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On the use of the Population Balance Equation for the Turbulent Transport of Polydispersed Inertial Particles

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Abstract

This paper presents a probability density function (PDF) form of the population balance equation (PBE) for polydispersed particles in turbulent flows and, for the first time, it includes explicit consideration of inertial effects in the PDF-PBE formulation. This model has wide application but has particular potential for understanding and improving liquid fuel spray in diesel engines. In this first step towards modelling inertial particles, the number density is taken as a function of particle size (volume) and velocity as well as space and time. Inertial effects are quantified through the Stokes number, leading to accurate modelling of the different trajectories that are followed by particles with different sizes. To treat these effects, a new affordable numerical approach is proposed which we call the *binned Stokes* method. In this approach, particles accelerate due to fluid dynamics forces associated with an averaged numerical Stokes number in each bin and hence the dimensionality of the model is determined by the number of such bins. A test case is constructed involving the turbulent jet dispersion of particles ranging in size from 1 μm to 100 μm. The results confirm the ability of the approach to accurately model the particle dispersion using as few as six Stokes bins thus offering the potential to greatly reduce the computational cost of the PDF-PBE equations for inertial particles.

Introduction

The transport of polydispersed particles in turbulent flows is relevant to many applications such as liquid spray fuel injection in diesel engines and gas turbines. An efficient liquid fuel injector can reduce the droplet size leading to shorter evaporation times, higher volumetric heat release rates, wider burning ranges and reduced pollutant emissions. The dynamics of droplets and other particles transported by a turbulent flow involves a complex series of inter-related phenomena including particle dispersion, surface growth (or shrinkage), breakage and agglomeration. In the present work we focus on modelling dispersion, noting it has a strong influence on the subsequent downstream processes [3]. Particles cannot be treated as point-like fluid tracers due to their mass density being, in general, vastly greater than that of the carrier phase. As a consequence of their size-related inertia, inhomogeneities develop in the particle spatial distribution, a phenomenon that is frequently referred to as preferential concentration [2]. The inertia of the dispersed phase also has a dissipative effect on the turbulence of the carrier.

Despite recent advances [1, 4, 8], the simulation of inertial particle dispersion remains challenging, not least because of the difficulty of capturing the preferential concentration in a computationally tractable fashion. For example, the PDF method of Bini and Jones [3] incorporates inertial particles on size dependent numerical parcels whereby the number of parcels is not fixed but can increase greatly due to growth, breakage and agglomeration making computational load balancing next to impossible. This problem increases exponentially as additional characteristics of the inertial particles (e.g. shape and morphology) are added. The population balance equation (PBE) approach postulates a number distribution of a dispersed phase with the physical properties introduced as internal coordinates of the number density function thus allowing, at least in its mathematical formulation, representation of polydispersed distributions on a fixed but possibly large computational grid. Nearly six decades ago Williams [12] provided a number density derivation for sprays and several more recent reviews of the PBE for a range of physical applications exist in the literature [7, 9, 10]. Rigopolous extended the PBE method to turbulent flows by introducing the probability density function (PDF) of the PBE (termed PDF-PBE) [9, 10]. To the best of our knowledge applications of the PBE, including applications in turbulent flows, have been limited to cases where the relative velocity between the continuous and dispersed phases may be neglected [9]. As a result, particles travel with the carrier fluid velocity regardless of their size or shape. However, this assumption cannot be justified where the effects of inertia on particle motion are significant. To summarise the situation, the mathematical formulation of the PBE approach offers the potential of modelling the turbulent transport of polydispersed inertial particles but currently lacks a tractable computational method for solution when the particle dynamics involve inertial forces due to multiple physical characteristics of the particles.

The objective of this paper is to present a novel PDF-PBE approach that explicitly addresses inertial effects in a computationally tractable way. The governing equations are presented in general form but in this first step, the validation study focuses on the dispersion of inertial spherical particles of different sizes in a turbulent flow while neglecting growth, breakage and agglomeration.

