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Study of Random Particle Interactions for Analysis of Diffusion Lengths in Turbulent Combustion Modelling

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Abstract

Turbulent combustion is commonly modelled using probability density function (PDF) methods; to close these methods, micro-mixing models are required: these are most commonly based on stochastic particle interactions. While it is standard practice for the turbulent diffusion coefficient to be used to specify the amount of mixing, few models account for the corresponding diffusion length scale that defines interacting particle separation. This study investigates ensemble averages of the minimum, mean and maximum inter-particle distances for random realisations as a precursor to comparing with the diffusion length in real simulations. It was found that the ensemble of results for each type of inter-particle distance (minimum, mean or maximum) had a normal distribution. For 1 to 1000 dimensions, the minimum inter-particle distances for 100 particles were 0.0051 to 12.3406 and the average distances were 0.3297 to 12.7776.

Keywords: Particles, Diffusion Length, Turbulent Combustion

1. Introduction

The world's dependency on fossil fuel energy resources is an important consideration: the energy demand up to 2030 is estimated to be about 18 billion tons of oil equivalents; about 79 percent of this will be fulfilled by oil, gas and coal [1]. The desire to improve combustion efficiency with lower emissions has led to an increased interest in combustion modelling [2-3] and research, especially unresolved problems in turbulent combustion. Many researchers have studied and modelled turbulent combustion with some success, but improvements can be made. Improved control of the turbulence process will result in increased combustion efficiency. Turbulence increases the mixing rate and thereby enhances combustion, which then releases heat and generates flow instability by gas expansion which further enhances the turbulence process [4].

Combustion processes require fuel and oxidiser to be mixed at the molecular level and the combustion efficiency largely depends on the efficiency of molecular mixing process, which depends on the diffusion process. In order to produce efficient mixing, we have to understand the diffusion process at a molecular level. The mixing process will form eddies of different size, then the strain and shear between eddies will improve the mixing rate. This process of forming smaller eddies is called the eddy break-up process; strain and shear will increase and enhance the inter-molecular diffusion. Molecular mixing between oxidiser and fuel takes place during these eddy break-up processes. Because modern computers are not capable of simulating the mixing process to the smallest scales of turbulence, models are required for all scales below the grid resolution, which is normally of the order of the inertial interval.

Mixing processes in turbulent combustion range from premixed to non-premixed; the selection of the inflow conditions requires careful consideration to balance the advantages and disadvantages. The Probability Density Function (PDF) model [5] is commonly used for transport of scalars; a mixing model is required to close its molecular diffusion term. The molecular diffusion term – the last in (1) – represents transport in reactive scalar space by molecular fluxes ($J_{i,k}$). Mixing plays an important role in the non-premixed combustion process since mixing and combustion take place simultaneously. The fuel and oxidiser must be mixed sufficiently quickly for the chemical reactions to occur.

$$\frac{\partial \rho P}{\partial t} + \frac{\partial \rho u_i P}{\partial x_i} + \frac{\partial \rho S_k P}{\partial \psi_k} = -\frac{\partial}{\partial x_i}\left[\rho \langle u_i^{"} | \psi \rangle P\right] + \frac{\partial}{\partial \psi_k}\left[\frac{1}{\rho}\langle \frac{\partial J_{i,k}}{\partial x_i} | \psi \rangle P\right] \quad (1)$$

In (1), P is the Favre joint PDF of composition, ρ the mean density, u_i the Favre mean velocity vector, S_k the reaction rate for species k, $u"$ is the velocity fluctuation vector and ψ is the composition space vector. There are two commonly-used methods to solve (1): discretised partial differential equations (PDE) and stochastic particles method; the latter is normally used [5].

There are two types of liquid molecule movement: effusion and diffusion. Effusion is the escape of a liquid or gas molecule through a tiny hole and diffusion is the movement of a liquid or gas molecule through another fluid with random molecular motion. The understanding of how particles behave in their random motion interaction will be of benefit to turbulent combustion modelling. While all mixing models use a turbulent diffusion coefficient to determine the decay rates of the scalars, few are fully consistent. This is due to those models not organising the inter-particle interaction so that the separation of particles is based on the diffusion length scale.

The current work is a preliminary study of the effect of the number of stochastic particles and the number of dimensions on the inter-particle distance.

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Future work will include analysis of the behaviour of current models with the turbulent diffusion length scale. The principles of this study may also be used to develop improved mixing models.

