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LAGRANGIAN MODEL FOR SIMULATING TURBULENT DISPERSION AND AGGLOMERATION OF DROPLETS WITHIN A SPRAY

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ABSTRACT

Lagrangian modeling approach is for simulating turbulent dispersion and agglomeration of droplets within a spray. This model (Lagrangian) predicts droplet dispersion rate and shift in droplet size distribution due to agglomeration within the spray, over a wide range of droplet and gas flows, and for sprays with different size distribution at the nozzle exit. The computer time required for simulating agglomeration within a steady axisymmetric spray is of a similar order of magnitude regardless of which formulation, Lagrangian, is adopted. However the Lagrangian formulation is more practical in terms of the range of applicability and ease of implementation.

Keywords: Lagrangian, Dispersion, Agglomeration, Droplets, Turbulent, CFD, Spray

I. INTRODUCTION

Spray dryers are used to produce dried powder products by atomising liquid suspensions that contain solids into a stream of hot gas where the moisture is evaporated. Particle agglomeration is an important phenomenon in this process because it affects the size distribution of the particles, and hence the properties of the dry powder. Agglomeration kinetics are determined to a certain extent by the turbulent nature of the flow, which influences the dispersion rate of practices and hence the development of relative velocities between particles, a prerequisite for successful particle collisions. No fundamental theory has yet been applied to model turbulent dispersion and agglomeration simultaneously within a spray dryer, and this lack of fundamental understandings is the reason, that spray dryers are so difficult to design. In fact, dryer manufactures and users of spray dryers typically rely on simple empirical models or a trial and error approach to improve their designs and operating conditions. The aim of this work to address this gap in fundamental understanding and to develop a Computational Fluid Dynamics

(CFD) model to predict the turbulent dispersion and agglomeration of droplets within a spray. In the Lagrangian model, the spray is represented by a flow of gas, treated mathematically as a continuum, which carries numerous discrete droplet parcels, each parcel consisting of a group of physical droplets of similar size. The trajectory of each droplet parcel within the airflow is predicted by solving the Lagrangian equations of mass and momentum. The Monte-Carlo method is used to model the turbulent dispersion of droplets by effectively sampling the fluctuating velocities of the droplets randomly. Ruger at al. (2000) [10] and Berlemont et al. (1990) [1] have used Lagrangian calculations in their analyses.

Mostafa and Mongia (1987) [7] have been that Larangian approach is able to predict the main features of a turbulent spray, such as the decay of the entire line axial velocity and the turbulent dispersion of droplets. The Lagrangian method may have Fourier transport equations to solve numerically, but the trade off is the necessity of a three-dimensional, transient solution to properly model the effect of collisions and turbulence interactions on the trajectories of individual droplets. In this paper, the Lagrantian predicts of droplet turbulent dispersion and agglomeration within a spray are compared over a wide range of gas and droplet flows, and for sprays with different droplet size (1) to validate the numerical aspects of each mathematical formulation so that the models can be applied with more confidence in future simulations. (2) To determine whether each approach predicts similar droplet turbulent dispersion and agglomeration rates, and (3) To ascertain the weaknesses and strengths of each approach in terms of the case of application and subsequent computational effort required. The ultimate aim of the work is to develop a validated CFD model to predict the extent of particle agglomeration within a spray dryer, and the flow patterns and drying of particles, and to use this predictive tool to design more efficient spray dryer that produce higher throughputs.

II. MODEL DISCRIPTION

Lagrangian method is for calculating the velocity and turbulence fields, and the turbulent dispersion of droplets, are described in detail by Ruger et al.(2000)[10] and Nijdam et al.(2003)[8], respectively. Here, we provide only a description of the agglomeration models used in each approach. This model has been incorporated into a commercially available Computational Fluid Dynamics (CFD) program called CFX4 (AEA Technology). The Lagrangian approach requires a transient, three dimensional calculations.

