in which $C_\mu = 0.09$ and $C_\phi = 2.0$ [15].

Freely-propagating turbulent flame LES: Large Eddy Simulation is inherently three-dimensional however the molecular and turbulent transport within the resolved flame front is approximately one-dimensional, in the direction normal to the resolved flame front. The resolved flame front is typically thin relative to the curvature radius of the resolved flame front. It is relevant to investigate the local propagation of the resolved flame front by considering the propagation of planar turbulent flames, subject to the same sub-filter scale turbulence. In order to investigate resolution requirements in the LES context, further one-dimensional Stochastic Fields simulations are performed using sub-models for the sub-filter scale turbulent diffusivity and dissipation time scale that depend on a notional LES filter length scale Δ and the corresponding sub-filter scale velocity fluctuation u'_Δ. The one-dimensional simulations may be interpreted loosely as representing the transport along a line passing perpendicularly through a LES-resolved flame front, assuming that the LES-resolved flame front propagation is quasi-steady and unaffected by other flame fronts, by curvature, or by resolved strain (except to the extent that the resolved strain results in generation of sub-filter scale velocity fluctuations characterised by u'_Δ). The sub-filter scale diffusivity and dissipation time scales in Eq. (1) are then modelled by Eq. (2) and Eq. (3), replacing the turbulence length scale L_T with the filter scale Δ, and the turbulent velocity u' with the sub-filter scale velocity u'_Δ, and setting coefficients $C_\mu = 1$ and scaling C_ϕ with $1/Re_\Delta = S_L\delta_{th}/(u'_\Delta\Delta)$ as in Ref. [16].

The turbulent premixed combustion regime is characterised by the Karlovitz number Ka$= \left[(u'/S_L)^3\delta_{th}/L_T\right]^{1/2}$. For filter length scales in the inertial sub-range of the turbulence spectrum, the filter scale Karlovitz number $\mathrm{Ka}_\Delta = \left[(u'_\Delta/S_L)^3\delta_{th}/\Delta\right]^{1/2}$ is equal to the Karlovitz number, $\mathrm{Ka}_\Delta =$Ka, independent of filter length scale [13]. Since LES relies on selection of a filter length scale in the inertial sub-range, the effect of choosing different ratios of the filter length scale to laminar flame thickness (Δ/δ_{th}) for simulation of a particular turbulent flame regime can be investigated by fixing Karlovitz number and evaluating the corresponding sub-filter scale velocity fluctuation as,

$$u'_\Delta = S_L \mathrm{Ka}^{2/3}\left(\frac{\Delta}{\delta_{th}}\right)^{1/3}. \qquad (4)$$

Turbulent Bunsen flame configuration: The F3 turbulent premixed Bunsen flame described by Chen *et al.* [11] is simulated using Stochastic Fields-LES. The flame is characterised by Karlovitz numbers of order unity, indicating that combustion takes place across the flamelet and thin reaction zone regimes. The flame has simple boundary conditions and has served as the basis for numerous investigations of PDF modelling for turbulent premixed combustion [17–20, 9].

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 [9] 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 [9] are closed with the constant-coefficient Smagorinsky model for the sub-filter scale turbulent stresses [21], with Smagorinsky constant equal to 0.09. The turbulent diffusivity required in Eq. (1) is modelled assuming turbulent Schmidt number equal to 0.7 and the dissipation timescale in Eq. (1) is modelled by $1/\tau_T = C_{\phi\Delta}(D + D_T)/\Delta^2$, with model coefficient C_ϕ once again scaled as proposed in [16].

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

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O. \qquad (5)$$

The fuel reaction rate is modelled by the Arrhenius law,

$$\dot{\omega}_{CH_4} = A \cdot \left(\frac{\rho Y_{CH_4}}{M_{CH_4}} \right)^{n_{CH_4}} \left(\frac{\rho Y_{O_2}}{M_{O_2}} \right)^{n_{O_2}} \exp\left(-\frac{E_a}{RT} \right), \quad (6)$$

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 $S_L = 0.38\ \mathrm{ms}^{-1}$, 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 [22, 9]. 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 [3]. The chemical source terms are solved using a Newton method-based stiff solver.