The PDF-PBE model for inertial particles

The PBE governs the evolution of the particle number density function, N, in a phase space, R. The latter is decomposed into the coordinate space, $\boldsymbol{x} = (x_1, x_2, x_3)$, and the property (or state) space, $\boldsymbol{\xi} = (\xi_1, \dots, \xi_M)$, which can include particle size (commonly, volume), shape, surface area, etc. It may also include flow dependent quantities such as particle velocity to quantify inertial effects. $N(\boldsymbol{x}, \boldsymbol{\xi}, t) d\boldsymbol{x} d\boldsymbol{\xi}$ is defined as the ensemble of entities having coordinates in the range $(d\boldsymbol{x}, d\boldsymbol{\xi})$ around $(\boldsymbol{x}, \boldsymbol{\xi})$ at a given time, t. Using this definition, the PBE is written as [11]

$$\frac{\partial N}{\partial t} + \nabla_x(\boldsymbol{U}N) + \nabla_\xi(\dot{\boldsymbol{\xi}}N) = \nabla_x(D_x \nabla_x N) + \nabla_\xi(D_\xi \nabla_\xi N) + W, \quad (1)$$

where $\boldsymbol{U}(\boldsymbol{\xi}; \boldsymbol{x}, t)$ and $\dot{\boldsymbol{\xi}}(\boldsymbol{\xi}; \boldsymbol{x}, t)$ are the time rates of change in the physical and the property spaces, respectively, and $D_x(\boldsymbol{\xi}; \boldsymbol{x}, t)$ and $D_\xi(\boldsymbol{\xi}; \boldsymbol{x}, t)$ are the diffusion coefficients accounting for random thermodynamic fluctuations (e.g. Brownian motion) in those spaces. The source term, W, is the net outcome of discrete births and deaths of particles due to breakage and agglomeration.

The eventual goal of our research is to have a computational model for secondary atomisation of injected fuel. The physics of that problem allow us to simplify the above general formulation of the PBE. Experimental evidence of secondary atomisation [5] indicates that droplets may be characterised by size and shape. In this initial work we consider only spherical particles thus eliminating shape as a state variable i.e. $\boldsymbol{\xi} = (V)$. As is normal practice [11] it is assumed that $D_{\xi} = 0$, while D_x may also be neglected as it approaches zero for inertial particles. Further, growth due to evaporation and condensation is neglected due to it having a small effect relative to breakup in the secondary atomisation zone of an internal combustion engine. Hence, the PBE can be rewritten as

$$\frac{\partial N}{\partial t} + \nabla_{\boldsymbol{x}}(\boldsymbol{U}N) = W. \tag{2}$$

Various models for W are suggested in the literature [6]. Although we set the source to zero in the dispersion validation study below, we retain W in the derivation in order to demonstrate the closed form treatment of this highly non-linear term in the context of PDF methods.

Equation (2) holds for either laminar or turbulent flows although for the latter a numerical method to solve it directly needs to resolve all the scales of turbulence. Continuum DNS of particle laden flows has an even greater cost than single-phase DNS as one must resolve down to the Batchelor scale $\eta_B = \eta/\sqrt{Sc}$ where η is the Kolmogorov scale and $Sc \gg 1$ is the Schmidt number of the inertial particles. For practical simulations some form of averaging or statistical emulation of the turbulent field is required. We adopt a hybrid approach. Large eddy simulation (LES) is employed for the carrier phase whereby the large scale motions are resolved while the subfilter scales are modelled. An LES (i.e. filtered) version of Eq. (2) can also be derived but it introduces multiple unclosed terms for the non-linear fluid-particle interactions with closure of the filtered source term being particularly problematic. Following Rigopoulos [9] the subfilter fluctuations of the PBE are solved using a PDF method. The novelty of the present work is to introduce inertial effects into the PDF-PBE for the first time. The continuous number density function is approximated as a set of classes where each class represents a subset of the turbulent distribution of number densities. Each class includes a range of droplet sizes having similar inertial effects and the relevant velocity of this class is represented by $\boldsymbol{U_\alpha}$. The combination of classes reproduces the entire turbulent distribution.