2.1 Lagrangian Agglomeration Model

The Lagrangian agglomeration model is a modification of the O'Rourke model (1981)[9], for which parcels of droplets are tracked simultaneously in three-dimensional space and with time. The turbulent effect is included within the droplet transport model using the eddy-lifetime method of Gosman and loannides (1983)[2]. When considering a collision between two parcels, the parcel containing the larger number of droplets (N_i) is called the 'contributor" While the parcel containing fewer droplets (N_i) is called the 'collector'. Ruger et al. (2000) [10] have shown that the collision frequency v between the collector and contributor parcels is proportional to the mean number density, a collision cross-sectional area, and a relative velocity, as follows:

$$v = \frac{N_j}{V}\frac{\Pi}{4}(D_i + D_j)^2 u_r \qquad \ldots\ldots\ldots \quad (1)$$

Where V is the volume within which both parcels are located. This volume V is related to the cube of the distance l between parcels, so that eqn. (1) becomes

$$v = \frac{N_j}{b_1 l^3}(D_i + D_j)^2 u_r \quad \ldots\ldots (2)$$

Where b_1 is an empirical constant A “proximity” function is derived from Equation (2), as follows

$$P = \frac{N_j}{l^3}\Delta t (D_i + D_j)^2 u_r \quad \ldots\ldots\ldots \quad (3)$$

Which effectively represents the probability of collision between two parcels over a given time interval Δt. At the end of each time-step in the simulation, the proximity function is evaluated for every combination of parcel pairs. Collision of a pair of parcels is allowed when the proximity function P exceeds a critical value P_c,

$$P \ge P_c \equiv -\frac{b_1 \log 0.5}{1.5} \quad \ldots\ldots. \quad (4)$$

for any acceptable collision, the collector parcel absorbs a part of the colliding contributor parcel, so that every droplet in the collector parcel coalesces with a droplet in the contributor parcel on a one-to-one basis to form the group of agglomerates. The remaining diminished contributor parcel, which contains any excess droplets, is tracked further in the next time-step. The velocities of the parcels after collision are determined by conservation of momentum. The size of the droplets in the collector increases according to conservation of volume, as follows.

$$D^3 = D^3{}_i + D^3{}_j \quad \ldots\ldots\ldots \quad (5)$$

A more detailed description of the model can be found in Guo et al. (2003)[3].

III. RESULTS AND DISCUSSION

3.1 No Agglomeration Case

Figure 1 shows the Lagrangian predicts of the axial mean velocity profiles of the droplets at various axial locations downstream of the nozzle clearly, it predicts decay rate for the. axial mean velocity at the centre-line.

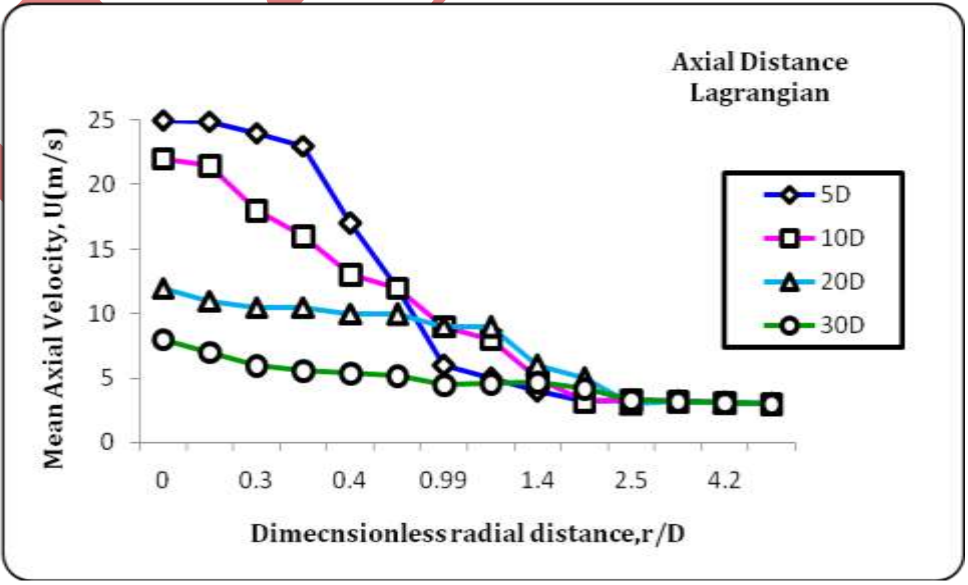

Fig1: Mean axial velocity U (mean of all droplet size classes) verses dimensionless radial distance at various axial locations from the nozzle exit.

Figure 2: shows that the spreading rate of droplets of different size is also similarly predicted in this model. . and implies that smaller droplets disperse radially more rapidly than larger droplets. This is physically reasonable because small droplets have relatively low inertia and therefore they readily follow the turbulent fluctuations of the carrier gas, whereas large droplets have relatively high inertia so that they are less affected by gas-flow turbulent fluctuations. The Lagrangian approach is able to predict the main features of a turbulent spray, including the decay of centerline velocity and the radial dispersion of droplets with axial distance from the nozzle.

