Reconstructing Polydispersed Multi–Phase Flow Joint Probability Density Functions Using The Maximum Entropy Method

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Moment transport methods are being developed to model polydispersed multi–phase flows by transporting statistical moments of the particle size–velocity *joint probability density function* (JPDF). A common feature of these methods is the requirement to reproduce the form of the JPDF from the transported moments for calculation of body force terms and closure of higher order moments. Two approaches that have been proposed are the use of a modified Rosin–Rammler size distribution parameterised by the transported moments of the particle size PDF, and the *maximum entropy formulation* (MEF) which uses the transported moments to constrain the JPDF of least bias. This paper examines the application of the MEF technique to real *phase doppler anemometry* (PDA) data sets from an electrostatically charged kerosene spray and attempts to assess which moments are required to reproduce the JPDFs to a sufficient level of accuracy. It is possible to reproduce the JPDFs to a high level of accuracy using a large number of moments, however, this is likely to incur large computational overheads. If the moments to be transported are chosen on the basis of physical reasoning (such as the relationship between size and velocity due to drag) it is possible to reduce the number of moments it is necessary to transport to obtain a reasonable approximation to the experimental distribution.

1 Introduction

1.1 Background

Dispersed multi–phase flows describe the transport of mass in the form of particles dispersed within a gas or liquid carrier phase. Typically, individual particles within a dispersed multi–phase flow may be characterised by position, velocity, diameter and temperature at any point in time. In a typical industrial application (such as diesel injection in an internal combustion engine) the flow may consist of millions of particles which interact with each other and with the carrier phase. The high dimensionality and complex interactions found in practical multi–phase flow applications provide many challenges for engineers attempting to predict these flows computationally. Several different

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models have been developed for this purpose, based around the two continua (Eulerian–Eulerian) and discrete particle (Eulerian–Lagrangian) methods. For poly–sized multi–phase flows the Eulerian–Eulerian method has traditionally been less popular due the computational penalties incurred by having to 'bin' the particle diameter and transport each 'bin' as a separate interpenetrating phase. Less obviously, the Lagrangian particle tracking method suffers from the drawback that it requires the injection of many particle 'packets' before meaningful statistical information can be obtained throughout the whole of the spray plume.

Moment transport methods, a subset of a general PDF approach, have been available at a theoretical level for several years and have recently been applied (in differing forms) by Archambault and Edwards [1, 2]; Beck and Watkins [3–5]; and White and Hounslow [6]. The moment transport method offers the possibility of modelling the dynamics of the dispersed particle phase by transporting the statistical moments of a particle state JPDF. Clearly, for accurate and efficient simulation of dispersed multi–phase flows using a moment transport model, it is essential to transport the required statistical moments accurately and economically.

1.2 Single Point Statistics and JPDFs

The foundation for the moment transport methods is the concept of a single point statistical description of a spray, comprehensive details of which can be found in Edwards and Marx [7] and Subramaniam [8]. Single point statistics describe the stochastic processes within a spray at any single spatial location at a particular time in terms of JPDFs of dependent variables [9].

When describing a spray using a JPDF we would typically have $f(\mathbf{x}, \mathbf{v}, \phi)$ for a polydispersed non vaporising spray, where $\mathbf{x}$ is spatial location, $\mathbf{v}$ is particle velocity and ϕ is particle diameter. The particle JPDF of size and velocity in dispersed multi–phase flows are generally non–gaussian and will probably require higher order moment modelling to encompass the complexity and non–symmetrical character of the distribution.

