A physics-based advanced Euler-Lagrange framework for droplet-droplet interaction in dense spray systems

Kai Liu, Chandler Moore and S. Balachandar*

Department of Mechanical & Aerospace Engineering
University of Florida
Gainesville, FL

Euler-Lagrange (EL) methodology is the common approach used to simulate the collective dynamics of a very large number of dispersed droplets in the mid region of a spray. Traditional point-particle models used in these EL simulations assume the force on a droplets to depend only on mean Reynolds number and the mean volume fraction. This approximation ignores interactions among the droplets at the microscale and therefore significantly under-predicts fluctuations in droplet velocity and feed-back forces, resulting in incorrect mesoscale structures and macroscale dispersion. Furthermore, often the larger droplets under consideration are as large as the underlying Eulerian grid and this caused substantial error in the estimation of the undisturbed flow velocity for the drag force calculation. In this study we employ (i) the extended point-particle force (PIEP) model and rigorously account for the hydrodynamic influence of the neighboring droplets and (ii) the self-induced velocity correction (SIC) model for obtaining the true undisturbed fluid velocity which can then be used in the inter-phase coupling models. Both these models have been tested extensively for the cases of a random array of stationary and freely sedimenting particles. The overall objective of our project is to demonstrate multiphysics control of liquid sprays. The talk will also present the on-going simulation effort of a spray in the mid-field region, where the dispersed droplets in a turbulent flow is considered with the PIEP and SIC models. Mid-field control of spray using electrostatic and acoustic forcing will be systematically explored. This study is part of a multi-disciplinary university research initiative (MURI) funded by the Office of Naval Research to experimentally and computationally explore multi-physics spray control.

* Corresponding author, bala1s@ufl.edu
Introduction

Efficient and effective control of droplet spray is a problem of great interest in many engineering applications. The present work is part of a Multidisciplinary University Research Initiative (MURI) that has been funded by the Office of Naval Research to explore active control of the atomization process with an integrated simulation and experimental approach. The coordinated effort is further divided into near-field and mid-field control of the spray. This conference paper is to provide an update of our progress towards improved modeling capability needed for large-scale simulations of mid-field control of spray droplets and their dispersion using acoustic and electrostatic forcing.

We define the near-field as the region where all the primary breakup of the liquid jet into droplets, and most of the subsequent breakups into a fine droplet spray is complete. Thus, control of droplet size spectra is primarily in the near-field. Control of the spatial distribution of the droplet spray in the radial direction, using active acoustic and electrostatic forcing is the primary goal of the mid-field simulation. With this in mind, we pursue an Euler-Lagrange (EL) dispersed turbulent multiphase flow simulation strategy for the mid-field.

In the EL methodology, the location of all the droplets, or a subset of computational droplets that accurately represent the actual distribution in a statistical sense, is tracked. Since the flow around the individual droplets is not resolved, a point-particle (PP) model is used to track the trajectory of the computed droplets by solving their equations of motion. The accuracy of the Eulerian-Lagrangian point-particle (EL-PP) technique is dependent on the fidelity of the force, thermal and mass transfer couplings laws used for representing the fluid-droplet mass, momentum and energy exchange that occurs at the microscale. These closure models must account for the net effect of the droplet-flow interactions that happen at the microscale, which are unresolved in the EL-PP approach.

In the dilute limit when the droplet size is smaller than the ambient flow scales, force models, such as the standard drag law, provide an excellent closure [1]. At intermediate droplet volume fraction, the effects of indirect interaction between the droplets as mediated by the surrounding gas flow starts to become important. With further increase in volume fraction, the probability of direct collisions between the droplets increases, which further can lead to collision-induced agglomeration and breakup of droplets. Recent EL-DEM (discrete element method) simulations of dispersed multiphase flow partially account for these effects through volume fraction dependent drag coefficient and collision detection [2-5]. Such models however do not make use of information on the location of neighboring droplets on the motion of each droplet, except abruptly when they collide.

The purpose of this paper is to describe the pairwise interaction expended point-particle (PIEP) model that systematically accounts for the effect of neighbors on the motion of individual particles. The PIEP model includes not only the direct collisional force as the particles are in contact, but also the force due to gas-mediated interaction between neighboring particles. In this paper we will also briefly describe the self-induced correction (SIC) model that accounts for the self-induced velocity perturbation induced due to two-way coupling from a particle of size comparable to the Eulerian grid. We will also present preliminary results of a spray system with and without PIEP and SIC models included in the simulation. The difference between the two simulation results will highlight the importance of neighbor-neighbor interaction and self-induced velocity correction. We will also briefly present our initial progress towards swirl induced modulation of the mid-field of a spray.