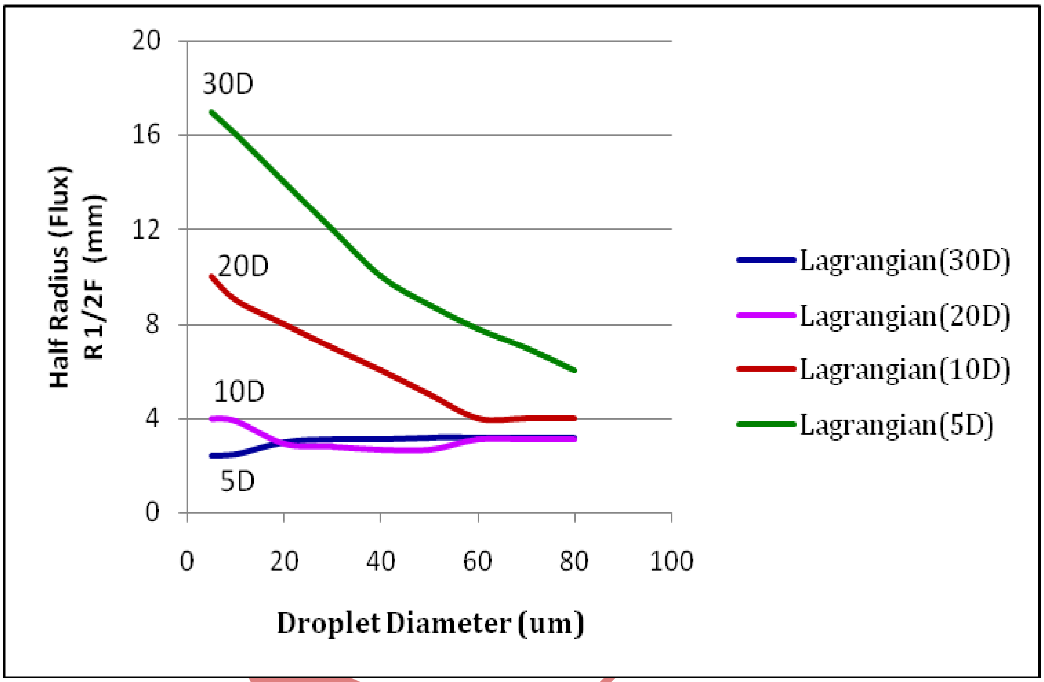

Fig 2: The half-radio $R_{1/2F}$ of the radial profiles of droplet volume flux for different droplet size classes at various axial locations from the nozzle exit.

3.2 Agglomeration Case

The Lagrangian model is first fitted to one set of spray conditions by arbitrarily choosing a value of 3.2 for the Lagrangian parameter b_1. A second set of parameters – double the Lagrangian parameter (b_1=6.4) is also tested over a range of droplet flows. This test gives an indication of the compatibility for predicting droplet – droplet interactions with different agglomeration efficiencies. Here, the critical agglomeration probability (eq. 4), and accounts for the reduced probability of collision and subsequent coalescence due to 1) unsuccessful wake capture of a portion of droplets as they are accelerated within the wakes of other droplets, and 2) insufficient contact times for the film separating collided droplet pairs to drain and rupture. Figure 3 shows the Lagrangian predicts of the Sauter-mean diameter D_{32} for sprays having the same normalized droplet volume distribution, and air velocity and turbulence profiles at the nozzle exit, but having different total droplet flows in this model predicts similar increases in D_{32} with droplet flow for two different sets of agglomeration parameters (b_1 and β_o). Firstly, this verifies to a certain extent of the Lagrangian numerical code, so that it can be used with confidence in future agglomeration calculations. Secondly, this result implies that a sufficient number of droplet size classes (15 droplet size classes) and parcels (about 20000 parcels are tracked at any given time) have been chosen for the Lagrangian approach, to ensure that the solution is independent of these quantities.