1.3 The Spray Equation and Moment Transport Equations

If an intensity based statistical description of the spray is used [1, 7] we can define the JPDF for obtaining a particle at a particular time and spatial location[1] as $\lambda(\mathbf{x}; t)$. If we choose (for the sake of simplicity) to restrict our particle characteristics to velocity, position and diameter we can define a normalised JPDF that describes the probability of finding a particle of particular velocity and size, conditioned on the existence of a particle at a particular spatial location and time, $f(\mathbf{v}, \phi; \mathbf{x}, t)$. The expressions for spray intensity, λ, and particle characteristics, f, can be combined to form an unnormalised single particle distribution function for the spray, F.

$$F(\mathbf{v}, \phi, \mathbf{x}; t)\, d\mathbf{v}\, d\phi\, dV = \lambda(\mathbf{x}; t)\, f(\mathbf{v}, \phi; \mathbf{x}, t)\, d\mathbf{v}\, d\phi\, dV. \tag{1}$$

From this single point statistical description of the spray it is now possible to derive

[1] It should be noted that this expression is also the expected number density of particles in space and time and consequently is a measure of concentration and not strictly a PDF because it is not normalised.

a general transport equation for F, more commonly known as the spray equation, first performed by Williams [10]. If we once again restrict the particle state vector to size, position and velocity and ignore source terms (such as collisions and breakup) we obtain the following version of the spray equation using the same nomenclature as Archambault [1].

$$\frac{\partial F}{\partial t} + \nabla_x \cdot (F\mathbf{v}) + \nabla_v \cdot (F\mathbf{a}) = 0. \tag{2}$$

The spray equation describes the evolution of the particle JPDF, F, through phase–space. From this equation we can derive transport equations for the moments of f that represent physical quantities that define the problem of interest. Transportation of the statistical moments does not suffer from the drawback of statistical bias.

Multi–phase moment transport methods are still in the early stages of development and many issues remain unresolved. Specifically, difficulties are encountered when attempting to evaluate body force terms such as particle drag forces, breakup and collisions. To evaluate these terms the complete form of the particle size–velocity JPDF is required and for moment transport models we must reconstruct the JPDF from the available information. In the case of interphase drag, it is important to achieve an accurate representation of the JPDF because although the 'tail' of the size–velocity JPDF contains relatively few particles their mass fraction is relatively large. Consequently apparently small inaccuracies in the JPDF tail can lead to large errors in the overall multi–phase prediction.

Previous work in this area has adopted two different methods for the reconstruction of the JPDF. Beck [3] approximates the particle size distribution using a modified form of Rosin–Rammler distribution, parameterised by two of the transported moments. Archambault [1] outlines the use of the *maximum entropy formulation* [11] (MEF) to calculate the higher order moments, required for closure, using the transported moments of the droplet size-velocity JPDF. Of these two methods the MEF method appears to offer promise for both the present problem and for future ones. It can be easily extended to incorporate additional or higher order moments for greater accuracy and additional phase–space dimensions for JPDFs of higher dimensions at some increase in cost. However, to date little research has been conducted to quantify the suitability of the MEF method to this application. If the moment transport method is to provide a reliable and accurate alternative to the established spray modelling techniques, it necessary to assess the performance of the MEF technique in terms of accuracy, reliability, computational efficiency and computational stability.

Transportation of higher order moments is accompanied by significant computational burdens. It is therefore appropriate to first analyse the accuracy of JPDF outputs from the MEF procedure using different levels of constraints. This paper attempts to reconstruct real particle JPDFs using statistical moments calculated from experimental PDA data with the specific objective of determining how many, and which moments are required to reproduce, using the MEF technique, JPDFs at a satisfactory level of accuracy.

2 The PDA Data

For the purpose of this investigation PDA data providing the correlation of v_x, v_y and ϕ for a steady electrostatically atomised kerosene fuel spray were investigated. The atomiser has an orifice diameter of $d_o = 250\,\mu m$, a flow rate of $\dot{Q} = 1.67\,mls^{-1}$ and charge density of $\rho = -1.8\,Cm^{-3}$ [12].

JPDFs were constructed from the PDA data by 'binning' the diameter and velocity axis, and calculating the droplet frequency in each of these bins. For comparison between the experimental distributions and the MEF predictions for the charged spray, a data point on the spray axis 150 mm from the injector has been selected for presentation in this paper. The charge field on the spray axis is zero, thus any electrostatic effect may be neglected for this position. An example JPDF for a point on the axis 150mm downstream of the nozzle is presented in figure 1.

