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A Stochastic Micromixing Model based on the Turbulent Diffusion Length Scale

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Abstract

A new micromixing model to close probability density function (pdf) models is proposed. The model is based on the proposition that each computational timestep, stochastic particles move within the scalar space (on average) by a distance equal to the turbulent diffusion length scale. At each timestep, the model evaluates the distance in scalar space between all particles. During the timestep, a discrete pdf is computed for the distance between unmixed particles and the cumulative integral for the mean calculated. A filter is applied to retain the lower portion of the distance domain so that the cumulative integral is equal to the average diffusion length required to decrease the scalar variance. A sample (a pair of particles) is chosen from this filtered part of the domain and the particles mixed using Modified Curl's model. The complete interparticle-distance pdf is re-evaluated for each pair to ensure that there is sufficient capacity to mix to meet the variance decay requirements. Preliminary tests show that this model obeys several fundamental properties required of micromixing models, including conservation, correct decay of variance and relaxation to Gaussian pdf.

Keywords: Micromixing Model, Diffusion Length, Stochastic Particles

1. Introduction

Numerous turbulent combustion models have been developed for the diffusion process (commonly modelled by scalar micromixing in probability density function [pdf] models [1,2,3]). Some of the most commonly-used models are: Curl's Model [4], Modified Curl's Model [5,6], Interaction by Exchange with the Mean (IEM) [7,8], the Flamelet model [9], Conditional Moment Closure (CMC) [10], Euclidean Minimal Spanning Tree (EMST) [11] and Multiple Mapping Conditioning (MMC) [12].

A number of these models (Curl's, EMST, stochastic MMC) use particle interaction to model the micromixing process and a major distinction between them is the selection process of which particle is chosen to share its values with the particle of interest. In Curl's model, the particles are chosen at random, so they can be separated by any distance, leading to potentially non-physical effects because locality is violated. EMST is founded on the principle that a particle should only interact with the particle that is closest to it. This leads to an undesirable stranding effect where clusters of particles interact exclusively within that cluster, causing them to locally collapse towards the same value [11, 13]. To alleviate this problem of over-localisation, an age parameter was introduced so that approximately half the particles are available for mixing in any given timestep [11]. Different perspectives have been utilised in the MMC framework. One method for MMC-LES (Large Eddy Simulations) [14] is similar to that used in EMST, where a normalised distance is minimised; a distinction between this MMC-LES method and EMST is that a weighted average of physical and scalar distances is used in the former, while only scalar distances are used in the latter. Note that EMST used at LES scale produces good results [13].

A fundamental principle used in another MMC method is that particles should only be able to interact if they have to travel no more than a diffusion length to reach a coincident location (previously alluded to [15] and explicitly stated [16]). This can be considered a relaxation of the EMST and MMC-LES methods where the closest particles are forced to interact with each other. Consider the Ito form of the MMC model [12]:

$$d\xi_k = A_k dt + b_{kl} dw_l \tag{1}$$

where ξ_k is the kth reference variable, A_k its drift coefficient, the diffusion coefficient is $2B_{kl} = b_{ki}\, b_{li}$ and dw_l a Wiener process. Since the Wiener process is commonly modelled by

$$dw_l = \omega_l \sqrt{dt}\,, \tag{2}$$

where ω_l is a random variable with a standard Gaussian distribution, this scalar ξ_k varies by (on average) $b_{kl}\sqrt{dt}$ from the relaxation towards the mean imposed by the drift. If there is a single scalar, this would commonly be represented by

$$\sqrt{2Bdt}\,, \tag{3}$$

which is the definition of the (scalar) diffusion length scale. Therefore, particles with similar values of A can only reach coincident values of ξ_k (i.e. meet) if they are separated by no more than (on average) $2\sqrt{2Bdt}$. Because of the random nature of ω_l, it is possible that any pair of particles could be separated by more or less than $2\sqrt{2Bdt}$ and still be coincident. The definition in

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(3) has similarly been used for the diffusion in physical space, for example using the molecular and Smagorinsky turbulent diffusivities (D and D_t respectively) [14]:

$$d\mathbf{x} = \left[\tilde{\mathbf{u}} + \frac{1}{\bar{\rho}} \nabla \bar{\rho} \left(D + D_t \right) \right] dt + \sqrt{2\left(D + D_t \right)} d\mathbf{w} \ . \quad (4)$$

The drift coefficient is a function of the filtered velocity vector and mean density.

The remainder of this paper will describe the model and present results from validation tests.

