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

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ABSTRACT

Lagrangian and Eulerian modelling approaches are compared for simulating turbulent dispersion and agglomeration of droplets within a spray. Both models predict similar droplet dispersion rates and shifts in droplet size distribution due to agglomeration within the spray, over a wide range of droplet and gas flows, and for sprays with different droplet size distributions 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, Eulerian or Lagrangian, is adopted. However, the Lagrangian formulation is more practical in terms of the range of applicability and ease of implementation.

NOMENCLATURE

b_1	Lagrangian model constant
D	droplet diameter or nozzle diameter (m)
k	turbulent kinetic energy (m^2/s^2)
l	inter-parcel distance (m)
$\dot{m}$	inter-phase mass-transfer rate (kg/m^3s)
N	droplet number density (m^{-3}), or droplet number in a tracked parcel
N_P	number of droplet phases
P	proximity function (Lagrangian model)
r	volume fraction (m^3/m^3), or radial distance (m)
t	time (s)
u'	fluctuating velocity (m/s)
u_r	instantaneous relative velocity between two droplets (m/s)
U	mean velocity (m/s)
v	droplet volume (m^3)
Z	ratio of axial distance from nozzle and nozzle diameter
β	agglomeration kernel (Eulerian model)
ρ	density (kg/m^3)

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 particles 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 understanding is the reason that spray dryers are so difficult to design. In fact, dryer manufacturers and users of spray dryers typically rely on simple empirical models or a trial and error approach to improve their designs and operating conditions.

It is 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. Two different modelling approaches are compared: the Lagrangian and Eulerian approaches. 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. Rüger *et al*. (2000) and Berlemont *et al*. (1990) have used Lagrangian calculations in their analyses. In the Eulerian approach, the airflow and droplet phases are both treated as interpenetrating interacting continuums. The governing equations for each phase are similar to the Navier-Stokes equations, with extra source terms in the momentum equations to account for the turbulent dispersion of droplets. The Eulerian approach has been adopted by a number of researchers including Simonin (1991) and Issa *et al*. (1994). The gas-flow turbulence is treated similarly in both the Eulerian and Lagrangian approaches.

Mostafa and Mongia (1987) have shown that both Eulerian and Lagrangian approaches are able to predict the main features of a turbulent spray, such as the decay of the centre-line axial velocity and the turbulent dispersion of droplets. The Eulerian strategy is attractive from a computational point of view because these calculations are easier to parallel process, which can have advantages when modelling complex flows that require considerable computational effort. However, in order to model coalescence and evaporation of droplets using an Eulerian formulation, the droplet-size distribution must be divided into a number of separate size classes, each size class requiring its own set of transport equations, which increases the computational effort expended considerably. The Lagrangian method may have fewer 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. The

Eulerian formulation requires only a two-dimensional steady-state calculation for many simple flows, such as a turbulent axisymmetric round jet, although less information is provided about the trajectories and residence times of these droplets with this approach.

In this paper, the Lagrangian and Eulerian predictions 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 distributions at the nozzle exit. The aims of this paper are 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 ease of application and subsequent computational effort required. The ultimate aim of this 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 dryers that produce higher throughputs.

MODEL DESCRIPTION

Both Eulerian and Lagrangian methods for calculating the velocity and turbulence fields, and the turbulent dispersion of droplets are described in detail by Rüger *et al*. (2000) and Nijdam *et al*. (2003), respectively. Here, we provide only a description of the agglomeration models used in each approach. These models have been incorporated into a commercially available Computational Fluid Dynamics (CFD) program called CFX4 (AEA Technology).

The Eulerian approach uses a steady-state, two-dimensional (axisymmetric, cylindrical coordinate system) calculation to model the collision and subsequent agglomeration of droplets within the spray, whereas the Lagrangian approach requires a transient, three-dimensional calculation.