The turbulent distribution of each set is represented by the filtered one-time, one-point joint PDF of number density $\overline{F_N}(\boldsymbol{n_\alpha}; x, t)$, where $\boldsymbol{n_\alpha}$ is the sample space for $\boldsymbol{N_\alpha}$. Significantly, W is not filtered but instead appears naturally in exact form. $\overline{F_N}$ is highly dimensional making solution via a finite volume scheme intractable. Instead the PDF is represented by an ensemble of statistically independent notional particles which are computational elements that should not be confused with real inertial particles. The notional particles evolve according to stochastic differential equations

$$d\boldsymbol{x}^{(p)} = \boldsymbol{U}^{(p)}\, dt \tag{3}$$

$$d\boldsymbol{U}^{(p)} = \boldsymbol{A}dt = -\frac{1}{\tau_p}\left(\boldsymbol{U}^{(p)} - \overline{\boldsymbol{\mathcal{V}}}^{(p)}\right)dt + \frac{\rho_p - \overline{\rho_f}}{\rho_p}\boldsymbol{g}dt + \sqrt{b}d\boldsymbol{w} \tag{4}$$

$$d\boldsymbol{N}^{(p)} = \boldsymbol{W}^{(p)}dt. \tag{5}$$

The superscript (p) denotes values on, or at the location of, the notional particles. The deterministic part of acceleration due to the drag force is only considered here and hence the acceleration is $-\frac{1}{\tau_p}\left(\boldsymbol{U}^{(p)} - \overline{\boldsymbol{\mathcal{V}}}^{(p)}\right)$ where $\overline{\boldsymbol{\mathcal{V}}}$ is the LES filtered carrier velocity and τ_p is the response time due to fluid-particle interaction forces and for spherical particles of dimeter d_p may be defined as

$$\frac{1}{\tau_p} = \frac{6}{8}\frac{\overline{\rho_f}}{\rho_p}\frac{C_D}{d_p}\left|\boldsymbol{U}^{(p)} - \overline{\boldsymbol{\mathcal{V}}}^{(p)}\right| \tag{6}$$

where ρ_p and $\overline{\rho_f}$ are the dispersed phase density and the LES filter density, respectively. C_D is the drag coefficient modelled for spherical particles as [3]

$$C_D = \begin{cases} \frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right) & \text{for } 0 < Re < 1000 \\ 0.424 & \end{cases} \tag{7}$$

where $Re = \left|\boldsymbol{U}^{(p)} - \overline{\boldsymbol{\mathcal{V}}}^{(p)}\right| d_p/\nu$ is the Reynolds number.

Binned Stokes Method

If the dispersed phase was not subject to inertial forces it would be possible to solve Eq. (3) – (4) on an ensemble of notional particles where each particle represents a single turbulent realisation of the entire number density function. However, since inertial forces are important it is not possible to use a single notional particle moving at a certain velocity to represent the number density function over a large range of inertial particle sizes. The brute force, and therefore expensive, option is to ensure that each notional particle represents only one size class and as the inertial particles breakup additional notional particles are added. This is essentially the method used by Bini and Jones [3] although their method was not derived from the point of view of the population balance equation. Computational cost in that approach can easily grow by two orders of magnitude and more viable methods are required.

The effects of inertia are usually quantified through the Stokes number defined as $St = \frac{\tau_p}{\tau_f}$ where τ_f is the fluid characteristic time scale. The Stokes number expresses the response of an inertial particle to changes in the carrier flow (e.g due to eddies). Particles with different sizes experience a different drag force and therefore exhibit different accelerations. For $St \ll 1$, particles have small inertia, quickly accelerate to the local flow velocity and thus closely follow the flow streamlines. For $St \gg 1$, particles have large inertia and are increasingly less affected by the variations in the carrier flow. We can therefore define specific Stokes number ranges (or bins) in which inertial particles may be assumed to have the same dynamic response to the carrier flow. In the *binned Stokes* approach for our PDF-PBE model individual notional particles represent the number density for inertial particles within a single bin and the acceleration is obtained according to an average Stokes number for that each bin. An optimal choice of the Stokes bins can reduce the required number of notional particles leading to a significant reduction in computational cost compared to brute force method while maintaining a high level of accuracy. Our aim is to develop a rigorous procedure for selecting the Stokes bins for any range of inertial particles sizes. Eq. (4) can be integrated in fractional steps. Here we deal with the first term which accounts for the inertial forces through the time scale, τ_p, and the slip velocity. Integration of this term over the flow time scale, τ_f, yields