2. Particle Diffusion

Diffusion is the random movement of small particles arising from motion due to thermal energy, with length scales ranging from nanometres to millimetres. For the larger length scales, the bulk movement of the fluids is normally due to convection [6]. When large molecules diffuse, Brownian motion is observable under a microscope but for small-molecule diffusion the Brownian motion is hard to observe except under carefully controlled experimental conditions. Particles and molecules are very dynamic and always moving from one space to another especially from areas of high to low concentration.

2.1 Brownian Motion

The mechanism for Brownian motion was discovered in 1785 by Ingenhousz, who noticed the irregular motion of coal dust particles on the surface of alcohol [7]. In 1827 Brown observed the movement of suspended pollen grains in water [8] and further research was initiated by Einstein, Smoluchowski, Perrin, Langevin and Lorentz which shows that it was caused by very frequent collisions of the particles with other particles, resulting in random or thermal motion. The notable development in diffusion seems to be the theoretical solution by Einstein in 1905 [9].

2.2 Molecular Diffusion

Fick's law [10–13], describing the variation of non-uniform particle distributions, is derived from the model of random motion or random walks. If we know the number of particles at each point along the *x*-axis at time *t*, then we can find how many particles will move across unit area in unit time from point x to point $x + a$. Brownian motion [14] states that the average distance δl a particle moves in duration (δt) is:

$$(\delta l)^2 = 2D(\delta t) \tag{2}$$

where the molecular diffusion coefficient is:

$$D = \frac{RT}{6\pi N_A v r} \tag{3}$$

R is the gas constant (8.3145 J/mol K), T is absolute temperature, N_A is Avogadro number ($6.22\text{x}10^{23}$ mol^{-1}), v is viscosity and r is the radius of the particle.

2.3 Turbulent Diffusion

Turbulent diffusion is the modelling of the mixing process for all scales of turbulence below the grid resolution. For the mixture fraction Z, this is conventionally represented by the scalar dissipation rate:

$$N = D\left(\frac{\partial Z}{\partial x}\right)^2 \tag{4}$$

In Curl's [15] and modified Curl's mixing models [16,17], when particle pairs are selected, the average distance between the pairs is equal to the overall mean inter-particle distance in the ensemble. In reality, the closer a particle is to another, the more likely it is to mix and this is the weakness of Curl's and modified Curl's model. This localness was solved by mixing the nearest pairs of particles in the Euclidean Minimum Spanning Trees (EMST) model [18]: the average distance between interacting particles is equal to the average minimum inter-particle distance. In two implementations of the Multiple Mapping Conditioning (MMC) model, pairs of stochastic particles were selected so that their spacing in reference space was small (but not necessarily closest), thus preserving the localness [19,20].

3. Methodology

Gas molecules are in constant, rapid, random motion and diffuse quickly throughout any space. The molecular diffusion process can be modelled by making the stochastic particles interact. Note that the inter-particle distance is a consequence of the ensemble of realisations and the diffusion length is a property of the turbulence. In order to provide an estimate of the inter-particle distance, a pseudo-random generator was utilised to produce multi-dimensional ensembles. Particles were uniformly distributed within each dimension, taking values between 0 and 1 (although in practice particles are almost certainly distributed differently, this is an indicative study of the behaviour). The values for the minimum, average and maximum inter-particle distance were determined for up to 1000 particles and up to 1000 dimensions; multiple realisations were averaged to reduce the stochastic error. Table 1 lists the numbers of particles (P) tested and corresponding number of realisations (R).

Table 1: List of number of particles (P) and realisations (R).

P	5	10	20	30	40	50	100	200	300	400	500	1000
R	1000	500	300	250	220	170	100	75	50	40	30	20

There were fifteen different dimensionalities simulated: 1, 2, 3, 5, 10, 20, 30, 50, 100, 200, 300, 400, 500, 750 and 1000. Every particle realisation was simulated for each number of dimensions.

4. Results and Discussion

The results for the inter-particle distances are described in this section. Figure 1(a) shows the ensemble average for 1000 particles as a function of dimensionality. The average minimum, average mean and average maximum distances increase with the number of dimensions. This is guaranteed because for one dimension the maximum possible inter-particle distance is 1.0; for two dimensions, the max is $\sqrt{2}$ (=1.414); for three dimensions, the max is $\sqrt{3}$ and so on. From dimension 1 to 100, all distances rapidly increase but the rate of increase diminishes as the dimension increases with the rate approximately linear.

The ensemble standard deviation in Fig. 1(b) indicates the accuracy of the ensemble means in Fig. 1(a). For dimensions 1–50, the values for the maximum distance had significantly greater spread than the minimum and average distances. For higher dimensions, the spread stabilised and the average standard deviations throughout dimension 50 to 1000 for minimum, average and maximum are 0.00626, 0.00673 and 0.00821 respectively.