PIEP Model

The PIEP-physics model is built upon two basic ideas. First, the undisturbed flow at each droplet location, defined as the flow that would exist at a droplet location in the absence of that droplet but with all other droplets present, is separated into two parts: a macroscale flow that accounts for the collective action of all the droplets and a microscale flow that accounts for the presence of all the neighbors taken one at a time (this is the pairwise interaction approximation). Second, the above defined undisturbed flow is used to calculate the net aerodynamic force and torque on the droplet using the Faxén form of the quasi-steady, added-mass, Basset history, and vorticity-induced (lift) forces relation (and similarly for the torque), since the undisturbed flow obtained from the first step is non-uniform.

The important aspect of the PIEP model is it attempts to systematically account for the microscale flow induced by the neighbors by making use of their precise location, an information which is readily available in EL simulations. By accounting for the precise location of neighbors, the PIEP model goes beyond the mean neighborhood information of local droplet volume fraction, and distinguishes the influence of upstream, downstream and laterally located neighbors. Such droplet-droplet interaction information is critical in order to capture phenomenon such as collision and close-range interaction of droplets.

It is important to note that PIEP model retains the computational efficiency of the standard Euler-Lagrange...
PP approach. The microscale perturbation field induced by a neighbor can be easily computed for a range of Reynolds number and ambient conditions. Which can then be used to pre-compute the pairwise interactions and store as PIEP maps. These maps are then used repeatedly to calculate the microscale contribution to hydrodynamic force and torque.

The implementation of the PIEP model requires the generation of streamwise force, transverse force and torque maps. Here streamwise direction is along the macroscale ambient flow seen by the moving particle and transverse direction is perpendicular in the plane formed with the neighbor (see [6, 7] for details of the model and notations). Each map is a function of streamwise and transverse distance between the “reference” particle and the neighbor, whose effect on the reference particle is being computed, and the flow Reynolds number.

Hybrid PIEP model

The PIEP-physics models was tested extensively by comparing DNS results for a pair of falling and colliding particles, sedimentation of a system of 5 particles and a larger system consisting of 80 particles [7]. In all three cases the PIEP-physics model was shown to capture the essential features of the fully-resolved simulations that would not be captured in a typical point-particle Euler-Lagrange simulation. However, the accuracy of the PIEP-physics models was limited to moderate volume fraction. With increasing volume fraction the performance of PIEP-physics model started to suffer. For example, DNS of fully resolved simulations of flow over a random array of particles at 45% volume fraction showed that the agreement between the DNS values of drag and lift forces on the particle could not be accurately calculated with the PIEP-model (not as well as at 10% or 20% volume fraction). The difficulty was due to the use of results from single and two particle simulations in the construction of the PIEP-physics model. While these results made good sense at lower volume fraction, at higher volume fraction the presence of large number of neighbors modified the flow substantially.

Here we will explore an hybrid approach to modeling that combines the physics-driven and data-driven approaches. While the data-driven approach has an advantage when the flow becomes complex for simple physical description, the physics-driven approach offers significant advantage in regimes where available data is limited. Furthermore, the data-driven approach is most effective when guided by the physics-driven approach. Finally, the data-driven approach yields considerable insight into the physics of the problem.

The data-driven approach which depends on the DNS data itself is able well capture the influence of the neighboring particles in restructuring the wake. Similar differences are seen in the transverse force and torque maps for the higher volume fraction. However in the modest volume fraction regime the PIEP-physics results are in good agreement with those from the data-driven approach. A comparison of the PIEP-physics and PIEP-hybrid models against actual DNS data for drag for two different volume fractions is shown in the Table below.

It is clear that the data-driven approach has a great potential in capturing the microscale physics at higher volume fraction. It helps improve the $R^2$ values even at lower volume fraction.