$$\boldsymbol{U}^{(p)}(t + \tau_f) = \overline{\boldsymbol{\mathcal{V}}}^{(p)} - \left(\overline{\boldsymbol{\mathcal{V}}}^{(p)} - \boldsymbol{U}^{(p)}(t)\right) exp\left(-\frac{\tau_f}{\tau_p}\right) \tag{8}$$

It can be seen that the particle acceleration is governed by an exponential function, $g = exp\left(-\frac{1}{St}\right)$. Figure 1 shows this function versus the St number. For low Stokes number the function asymptotes to zero indicating that any slip velocity will result in a particle immediately accelerating to match the carrier flow. We choose $St = 0.25$ corresponding to $g \approx 0.02$ as a lower cut-off with particles in the range $0 < St < 0.25$ deemed to be non-inertial. For large Stokes number the function asymptotes to unity indicating that a particle is not sensitive to a slip velocity. We choose $St = 50$ corresponding to $g \approx 0.98$ as an upper cut-off with the trajectory of particles in the range $50 < St < \infty$ deemed to be non-responsive to fluid-particle interactions. All particles in either of these Stokes ranges can be binned for determining their dynamic response to the flow.

The interval $0.25 < St < 50$ exhibits strong fluid-particle interactions and it is not obvious a priori how particles in that range should be binned (i.e. number and spacing) but obviously we want the minimum possible number of bins while maintaining accuracy. Our testing has revealed that constant spacing in logarithmic space $\Delta(\log St)$ works best with a series of numerical trials conducted below to find the optimum number of equally sized bins. To illustrate Fig. 1 shows bins corresponding to $\Delta(\log St) = 0.57$ obtained from five points on the curve resulting in six bins in total (including the non-inertial and non-responsive bins in the low and high Stokes limits). Since the shape of the function g is unaffected by the range of Stokes numbers accessed in any particle laden flow, it is only necessary conduct the tests once for a range of flow types to determine the optimum value of Δ. The number of Stokes bins in a given computation is then dependent only on the Stokes number range that is present.

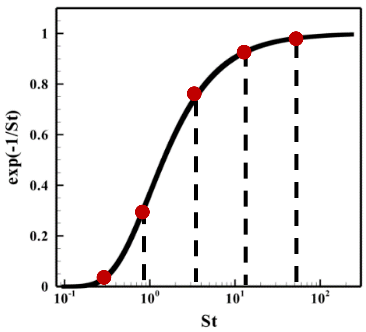

Figure 1. Exponential function g versus St number.

Test Cases Studied and Numerical Setup

To validate the postulated Stokes binning method for the PDF-PBE we construct a numerical test case of inertial particle dispersion in a turbulent mixing layer. For this purpose, the evolution of a relatively high velocity air jet at atmospheric pressure is simulated using a compressible LES code with a standard Smagorinsky subgrid model implemented in an open source C++ code known as OpenFOAM. The mean jet velocity is 50 m/s whereas the coflow velocity is 1 m/s. The jet diameter, D, is 4 mm. The computational domain is a three-dimensional rectangular mesh of 20D in the axial direction and 10D in both transverse directions. Time-varying realistic turbulent velocity boundary conditions are applied for the inflow jet based on a turbulence intensity of 15% and an integral length-to-jet diameter ratio of 0.125. The hexahedral mesh has about 1M cells uniformly distributed in all directions with a mesh size of 0.5 mm. Once a statistically stationary carrier flow was obtained, inertial particles with different diameters were homogenously injected from the jet with the mean jet carrier velocity. For simplicity, the effects of the inertial particle motions on the carrier phase are not taken into account. The particles have uniform density of 780 kg/m^3 (typical of hydrocarbon fuels) and a mass loading is 0.2 g/s. The main case consists of particles size ranging from 1 μm to 50 μm. Two additional cases with particle sizes in the range 1-100 μm and 1-10 μm are also considered. Table 1 shows the range of (numerical) St number obtained based on a numerical time step of 20 μs, for each set of particle size. For each case the simulation was initially conducted without binning followed by simulations with Stokes binning with progressively smaller bin sizes.