The one-dimensional simulations assume constant density, such that the mean velocity is constant through the flame. The inflow velocity is controlled in order to keep the flame brush position stationary in the domain. The grid spacing is uniform and set according to the resolution requirements of each test case. 512 Stochastic Fields are used in the one-dimensional calculations which is substantially more than are currently used in 3D LES.

The turbulent Bunsen flame is simulated using two different computational grids: a fine grid characterised by 0.5 mm grid spacing at the inlet, and a coarse grid 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 respective cases are $4.6\mu s$ and $2.3\mu s$ respectively. The turbulent inflow is modelled with the digital filter based method of Klein *et al.* using the mean and rms velocity profiles from [11].

Results and Discussion

Freely-propagating turbulent flame RANS: The one-dimensional RANS model is applied to the freely-propagating turbulent premixed flame for a range of u'/S_L and L_T/δ_{th}, and the turbulent flame speed predictions are reported in Fig. 2 alongside experimental data for methane-air flames at $L_T/\delta_{th} \approx 35$ from Abdel-Gayed *et al.* [23]. The experimental data lie close to the RANS Stochastic Fields predictions for $L_T/\delta_{th} = 25$ across a wide range of u'/S_L. Even though use of non-local mixing models is known to be deficient in Lagrangian particle RANS-PDF modelling of premixed flames [18], the RANS-Stochastic Fields simulations using the IEM model successfully describes the correct premixed combustion physics, and even, to the same extent that it is seen in the data of Abdel-Gayed *et al.* [23], the onset of the "bending" effect, whereby the increase of turbulent flame speed saturates at higher u'/S_L. The relative success of the Stochastic Fields PDF implementation in premixed

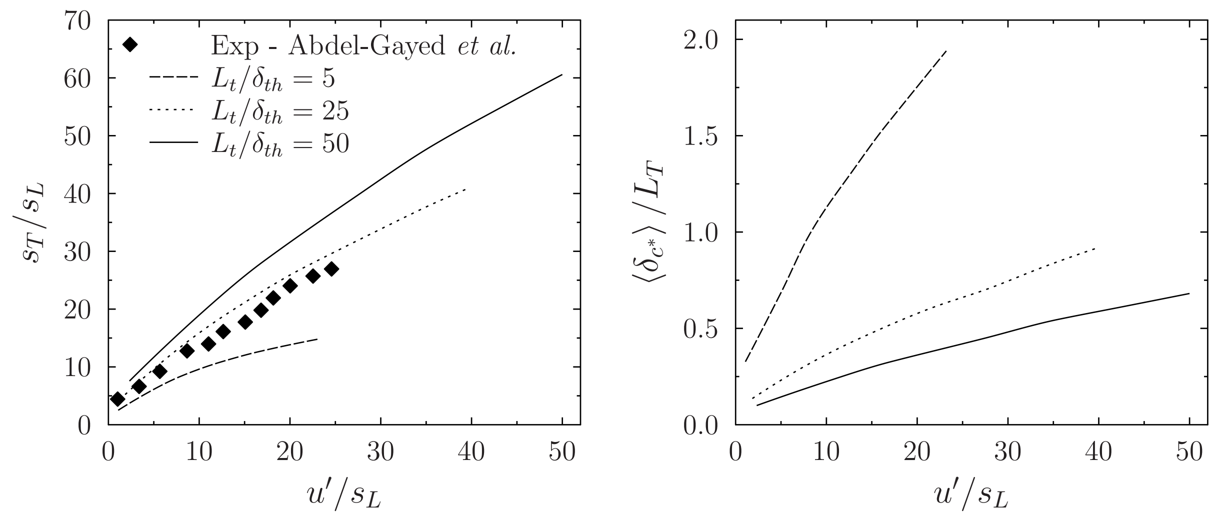

Figure 2: RANS Stochastic Fields results for freely-propagating turbulent flame speed (left) and for the average thermal thickness of the stochastic fields (right) versus u'/S_L for $L_T/\delta_{th} = 5, 25, 50$, and experimental results from Abdel-Gayed *et al.* [23].