2. The Stochastic Particle Diffusion Length (SPDL) Model

The current model relies on the discussion following (3) that particles can be expected to meet, thereby be able to interact, if they are separated by approximately double the diffusion length scale. Let d^{pq} be the distance between particles p and q and $P_d(d^{pq})$ be the pdf of inter-particle distance for all p and q that are deemed to be allowed to interact (in a finite volume description, all those particles in the same physical cell). It is desirable to choose a maximum interaction distance $d_{\max}$ so that

$$\int_0^{d_{\max}} d^{pq} P_d\left(d^{pq}\right) \cdot d\left(d^{pq}\right) = 2\sqrt{2Ddt} \quad (5)$$

i.e. the mean inter-particular distance is equal to twice the diffusion length, where D is the appropriate diffusivity corresponding to the variable d^{pq}. The pair of particles to be mixed (p,q) is randomly selected from those that satisfy

$$d^{pq} \le d_{\max} \ . \quad (6)$$

Ostensibly, this pair of particles mix using Curl's model; in practice, to remove the known difficulty with Curl's model only producing discrete values from initial δ-functions, a weak Modified Curl's model is proposed. Let b be the extent of mixing (b = 0 for no mixing; b = 1 is Curl's model). To allow a continuous distribution to form, b was set to be

$$b = \frac{n - 2i + 1}{n - 2i + 2} \ , \quad (7)$$

where the total number of particles to be mixed together is n, and the ith pair is to be mixed.

In practice, to ensure that the set of particles mixes the correct amount specified by the decay of variance,

$$\frac{d\sigma^2}{dt} = -2D \ , \quad (8)$$

a numerical form of (5) is required. For the ith particle pair (p,q) there is a target diffusion length L_i which has the property

$$\frac{2}{n} \sum_{i=1}^{n/2} L_i^2 = 2Ddt \ . \quad (9)$$

If $i > 1$, then for all $j < i$, the value of the target diffusion length is set to the actual inter-particle distance for pair i:

$$\underset{j<i}{\forall} L_j = d^{pq} \quad (10)$$

and the value of the target diffusion length for all $j \ge i$ is set to:

$$\underset{j\ge i}{\forall} L_j^2 = \frac{1}{\frac{n}{2} - i} \left(\frac{n}{2} 2Ddt - \sum_{k=1}^{i-1} L_k^2 \right) . \quad (11)$$

This value is used in (5) to determine $(d_{\max})_i$:

$$\int_0^{(d_{\max})_i} d^{pq} P_{d,i}\left(d^{pq}\right) \cdot d\left(d^{pq}\right) = 2L_i \quad (12)$$

Note that $P_{d,i}(d^{pq})$ excludes all those distances d^{pq} where either p or q had been selected for $j < i$.

It is necessary to ensure that once the ith pair has been selected, the remaining n–2i particles are able to dissipate sufficiently to satisfy (11). The maximal change in variance that can be achieved by a pair of particles using Curl's model is:

$$\left(\Delta\sigma^2\right)_{\max,i} = -\frac{\left(d^{pq}\right)^2}{2} \quad (13)$$

therefore the maximal amount by which the n–2i particles are able to reduce the variance is

$$\sum_{k=i+1}^{n/2} \left(\Delta\sigma^2\right)_{\max,k} = -\sum_{p=1}^{n-2i} \max\left(\frac{\left(d^{pq}\right)^2}{2} \right) . \quad (14)$$

The summation on the rhs of (14) is non-repetitive, i.e. every q that is selected is not allowed to be considered p in the summation, so that the summation has only n/2–i terms. If it is observed that

$$\sum_{k=i+1}^{n/2} \left(\Delta\sigma^2\right)_{\max,k} < 2Ddt - \sum_{j=1}^{i} L_j^2 \ , \quad (15)$$

then the pair (p,q) needs to be reselected to provide the maximal d^{pq}. This process almost guarantees that the set of particles does not undershoot the decay of variance required: along with every other procedure of pairing, it fails if dt is too large for that realisation of particle values, and the computational timestep must be split.

Finally, if the amount of mixing for pair (p,q) using Curl's model overshoots the required total variance dissipation, then Modified Curl's model is used to reduce the mixing amount so the total variance dissipation satisfies (8).

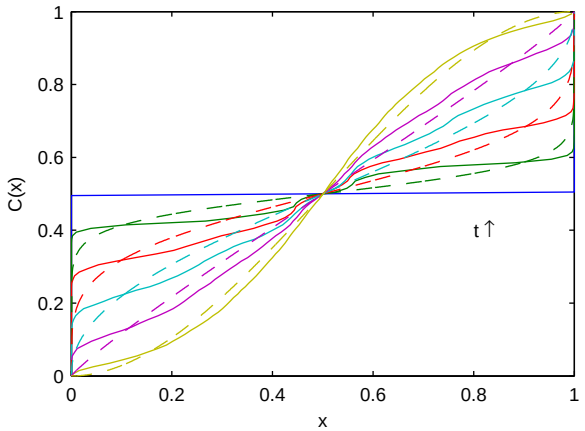

Figure 1: Cumulative distribution functions (cdf) from initial double δ-function pdf at $x = 0$ and 1. Solid lines: sample data $n = 100$, ensemble average of 100; dashed lines: β-function cdf with same mean and variance as ensemble. Lines of the same colour are from the same time.