d (μm)	Stokes number
1-50	0.097-220
1-100	0.097-900
1-10	0.097-11

Table 1. Stokes number range for each set of particle size

Results and Discussion

Figure 2a, b, and c show liquid particles concentration at 2 ms after injection for various range of diameters presented in Table 1. Each point represents a liquid particle accelerated based on Eq. (8). The particles are coloured by their diameter. As presented in Fig. 2a and b, the heavy (larger) particles mostly corresponding to high Stokes numbers follow their own trajectories and they are simply convected downstream with only a slightly detectable response to fluid-particle interactions. While light particles with small Stokes numbers follow the fluid pattern and disperse from the centreline. On the contrary, as shown in Fig. 2c, a larger numbers of particles follow the carrier fluid streamlines when the range of particles size is from 1 μm to 10 μm. Figure 2d presents dispersion of particles with the same size range shown in Fig. 2c (1-10 μm), however, all particles, regardless of their St number, have been forced to follow the carrier flow. The level of dispersion for this case is similar that that in Fig. 2c where particles accelerate according to their St number.

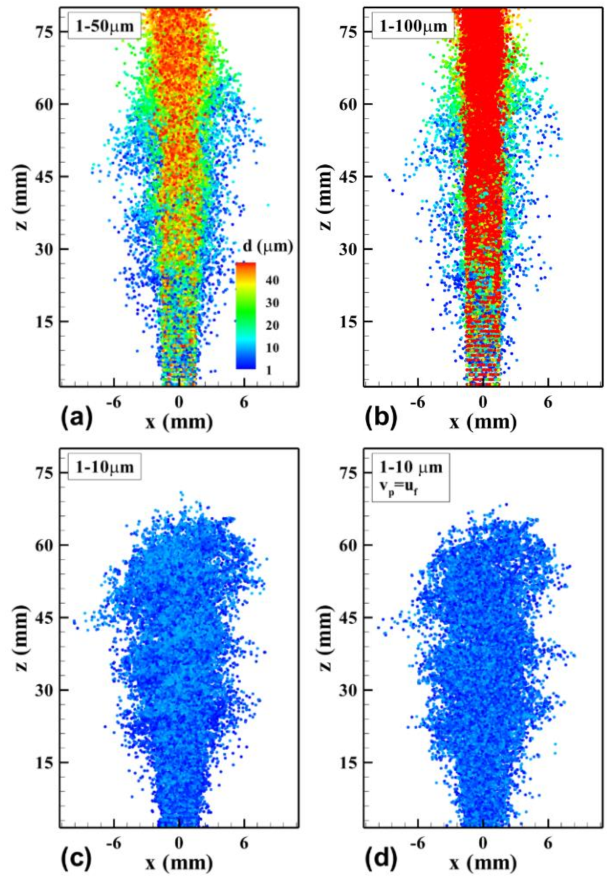

Figure 2. Particle distribution where particles move based on Eq. (9) for particles ranging in size of a) 1 μm-50 μm, b) 1 μm-100 μm, and c) 1 μm-10 μm and d) Particle distribution where particles move with the carrier fluid velocity for particles ranging in size of 1 μm-10 μm.

To demonstrate the optimal number of Stokes bins, we repeat the simulation with Stokes bins included. As shown in Table 2, we consider 3, 5 and 7 internal St points (corresponding to 4, 6 and 8 bins). The last row shows St points where Δ is same as 7-points while the St points smaller than 1 are neglected and hence less St bins are required. This will discussed later.