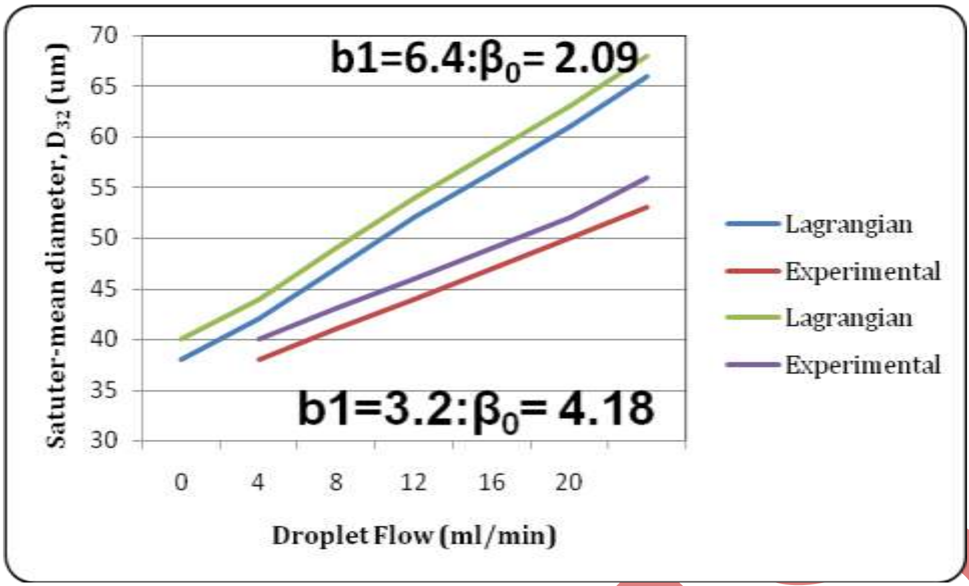

Fig:3 Lagrangian predictions of the integral Sauter-mean diameter D_{32} at an axial location of 30D for sprays with different droplet flows, and with different agglomeration efficiencies

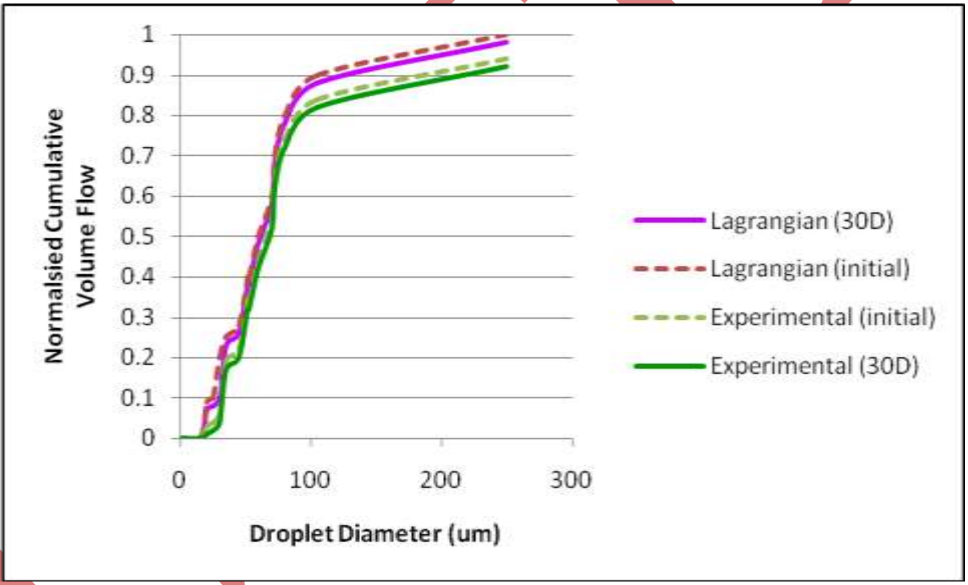

Fig: 4 Lagrangian predictions of the droplet size distribution at an axial location of 30D for a spray with a poly – disperse droplet size distribution (droplet flow is 10ml/min b_1 is 3.2).

Additionally, the discretisation of the droplet size distribution used in Lagrangian model is small enough so that further refinement would not effect the solution significantly. Finally, this result shows that this method predicts agglomeration rate, over a wide range of droplet flows and for different agglomeration efficiencies. The development of a poly-disperse droplet size distribution downstream of the nozzle is for the Lagrangian model, as shown in Figure 4. This agreement is also found when simulating the downstream development of a mono-size (36µm) droplet dispersion, as shown in Figure 5. Thus, this model predicts agglomeration of droplets in sprays with different droplet-size distributions at the nozzle exit.