Figure 1(c) shows that the distributions of the minimum, average and maximum distances fit the normal distribution as expected by the central limit theorem, and also found for 50,000 particles in a diffusion flow [21]. The cumulative distribution function (cdf) for the lower (cdf(X) = 0.0015), middle (cdf(X) = 0.5005) and upper (cdf(X) = 0.9995) values of the distribution are reported in Table 2.

To confirm that the corresponding distributions for all tests were normal, a *t*-test was performed on each ensemble of data, with the null hypothesis that each ensemble had a normal distribution. The result from the t-test was a failure to reject the null hypothesis with probability 1, at the 5% significance level. The results for the confidence interval were calculated using (5) and shown in Fig. 2.

$$CI_X = \overline{x} \pm \left(t_{2,\alpha,df} \times \frac{s}{\sqrt{n}} \right) \qquad (5)$$

Here X is the interval (normally 0.90, 0.95 or 0.99; 0.95 was chosen here), α is 1-X and df is the degrees of freedom.

From Fig. 2, the largest (worst) confidence intervals were for low dimensionality and particles, which correspond to the smallest inter-particle distances. This is to be expected because the random error increases as the number of particles decreases (mitigated to some extent by having a much larger ensemble). In addition, because the mean value is close to zero, it is possible that the distribution is bounded, which would result in a violation of the normal distribution. The ensemble mean values for each of the minimum, average and maximum inter-particle distance for all cases are shown in Fig. 3. As noted previously, the inter-particle distance increases with the number of dimensions. Figure 3(a), which is the average minimum inter-particle distance, shows that the isolines are angled up, which is to be expected. Consider an ensemble containing two particles in a domain where the possible location is bounded. If another particle is added, the average minimum distance is likely to reduce because the new particle is expected to be at least as close to one of the original particles as the original pair was to each other. As more particles are added with a consistent distribution, the average minimum distance will continue to diminish.

Table 2: The lower, middle and upper values for the cdfs in Fig. 1(c).

cdf(X)	0.0015	0.5005	0.9995
Minimum	11.77	12.18	12.53
Average	12.60	12.90	13.18
Maximum	13.25	13.62	13.95

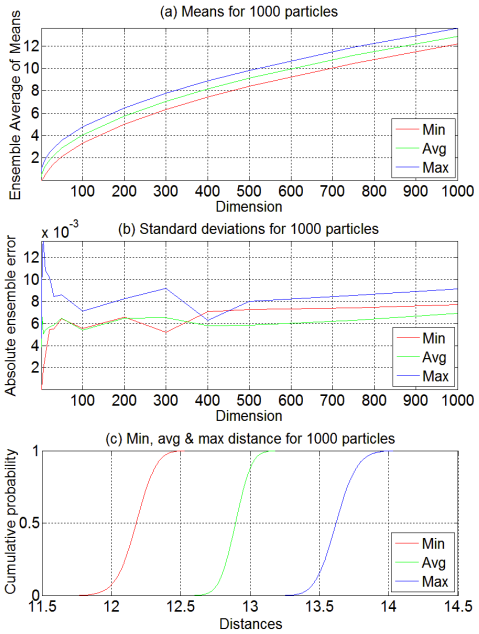

Figure 1: Statistical analysis for 1000 particles. (a) Ensemble mean (b) ensemble standard deviation (c) distribution of 1000 realisations for 1000 particles and 1000 dimensions.

The opposite behaviour is expected for the average and maximum distance [Figs. 3(b) and 3(c)]. There is a lot of empty space in the domain when the ensemble is only 2 particles. An additional particle will either be located between the original pair or closer to the edge of the ensemble; the latter case is more likely to occur, therefore the average and maximum distance will be larger for the two extreme particles than when there were only 2 particles. For large numbers of particles, the average and maximum inter-particle distances show asymptotic behaviour: an additional particle has little effect because when the number density of the particles is already high, the new particle is likely to be located very close to an existing one. Therefore the average and maximum distances will not be significantly affected.

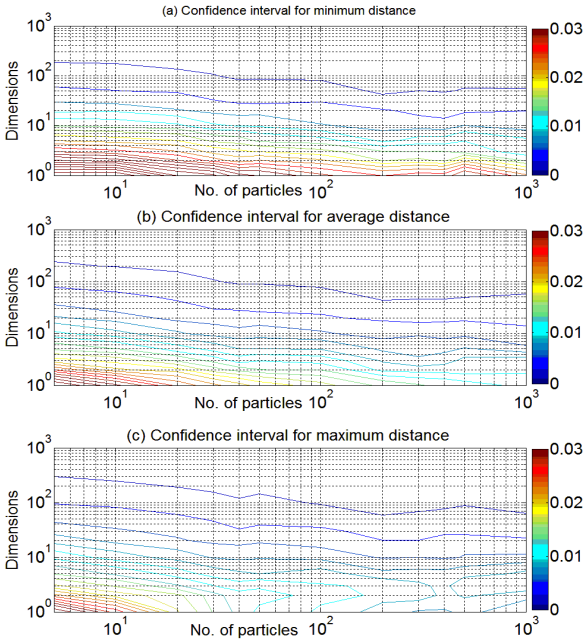

Figure 2: Confidence interval for particle distance, a) minimum, b) average and c) maximum.