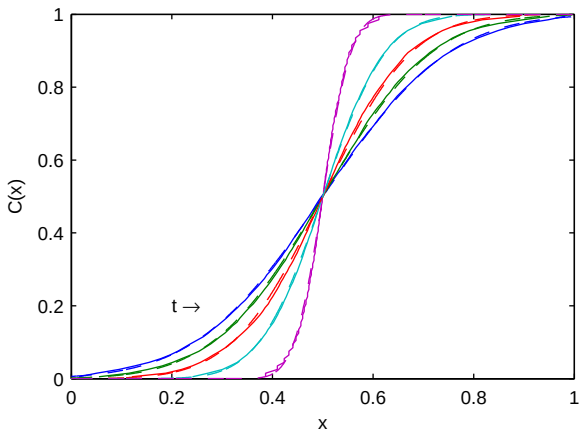

Figure 2: Cumulative distribution functions from later times to Fig. 1. Dashed lines: Gaussian cdf with same mean and variance as ensemble.

3. Testing of SPDL Model

Initial tests on the ability of SPDL to model cases accurately have been performed. The first test was to validate that the procedure satisfied (8), which it did to the level of computational precision.

Figures 1 and 2 show the results of the relaxation to Gaussian test for an ensemble average over 100 realisations with 100 particles. Curl's model causes the cumulative distribution function (cdf) at early times to not be smooth in the vicinity of $C = 0.5$ (Fig. 1), but this eventually disappears. [This cannot be remedied by using (7).] This is likely to be the cause of the sample cdf to have decayed more than the β-function cdf for $0.2 \le x \le 0.8$; for the variance to be identical, the sample cdf lags the β-function cdf near the tails. However, it is apparent that the sample data does relax to Gaussian (Fig. 2), with a much smaller over-decay in the centre of the cdf, so this is evidence that the scheme satisfies this fundamental property.

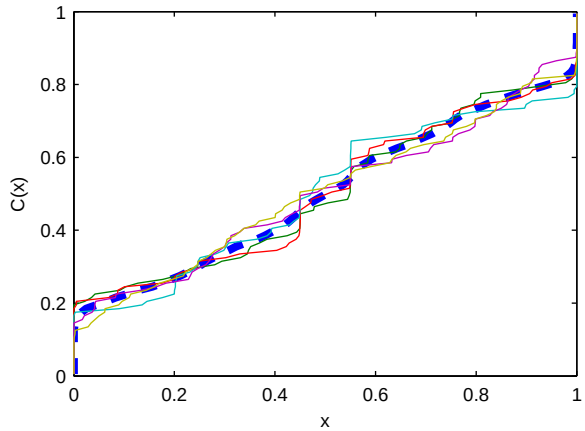

Figure 3: Cumulative distribution functions (cdf) from fourth sample in Fig. 1. Dashed line: ensemble average; other lines: 5 individual realisations.

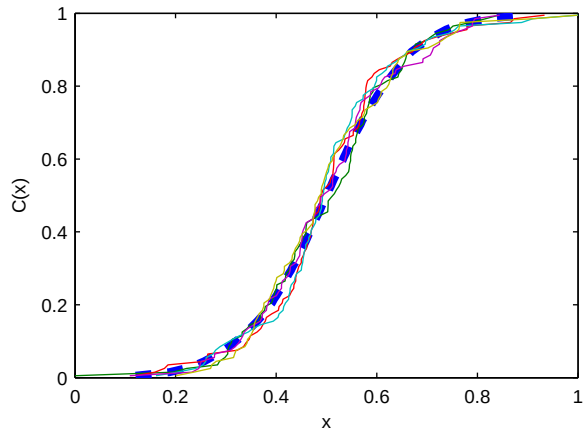

Figure 4: Cumulative distribution functions (cdf) from third sample in Fig. 2. As per Fig. 3.

Figures 3 and 4 show individual realisations compared to the ensemble average. The (almost) Curl's model (7) causes the occasional large deviation early on (Fig. 3), but otherwise the deviation from the ensemble average is relatively small.

4. Conclusions

A new turbulent combustion model, the Stochastic Particle Diffusion Length (SPDL) Model has been proposed. This micromixing model aims to cause stochastic particles to interact so that, on average, pairs are separated by twice the (turbulent) diffusion length scale. A Modified Curl's model is proposed for the mixing of the particles. Initial tests of the model for double δ-function initial conditions show that this model obeys the relaxation to Gaussian rule. Further tests are to be undertaken for more complex cases.

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