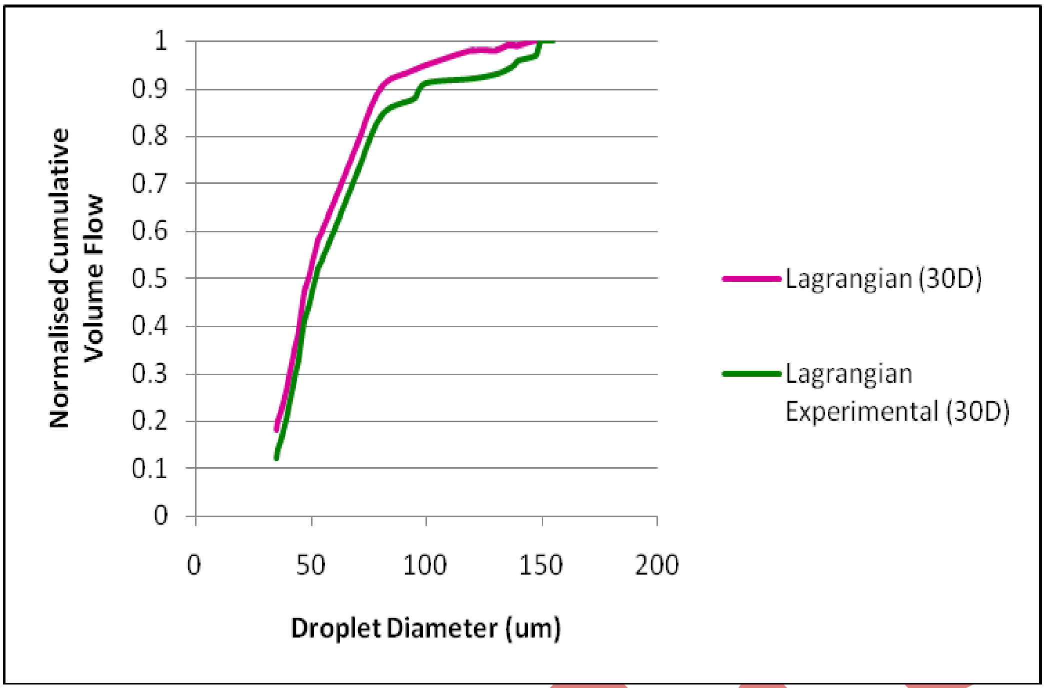

Fig 5: The Lagrangian predictions of the droplet size distribution at an axial location of 30D for a spray with an initial mono-sized distribution with 36 µm droplets (droplet flow is 10ml / min, b_1 is 3.2).

The effect of the gas-flow velocity and turbulence on the extent of agglomeration is shown in Table 1. In this part of the investigation, the velocity of the carrier gas at the nozzle exit is doubled and the turbulence kinetic energy is quadrupled (in order to retain the same turbulence intensity), while keeping the droplet flow constant at 10 m1/min. This effectively halves the number density of droplets at the nozzle exit, and hence reduces the extent of agglomeration within the spray, so that D_{32} at 30 nozzle diameters reduces from 52 µm to 45 µm. When the droplet flow is doubled from 10ml/min to 20 ml/min, while keeping the gas velocity and turbulence kinetic energy constant at the higher values, the number density at the nozzle exit increases back to the original value, and consequently D_{32} at 30 nozzle diameters, increases from 45µm to 53 µm. According to the Lagrangian predictions, D_{32} at 30 nozzle diameters only increases marginally from 51.8 µm to 52.5 µm when the gas velocity is doubled while keeping the droplet number density constant. Thus, the extent of agglomeration within a single spray is relatively insensitive to the carrier gas velocity and turbulence levels generated within the shear layer of the spray, and reasonably sensitive to the number density of droplets at the nozzle exit. In practice, it is considerably easier to change the number density of droplets over a wide range of values than the gas-flow velocity, which suggests that droplet number concentration is a particularly effective variable for controlling agglomeration.

Table 1 shows that Lagrangian model predicts the above mentioned trends. We have found that the computation time required to complete an agglomeration simulation is of a particular order of magnitude in its approach. The Lagrangian approach as a three dimensional calculation is realistically possible, so that it is more applicable for a wider range of different flows.

TABLE 1: Sauter-mean diameter D at an axial location of 30D for poly-disperse sprays with different air velocities and droplet flows: Lagrangian predictions ($b_1$is 3.2).

Droplet Flow (ml/min)	Velocity	D_{32}@ 30D (μm)
		Lagrangian
10	1x	51.8
10	2x	45.4
0	2x	52.5

The Lagrangian approach is not limited in this manner, so that droplets of similar size originating from different nozzles that point towards each other can cross-over the central axis of the impinging spray system, provided they have sufficient inertia.

IV. CONCLUSIONS

The Lagrangian approach is able to simulate droplet turbulent dispersion and agglomeration for a wide range of droplet and gas flows, and for sprays from nozzles that produce different droplet size distributions. Moreover, the time required for simulating agglomeration within a steady axisymmetric spray is of the given

magnitude for this approach. The Lagrangian approach has a wide range with regard to the range of applicability and ease of implementation.

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