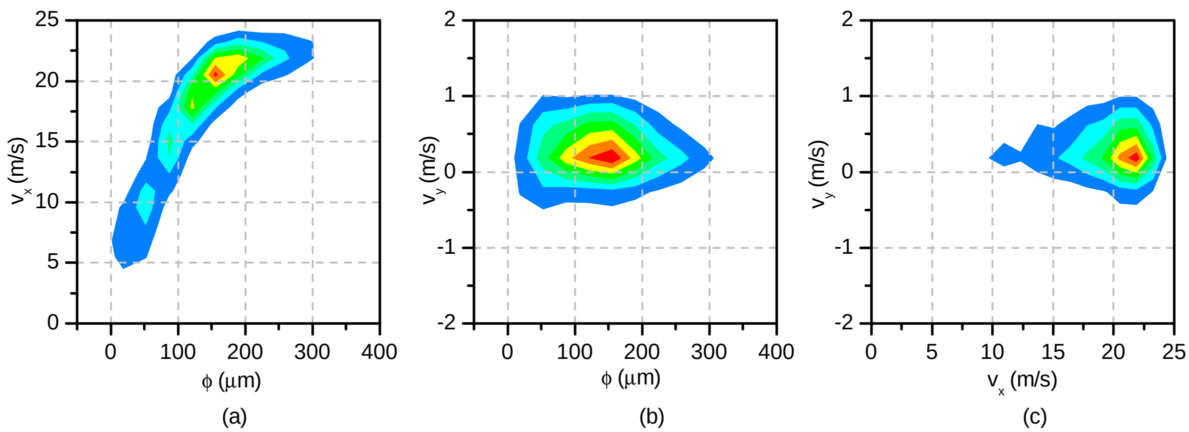

Figure 1: JPDF contour plots calculated from PDA data for position $z = 150\,mm, r = 0\,mm$. (a) $\phi - v_x$ (b) $\phi - v_y$, (c) $v_x - v_y$.

Figure 1(a) shows the non–linear relationship between droplet diameter and axial velocity with the larger 'ballistic' droplets travelling with higher velocity than the smaller droplets. The JPDF of droplet size and radial velocity in figure 1(b) shows an approximately Gaussian distribution with zero average velocity. This is to be expected because the point chosen is on the spray axis. The small transverse velocities can be assumed to be due mainly to turbulent 'diffusion' because negligible electric field should be present at this position and hence repulsive forces are small.

The JPDFs in figure 2 are more complicated due to influence of electrostatic charge effects. Modelling these details using the MEF method is more challenging and will most likely require higher order moments.

Using the distributions obtained from the discrete measurements, statistical moments of the distribution for use as constraints in the MEF code may be easily calculated according to

$$\langle A_r \rangle = \sum_i p_i A_{ri}, \tag{3}$$

where $\langle A_r \rangle$ is a moment of the JPDF, A_{ri} is an arbitrary function of the variables ϕ, v_x or v_y evaluated at location i in phase space and p_i is the probability at this location.