combustion applications may be that the stochastic fields are continuous in space and that a portion of the scalar dissipation processes are accounted for by the spatial diffusion term in the Stochastic Fields equation. The coupling between the spatial diffusion and reaction terms then drives the compositions in the Stochastic Fields solutions towards a physically-plausible composition manifold across the reaction front, even if the micromixing model lacks the localness property and might otherwise draw the composition into highly improbable regions of composition space.

In order to evaluate the resolution requirements of the Stochastic Fields equation, the thermal thicknesses of the reaction-diffusion fronts on the individual stochastic fields, δ_c^*, are evaluated as indicated in Fig. 3 and ensemble averaged. The average thickness of the RANS Stochastic Fields is presented in Fig. 2, showing that the thickness reduces towards the laminar flame thickness at low u'/S_L. The thickness remains on the order of the laminar

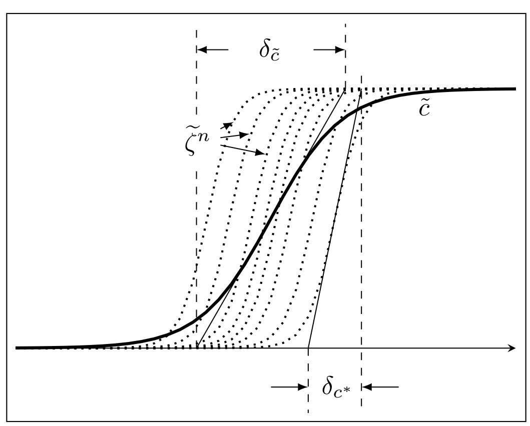

Figure 3: A schematic diagram showing the δ_{c^*} thickness of the individual stochastic fields progress variable profiles (dashed lines).

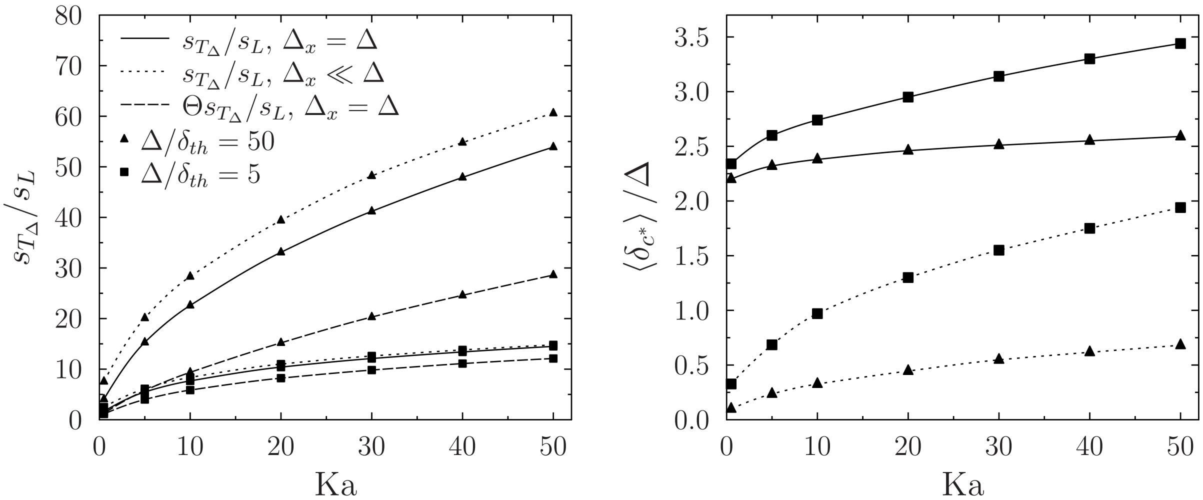

Figure 4: LES Stochastic Fields results for freely-propagating turbulent flame speed (left) and for the average thermal thickness of the stochastic fields (right) versus Ka for $\Delta/\delta_{th} = 5, 50$

flame thickness across a wide range of turbulence conditions. Since RANS simulations would otherwise resolve only the large scale flow features that drive the integral scale turbulence (i.e. length scales greater than L_T), the Stochastic Fields approach, requiring resolution at scales close to the much smaller laminar flame thickness, increases the resolution requirements dramatically when applied to premixed combustion.