<table>
<thead>
<tr>
<th>Volume Fraction</th>
<th>PIEP-Physics</th>
<th>PIEP-Hybrid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re</td>
<td>Drag</td>
<td>Lift</td>
</tr>
<tr>
<td>0.1</td>
<td>40</td>
<td>0.66</td>
</tr>
<tr>
<td>0.1</td>
<td>173</td>
<td>0.33</td>
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<tr>
<td>0.45</td>
<td>20</td>
<td>0.12</td>
</tr>
<tr>
<td>0.45</td>
<td>115</td>
<td>0.24</td>
</tr>
</tbody>
</table>

Table 1: Table showing $R^2$ values resulting from comparison between DNS drag and lift distribution over a cluster particles compared with the corresponding PIEP-physics and PIEP-hybrid model predictions.

Self-induced velocity correction model

The Self-induced velocity (SIC) correction model [10] is important for two-way coupled Euler-Lagrange simulations when the point particle being considered is of large size comparable to the underlying grid. The point particle model predicts the drag force on the particle based on the undisturbed velocity by two-way coupled feedback force and thereby affect the force model accuracy. In many conditions where two-way coupling needs to be considered, the particle size may be comparable to the grid size and the self-induced perturbation velocity may cause considerable error.

We have developed a correction model based on the analytical solution of Oseen’s equation. This model can explicitly evaluate the self-induced perturbation velocity as a function of feedback force and Gaussian filter Reynolds number. For both steady and unsteady conditions,

$$\mathbf{u}_{p, \text{un}}(t) = \mathbf{u}_{p, \text{in}}(t) + \mathbf{u}_{\text{SIC}}(t; F, Re_p)$$

This correction model can improve the quasi-steady force model accuracy in the two-way coupled conditions and will be implemented into the following simulations.

Mid-Field Spray Simulations

As a preliminary result we finally show results from an initial mid-field simulation of a gas jet of inlet Reynolds number of 400. An inlet Gaussian velocity distribution with random initial perturbation was applied.
The results obtained from two-way coupled simulations showing contours of axial gas velocity is shown in Figure 1. Also shown are the droplet locations and size at the time instant of the figure. The present coupled simulations include the ability to inject at the inlet with a specified inlet distribution of droplet spectra. We performed two-way coupled turbulent simulations with PIEP model implemented to account for both gas-droplet and droplet-droplet interactions. For each particle, we also apply the SIC correction model to predict the real undisturbed fluid velocity for the drag force model calculation. Nek5000, the code used for the above simulation, employs a higher-order accurate spectral element methodology to which Lagrangian droplet tracking capability has recently been added by us. The preliminary simulation shown in Figure 1 employs a modest grid of about 9 million grid points.

An important aspect of the present effort is to interface with experiments and simulations performed in the near-field of the spray. The measurements from these experiments and simulations can be used as input in the mid-field simulations, and this requires an integrated approach where measurements from the near-field should be converted into statistical information that can be used for time-dependent inflow condition for both the gas as well as spray droplets at the inflow boundary. Because of the turbulent nature of the simulation it is not sufficient to obtain only the mean statistics. The algorithm for statistical specification of the inflow is shown in Figure 2, where a comprehensive plan for both the gas and the droplets inflow conditions is presented.

In the case of the gas, in addition to the experimental and simulation data we also use information on jet instability. The self-similar nature of the multiphase jet flow with an appropriate time-dependent inflow condition is generated. Similarly the experimental measurements on number of droplets, size and velocity are used to construct a statistical picture of droplet inflow, which then is used for random injection of droplets as shown in Figure 2.

We also carefully studied the droplet dispersion taking into account several factors, such as density ratio, PIEP model, collision model, SIC model and inlet swirling flow. A sample particle dispersion is shown in Figure 8. Since the density ratio of two phases is as large as 1000, the particle trajectory is only slightly influenced by the flow field. However, if a swirling flow is included inside the nozzle, the spray cone angle will be increased accordingly. A comparison between two cases with and without swirling flow is illustrated in Figure 9. Here we have used a swirl amplitude of 10% of the spray centerline velocity.

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References
Figure 1: Streamwise velocity contours on the mid-plane passing through a cylindrical turbulent jet. A Gaussian inflow with random perturbation is specified as the inlet on the left. Also injected on the left end are droplets of varying size.

Figure 2: A stochastic approach for obtaining time-dependent inflow gas velocity and inlet droplet spectrum.
Figure 3: Mid-field particle dispersion with zoom-in views.

Figure 4: Mid-field particle dispersion without and with swirling flow. The yellow straight lines outline the spray angles.