Figure 3 presents radial profiles of axial velocity root mean square (v_{rms}) and particle diameter root mean square (d_{rms}) at an axial location 60 mm downstream of the jet exit plane. Symbols present results of the original (unbinned) solution while lines show results obtained with the binning method. It can be seen that d_{rms} changes only marginally as the number of bins increases while v_{rms} obtained using the binned method is sensitive to the number of bins but quickly converges as the number of bins is increased. The results obtained using Δ=0.38 are in an excellent agreement with the unbinned solution. As demonstrated in Fig. 2, particles with small St number follow the carrier flow trajectories and it is expected that fewer bins are required where $St < 1$. To confirm this, the results for Δ=0.38 but five points are also presented in Fig 3. It can be seen that they are very similar to the results obtained using seven points and Δ=0.38. It confirms five Stokes points are sufficient and lead to an excellent agreement for calculated v_{rms}.

For other cases, results are only shown for the 5-points and Δ=0.38. Similar profiles are presented in Fig. 4 and 5 for the cases including particles of 1-100 μm and 1-10 μm, respectively. It can be seen that for both diameter ranges, the results obtained using the Stokes binned method agree very well with the original results for individual particles.

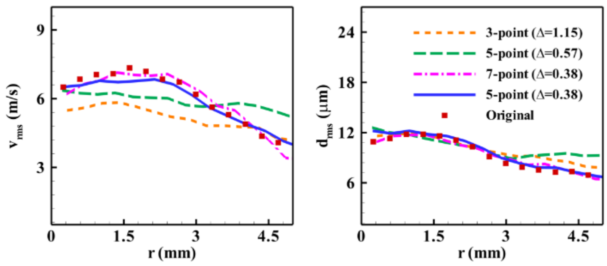

Figure 3. Radial profiles of v_{rms} and d_{rms} (1-50 μm). Symbols, original (unbinned) solution; lines, binned solutions.

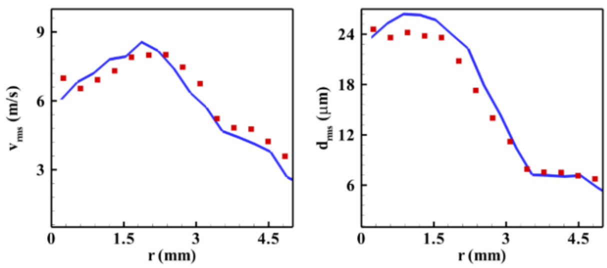

Figure 4. Radial profiles of v_{rms} and d_{rms} (1-100 μm). Symbols, original (unbinned) solution; lines, binned solution (5-points Δ=0.38).

Conclusions

This paper presented a PDF form of PBE for polydispersed inertial particles. A novel numerical method based on Stokes binning is proposed to explicitly include effects of inertia into the PDF-PBE for the first time. In this approach, particles accelerate according to an average Stokes number obtained within bins. The method was investigated using a test case involving the turbulent jet dispersion of particles ranging in size from 1 μm to 100 μm. The results confirm the ability of the approach to accurately model the particle dispersion using as few as six Stokes bins thus offering the potential to greatly reduce the computational cost of the PDF-PBE equations.

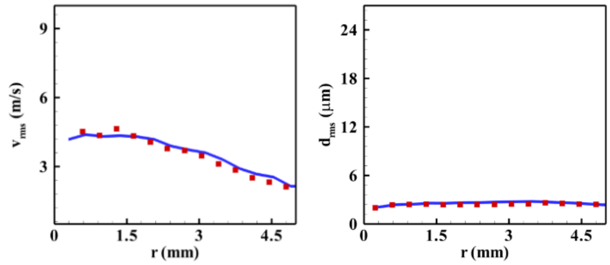

Figure 5. Radial profiles of v_{rms} and d_{rms} (1-10 μm). Symbols, original (unbinned) solution; lines, binned solution (5-points Δ=0.38).

Acknowledgments

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