Freely-propagating turbulent flame LES: Further one-dimensional simulations are performed in order to assess the effect of filter length scale on the spatial resolution requirements in the context of LES. Figure 4 shows that the average thickness of the reaction-diffusion fronts in the stochastic fields is close to the laminar flame thickness at low Karlovitz number, and increases with Karlovitz number and filter length scale due to the increasing contribution of sub-filter scale diffusivity. Given that an absolute minimum of five grid points are needed within a reaction diffusion front ($\delta_{c^*}/\Delta_x \geq 5$) in order to give an acceptable numerical resolution, it is evident that the setting $\Delta_x = \Delta$ does not give acceptable resolution anywhere in the wide range of combustion conditions considered.

The effect of the conventional approach of setting $\Delta_x = \Delta$ is to numerically thicken the reaction-diffusion fronts so that they extend across at least twice the grid spacing, making the reaction-diffusion fronts a factor of twelve thicker at Ka=0.5 and $\Delta/\delta_{th} = 5$. The numerical thickening is an error that changes the physical predictions of the model in two main ways. First, reduction of scalar gradients is expected to affect the local propagation speed of the reaction-diffusion fronts in the Stochastic Fields. Second, the numerically-thickened reaction-diffusion fronts are less-susceptible to wrinkling by the resolved turbulence leading to an under-prediction in the overall flame surface area.

The reduction in the local propagation speed of the reaction-diffusion fronts due to use of $\Delta_x = \Delta$ is shown in Fig. 4. The under-prediction of the local propagation speed is not significant for smaller filter scales $\Delta_x/\delta_{th} = 5$, but increases to around 15% at $\Delta_x/\delta_{th} = 50$. The effect of the numerical thickening on the under-prediction of flame surface area and consumption rate cannot be obtained directly from the one-dimensional simulations but it

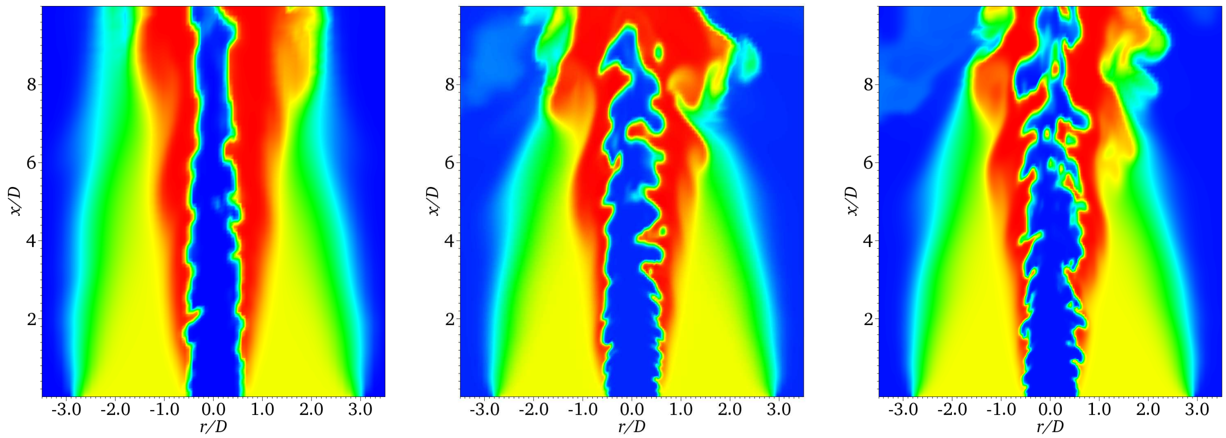

Figure 5: Instantaneous temperature field of an individual field from the turbulent Bunsen flame LES with $\Delta_x = \Delta = 1.0$ mm (left),$\Delta_x = 0.5$ mm & $\Delta = 1.0$ mm (mid), and $\Delta_x = \Delta = 0.5$ mm (right).