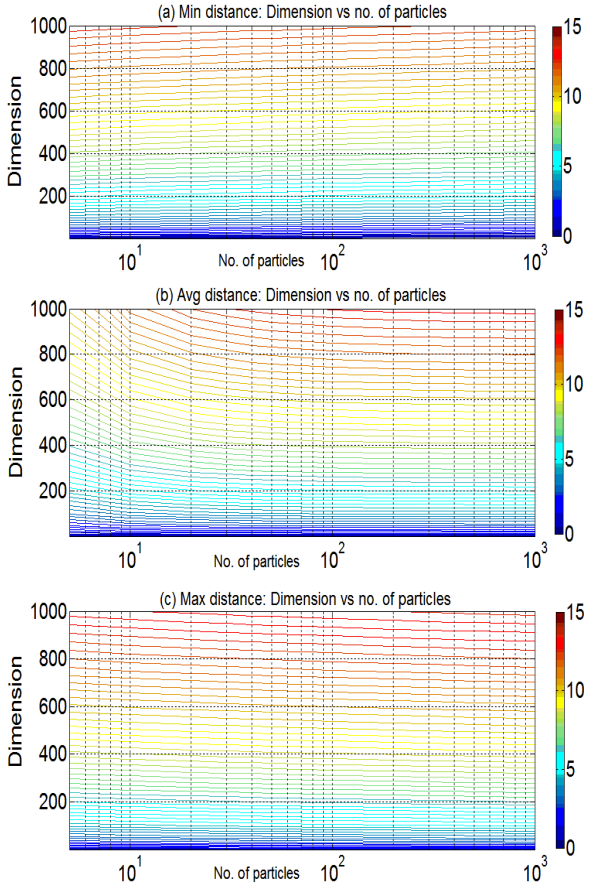

Figure 3: Inter-particles distances of every dimension for min, average and max distance.

The inter-particle distance for low numbers of dimensions is low and it increases with number of dimensions, due to the maximum possible inter-particle distance being proportional to the square root of the number of dimensions. The inter-particle distances for 100 and 1000 particles with 1000 realisations are summarised in Tables 3 and 4. For the range of 1 to 1000 dimensions, the minimum inter-particle distances for 100 particles are 0.0051 to 12.3406, the average and maximum distances are 0.3297 to 12.7776 and 0.7385 to 13.4612. Note that the values for 1000 particles are similar (except for the minimum at 1 dimension, which is a factor of 10 smaller as expected), indicating that this change in number of particles only affects the size of ensemble required to reduce errors.

Table 3: Summary of inter-particle distance for the particles (P) and dimensions (D): 100 particles.

(P,D)	(100,1)	(100,500)	(100,1000)
Minimum	0.0051	8.5575	12.3406
Average	0.3297	9.0344	12.7776
Maximum	0.7385	9.6796	13.4612

Table 4: Summary of inter-particle distance for the particles (P) and dimensions (D): 1000 particles.

(P,D)	(1000,1)	(1000,500)	(1000,1000)
Minimum	0.0005	8.3894	12.1760
Average	0.3317	9.1158	12.8952
Maximum	0.7476	9.8393	13.6237

5. Conclusions

The diffusion process in many turbulent combustion models is often simulated by mixing random pairs of particles. The distance between these particles is very important to ensure that locality of mixing occurs. Care must be taken that one particle does not repetitively mix with only one other (nominally the nearest), since their properties will at some stage reach their paired mean, terminating the mixing for that pair. To prevent this, it is necessary to randomise particle pairings by being less restrictive on the closeness of particle pairs without losing localness.

This study examined the inter-particle distance, implicitly used in popular turbulent combustion models, by generating ensembles of random particles. The analysis was carried out for up to 1000 particles, realisations and dimensions, showing the large variations as parameters are changed. By understanding the behaviour of the inter-particle distances, it may be possible to describe the shortcomings of models that neglect the diffusion length scale and devise new models that incorporate the diffusion length scale for potentially improved accuracy.

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7. References

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