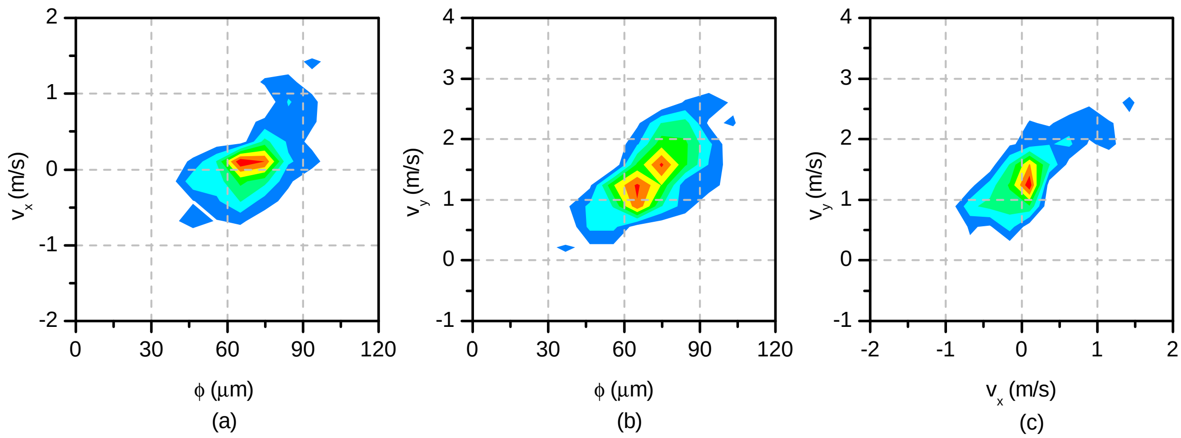

Figure 2: JPDF contour plots calculated from PDA data for position $z = 120\,mm, r = 40\,mm$. (a) $\phi - v_x$ (b) $\phi - v_y$, (c) $v_x - v_y$.

3 MEF Closure

3.1 Mathematical Background

The application of the maximum entropy formulation to spray modelling is not a new concept and has been previously to predict drop size distributions from primary atomisation [13]. The basis of MEF was established by Shannon [14] who showed that the entropy, S, for a discrete probability distribution, p_i, is given by the following expression

$$S = -\sum_i p_i \ln p_i. \tag{4}$$

The application of the maximum entropy principle for a PDF was first proposed by Jaynes [15] who showed that, given a set of M constraints of the form give in equation 5, the PDF that should be chosen is the distribution with maximum entropy.

$$\sum_i p_i = 1, \qquad \text{and} \qquad \langle A_r \rangle = \sum_i p_i A_{ri}, \qquad r = 1, \ldots, M. \tag{5}$$

The solution of maximum entropy problem can be achieved using the method of Lagrange multipliers, however this requires the solution of a set implicit non–linear equations. For problems of several phase–space dimensions with multiple constraints, solutions can be difficult to achieve and computationally expensive. An alternative to this method is to formulate a variational solution using the Lagrange multipliers as variational parameters. For the purposes of this investigation the method of Alhassid et al. [11] has been used in conjunction with a simplex minimisation algorithm [16]. The MEF code was tested by generating a multi–dimensional JPDF using a gaussian random number generator, taking the moments of this distribution, using these moments as constraints in the MEF code and comparing the results. Good correlations between distributions was achieved. Once the code was verified it was possible to generate MEF distributions using moments calculated from the PDA data sets shown in figures 1 and 2.

3.2 JPDFs constructed from MEF

Figures 3 and 4 show the JPDFs calculated from the PDA data compared with MEF distributions calculated with varying numbers of constraints. Each figure shows contour plots of the JPDFs of size with axial velocity (a), size with transverse velocity (b), and axial velocity with transverse velocity (c). Within each JPDF plot are four sub–plots of (i) the PDA data only (ii) MEF approximation using only central moments up to the sixth order (iii) MEF approximation using many moments and (iv) MEF approximation using a reduced set, where the aim is to achieve a reasonable representation of the JPDF with less computational effort.

When only central moments are used as constraints the MEF distribution is capable of reproducing the Gaussian nature of the size – transverse velocity JPDF (figure 3b(ii)) and the elongation shown in the axial – transverse velocity JPDF (figure 3c(ii) for the first spray location. Although the central moments reproduces the asymmetry of size – axial velocity JPDF (figure 3a(ii)), it is not capable of reproducing the non linear relationship between these variables and to do this accurately it is necessary to introduce higher order cross moments as shown in figure 3a(iv). Attempts were made to obtain a reasonable approximation to the PDA data using a reduced set of constraints. Sub–plot (iv) of figure 3 shows the MEF approximation using the first (mean) and second order central moments of each variable as constraints in addition to the $\langle \phi v_x \rangle$ cross–moment. Although using this reduced set of constraints has the disadvantage of losing the capability of modelling the asymmetry and elongation of the distributions it still makes a reasonable approximation to the original PDA data with reduced effort.