can be estimated using established models for sub-filter scale flame wrinkling in the context of artificially-thickened flame modelling [13, 24]. The efficiency function developed by Charlette *et al.* [13] provides an estimate for the contribution to flame surface area from turbulent motions below a particular length scale. Evaluating the efficiency function for the reaction-front thicknesses in Fig. 4, and taking the ratio Θ between the efficiency functions obtained with the $\Delta_x = \Delta$ and $\Delta_x \ll \Delta$ data gives an estimate for proportion of the flame surface area remaining after the numerical thickening. The impact of the loss of flame surface area on burning rate due to numerical thickening is illustrated in Fig. 4 by multiplying the propagation speed data for $\Delta_x = \Delta$ by Θ. The estimate indicates that the loss of surface area due to numerical thickening may be more significant than the effect on the local propagation speed: reducing the overall flame speed by around 20% at $\Delta_x/\delta_{th} = 5$, and between 50-75% at $\Delta_x/\delta_{th} = 50$.

Turbulent Bunsen Flame LES

The F3 turbulent Bunsen flame of Chen *et al.* [11] is simulated by LES-Stochastic Fields with coarse ($\Delta_x = \Delta = 1.0$ mm), fine ($\Delta_x = \Delta = 0.5$ mm) and improved ($\Delta_x = 0.5$ mm, $\Delta = 1.0$ mm) resolutions. The resolution of $\Delta_x/\delta_{th} = 1-2$ is much finer than can be achieved in simulations of industrial high-pressure combustion systems, however the previous analysis of one-dimensional simulations indicates that even these grid spacings are inadequate to fully-resolve the Stochastic Fields solution.

Instantaneous filtered temperature fields from the three simulations are shown as colour maps on a plane through the burner centreline in Fig. 5, and the radial variation of the time-averaged filtered methane mass fraction and axial velocity are compared with the experimental measurements at four axial positions in Fig. 6. The fine simulation gives velocity and fuel mass fraction predictions in reasonable agreement with the experimental data. The coarse resolution simulation shows slower flame propagation resulting in a longer flame length, and less fine-scale structure than the fine resolution case. The improved-resolution simulation yields mean velocity profiles similar to the coarse simulation but reactive scalar profiles similar to the fine simulation. This indicates that the velocity field is relatively insensitive to refinement of the computational grid spacing to less than the filter scale, whereas the reactive scalar fields are significantly affected by numerical diffusion when $\Delta_x = \Delta$. The

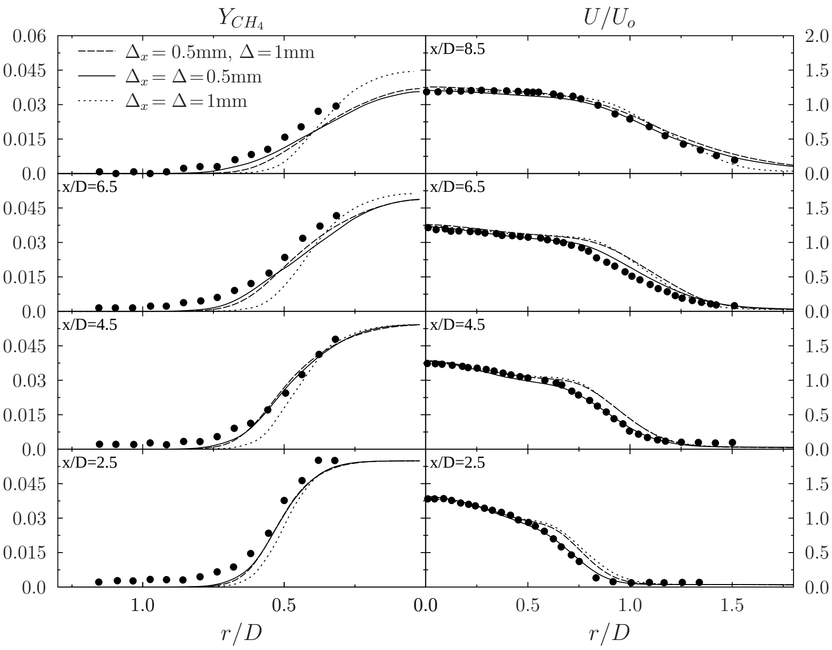

Figure 6: Radial distributions of the time-averaged methane mass fraction $\langle \widetilde{Y_{CH_4}} \rangle$ and the normalised mean axial velocity at various axial locations.

effect of numerical thickening is also demonstrated by evaluating the average progress variable gradient magnitude on the Stochastic Fields, conditioned on the progress variable giving maximum heat release, $\langle |\nabla \zeta_{c,(i)}| \mid \zeta_{c,(i)} = 0.68 \rangle^{-1}$: 4.6 mm in the fine simulation, 7.5 mm in the coarse simulation, and 4.6 mm in the improved resolution simulation – demonstrating that the stochastic field thickness is still set by the numerical resolution, even with $\Delta = 2\Delta_x$.

Conclusions

The Stochastic Fields formulation is an attractive way to apply transported probability density function approach to turbulent reacting flows, however the spatial resolution requirements become very demanding when applied to turbulent premixed combustion. One-dimensional analysis of resolution requirements in Stochastic Fields simulations of premixed turbulent combustion shows that the thickness of the reaction-diffusion fronts arising in the Stochastic Fields solution is on the order of the laminar flame thickness. In Large Eddy Simulation where the filter length scale can be much greater than the laminar flame thickness, the common practise of setting the LES filter scale equal to the grid spacing leads to very significant numerical thickening of the reaction-diffusion fronts. The numerical thickening reduces the predicted turbulent flame speed in two ways: First, reduction of scalar gradients reduces the local propagation speed of the reaction-diffusion fronts in the Stochastic Fields. Second, the numerically-thickened reaction-diffusion fronts are less susceptible to wrinkling by the resolved turbulence, leading to an under-prediction in the overall flame surface area. The combination of these effects leads to a projected underestimate of turbulent flame speed in the region of 20% for relatively well-resolved LES with filter length and grid spacing around five times the laminar flame thickness, and a 50-70% error for less well-resolved simulations, such as current advanced simulations of high-pressure industrial combustion systems, with filter length and grid spacing on the order of fifty times the laminar flame thickness. Three-dimensional Large Eddy Simulations of a laboratory turbulent Bunsen flame with the filter scale equal to twice the laminar flame thickness confirm that the Stochastic Fields solution is not numerically accurate when the grid spacing is equal to the filter length scale, whereas the flow field solution is relatively insensitive to further refinement of the spatial resolution. Even in the relatively well-resolved LES, the impact of numerical inaccuracy on the overall burning rate is substantial. The present results provide a guide to the resolution required in order to obtain numerically-accurate Stochastic Fields solutions. The general requirement is that the grid spacing should be finer than the filter scale and the same order of magnitude as the laminar flame thickness, but this is impractical for many industrial applications involving high pressure combustion. Techniques such as artificial thickening should be considered in order to reduce the resolution requirements while retaining the key advantages of the Stochastic Fields method.

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References

[1] Valiño, L., "A Field Monte Carlo Formulation for Calculating the Probability Density Function of a Single Scalar in a Turbulent Flow", *Flow, Turbulence and Combustion* 60:157–172 (1998).

[2] Valiño, L., Mustata, R., Ben Letaief, K., "Consistent behavior of eulerian monte carlo fields at low reynolds numbers", *Flow, Turbulence and Combustion* 96:503–512 (2016).

[3] Sabel'nikov, V., Soulard, O., "Rapidly decorrelating velocity-field model as a tool for solving one-point Fokker-Planck equations for probability density functions of turbulent reactive scalars", *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* 72:1–22 (2005).