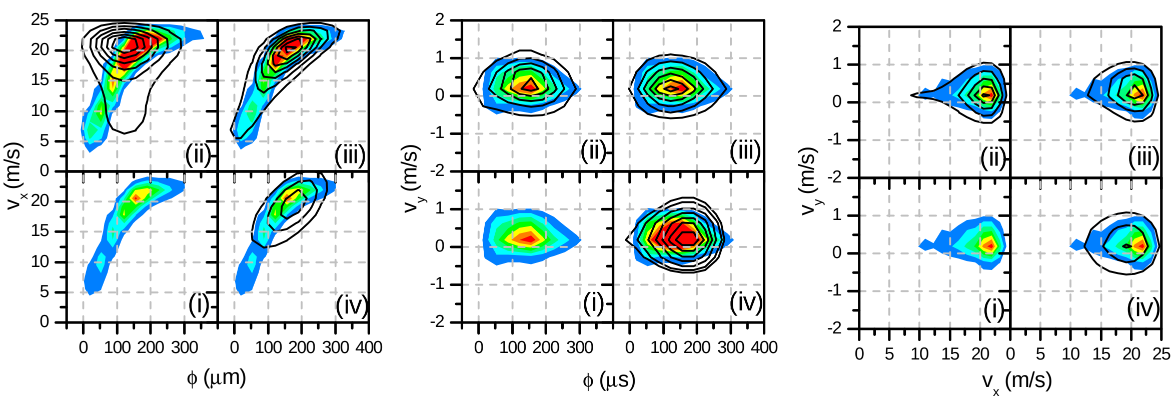

Figure 3: JPDFs calculated for position $z = 150\,mm, r = 0\,mm$. (a) $\phi - v_x$ (b) $\phi - v_y$, (c) $v_x - v_y$. (i) PDA data, (ii) Central moments only, (iii) with cross moments (iv) selected moments.

The distributions illustrated in figure 4 all show Gaussian characteristics. These plots show that there is little to be gained by modelling higher order moments for this position. Using only central moments (ii) and higher order cross–moments both give good approximations but acceptable distributions are achieved using only second order central moments in addition to $\langle \phi v_x \rangle$, $\langle \phi v_y \rangle$ and $\langle v_x v_y \rangle$ cross moments.

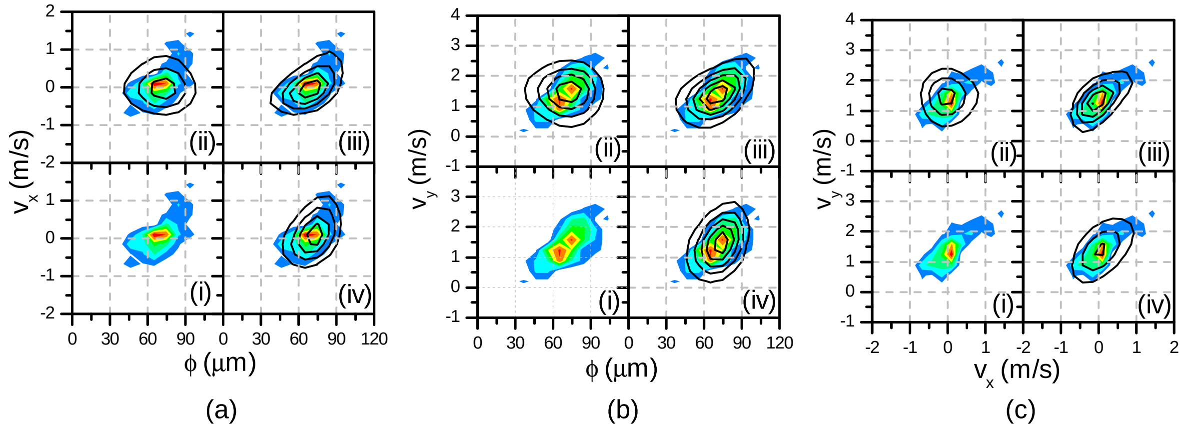

Figure 4: JPDFs calculated for position $z = 120\,mm, r = 40\,mm$. (a) $\phi - v_x$ (b) $\phi - v_y$, (c) $v_x - v_y$. (i) PDA data, (ii) Central moments only, (iii) with cross moments moments (iv) selected moments.