[4] Dopazo, C., O'Brien, E.E., "An approach to the autoignition of a turbulent mixture", *Acta Astronautica* 1:1239–1266 (1974).

[5] Jones, W., Navarro-Martinez, S., Röhl, O., "Large eddy simulation of hydrogen autoignition with a probability density function method", *Proceedings of the Combustion Institute* 31:1765–1771 (2007).

[6] Jones, W.P., Navarro-Martinez, S., "Numerical Study of n-Heptane Auto-ignition using LES-PDF Methods", *Flow, Turbulence and Combustion* 83:407–423 (2009).

[7] Jones, W., Navarro-Martinez, S., Röhl, O., "Large eddy simulation of hydrogen autoignition with a probability density function method", *Proceedings of the Combustion Institute* 31:1765–1771 (2007).

[8] Jones, W.P., Marquis, a.J., Prasad, V.N., "LES of a turbulent premixed swirl burner using the Eulerian stochastic field method", *Combustion and Flame* 159:3079–3095 (2012).

[9] Navarro-martinez, S., Dodoulas, I., "Large Eddy Simulation of Premixed Turbulent Flames Using the Probability Density Function Approach", *Flow, Turbulence and Combustion* 60:645–678 (2013).

[10] Jones, W.P., Marquis, A.J., Wang, F., "Large eddy simulation of a premixed propane turbulent bluff body flame using the Eulerian stochastic field method", *Fuel* 140:514–525 (2015).

[11] Chen, J.Y., Chang, W.C., Koszykowski, M., "Numerical simulation and scaling of NOx emissions from turbulent hydrogen jet flames with various amounts of helium dilution", *Combustion Science and Technology* 111:505–529 (1995).

[12] Peters, N., *Turbulent Combustion*, Cambridge Monographs on Mechanics, Cambridge University Press, 2000.

[13] Charlette, F., Meneveau, C., Veynante, D., "A power-law flame wrinkling model for LES of premixed turbulent combustion Part I: non-dynamic formulation and initial tests", *Combustion and Flame* 131:159–180 (2002).

[14] Vreman, B., Geurts, B., Kuerten, H., "Comparison of numerical schemes in large-eddy simulations of the temporal mixing layer", *International Journal for Numerical Methods in Fluids* 22:297–311 (1996).

[15] Pope, S., *Turbulent Flows*, Cambridge University Press, 2000.

[16] Prasad, N., *Large Eddy Simulation of Partially Premixed Turbulent Combustion*, Ph.D. thesis, Imperial College London (2011).

[17] Lindstedt, R.P., Vaos, E.M., "Transported PDF modeling of high-Reynolds-number premixed turbulent flames", *Combustion and Flame* 145:495–511 (2006).

[18] Stöllinger, M., Heinz, S., "PDF modeling and simulation of premixed turbulent combustion", *Monte Carlo Methods and Applications* 14:343–377 (2008).

[19] Stöllinger, M., Heinz, S., "Evaluation of scalar mixing and time scale models in PDF simulations of a turbulent premixed flame", *Combustion and Flame* 157:1671–1685 (2010).

[20] Yilmaz, S.L., Nik, M.B., Givi, P., Strakey, P.a., "Scalar filtered density function for large eddy simulation of a bunsen burner", *Journal of Propulsion and Power* 26:84–93 (2010).

[21] Smagorinsky, J., "General circulation experiments with the primitive equations", *Monthly Weather Review* 91:99–164 (1963).

[22] Jones, W., di Mare, F., Marquis, A., *LES BOFFIN: users guide.*, Imperial College London, 2002.

[23] Abdel-Gayed, R.G., Al-Khishali, K.J., Bradley, D., "Turbulent burning velocities and flame straining in explosions", *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* 391:393–414 (1984).

[24] Colin, O., Ducros, F., Veynante, D., Poinsot, T., "A thickened flame model for large eddy simulations of turbulent premixed combustion", *Physics of Fluids* 12:1843–1863 (2000).