3.3 Error calculation

The measure of the error between the PDA and MEF distributions was calculated separately for each position by summing the square of the differences at each location in the domain as shown in equation 6

$$\varepsilon = \frac{1}{n^2} \sum_i \sqrt{(p_i^{PDA} - p_i^{MEF})^2}, \tag{6}$$

where n is the number of 'bins' along each axis and hence n^2 points exist in the domain for each JPDF. Figure 5 shows the error plotted as a function of the central moment order for the two positions in the spray.

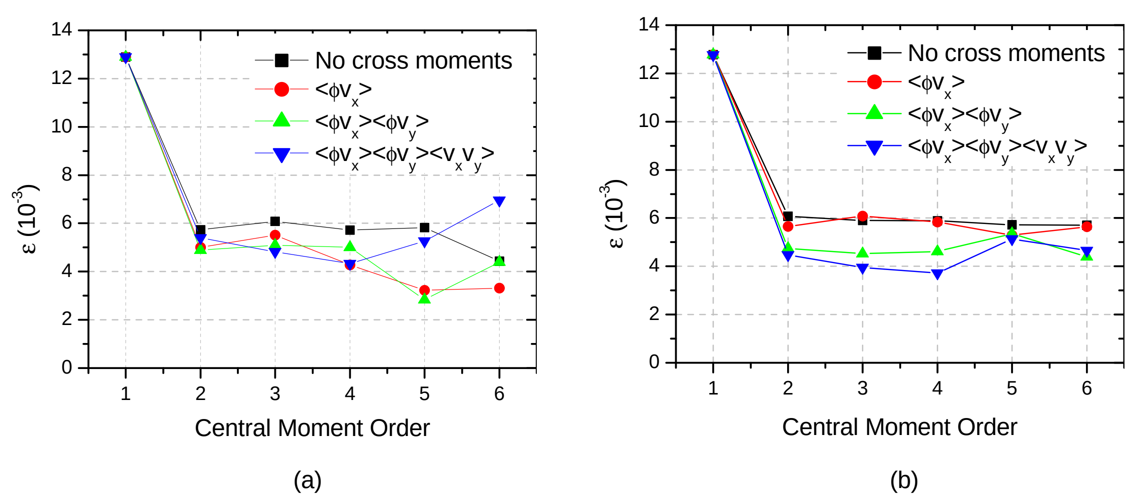

Figure 5: Measure of the error, ε, between the PDA and MEF distributions for increasing order of central moments and with additional cross moments as indicated. (a) position $z = 150\,mm, r = 0\,mm$ (b) position $z = 120\,mm, r = 40\,mm$.

Figure 5 shows a large reduction in the error when increasing the constraint order from one to two. This is to be expected because this effectively changes the MEF distribution from and exponential to Gaussian approximation to the 'real' PDA distribution.

The trend as higher order moments are added is a reduction in the error. There are exceptions to this trend where the addition of higher order moments increases the error. This may due to the increased rigidity of the MEF solution as additional moments are added. The MEF code attempts to find the distribution of maximum entropy for a given set of constraints, and this is not necessarily the distribution that most accurately reproduces the PDA data. Figure 5 also shows the effect of the adding cross–moments $\langle \phi v_x \rangle, \langle \phi v_y \rangle$ and $\langle v_x v_y \rangle$. For low order central moments the addition of these constraints can significantly reduce the error.

4 Conclusion

Comparisons between real JPDFs obtained from experimental PDA data and MEF reconstructions show that the MEF method is capable of reasonably accurate approximations to the JPDFs. The accuracy of the MEF method increases as additional constraints are added, although this has the drawback of the increased computation time necessary for solution. If constraints are selected on the basis of physical reasoning reasonable approximations can be achieved with less effort. Future work should look at the inclusion of constraints that represent physical features of the flow such as droplet drag.

The work documented in this paper covers single peak JPDFs only and future work should investigate the modelling of multi–peaked JPDFs for application in wall impacting flows etc. Numerical aspects of the MEF technique, such as speed, convergence properties and stability also need further attention.

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