Eulerian Agglomeration Model

One continuity equation is required to represent the air phase, while a number of continuity equations (N_P) are needed to represent the droplet phase in order to account for a range of droplet size classes. The continuity equation takes the general form,

$$\nabla \cdot \left(r_i \rho_i U_i \right) = \sum_{j=1}^{N_P} \left(\dot{m}_{ij} - \dot{m}_{ji} \right) \qquad (1)$$

The subscript i takes a value of zero for the air phase, while the droplet phases take values for i of unity or higher. The term on the right-hand side of Equation (1) represents inter-phase mass-transfer as droplets move from one size group into another due to agglomeration, where $\dot{m}_{ij}$ is the droplet mass flow per unit volume into droplet size class i from droplet size class j. This term vanishes for the air continuity equation, since no inter-phase mass-transfer occurs between the air and the droplet phases.

Agglomeration of droplets in a poly-disperse spray can be mathematically described by the population balance equation (Hounslow *et al*. 1998), which relates the rate of change of the droplet number in a given size class to the rates of birth and death in that droplet size class due to agglomeration. Hounslow *et al*. (1988) have produced a discretised form of the population balance for agglomeration that guarantees conservation of both droplet number and mass, and which can be readily solved numerically using conventional techniques. The droplet size distribution is broken up into discrete size classes according to the following geometric-series discretisation:

$$\frac{v_{i+1}}{v_i} = 2 \qquad (2)$$

Here, v_i and v_{i+1} are the lower and upper volume bounds of the i^{th} droplet size class. The droplet size distribution and index notation used in this work is shown in Figure 1.

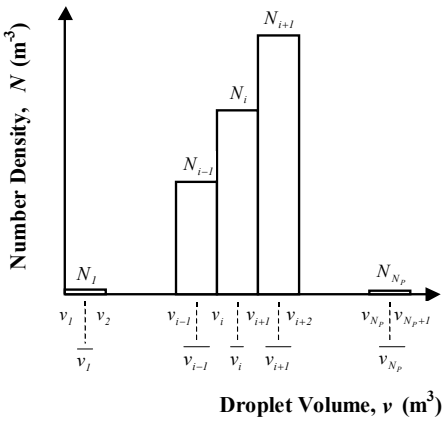

Figure 1: Droplet size distribution showing the index notation.

By identifying four possible types of droplet-droplet interactions, that either add droplets to or remove droplets from the i^{th} droplet size class, Hounslow *et al*. (1998) have derived the following discretised form of the population balance for agglomeration:

$$\left(\frac{dN_i}{dt} \right)_{agg} = + \sum_{j=1}^{i-2} 2^{j-i+1} \beta_{i-1,j} N_{i-1} N_j + \frac{1}{2} \beta_{i-1,i-1} N_{i-1}^2 - N_i \sum_{j=1}^{i-1} 2^{j-i} \beta_{i,j} N_j - N_i \sum_{j=i}^{N_P} \beta_{i,j} N_j \qquad (3)$$

Here, N_i is the number of droplets per unit volume in the i^{th} droplet size class, and $\beta_{i,j}$ is the agglomeration kernel, which is a measure of the frequency of collision and subsequent coalescence of droplets in size classes i and j. The first term on the right-hand side of Equation (3) represents the birth of a droplet in the i^{th} size class due to agglomeration of two droplets, one of which is in the $(i-1)^{th}$ size class and the other of which is within the first to the $(i-2)^{th}$ size classes. The second term

represents the birth of a droplet in the i^{th} size class due to agglomeration of two droplets both in the $(i-1)^{th}$ size class. The third term represents the death of a droplet in the i^{th} size class due to agglomeration with a droplet within the first to the $(i-1)^{th}$ size classes. The last term represents the death of a droplet in the i^{th} size class due to agglomeration with a droplet of the same size or larger. When i is equal to unity, all but the last term on the right-hand side of Equation (3) drop out, since no smaller droplets occur in the discretisation, and therefore droplets from this size class can only move out of the size class as they agglomerate with droplets of the same size or larger. Only the first term on the right-hand side of Equation (3) drops out when i is equal to two, for a similar reason. When i is equal to the number of droplet size classes N_P, the last two terms drop out, because these terms represent the death of a droplet within the largest droplet size class, and given that no larger droplet classes exist in the discretisation, no transfer of droplets into a larger size class is possible. Clearly, a sufficient number of droplet size classes is required to ensure that relatively few droplets exist in the smallest and largest droplet size classes at any time during the agglomeration process.

There are $\frac{1}{2}N_P(N_P-1)$ inter-phase mass-transfer $\dot{m}_{ij}$ (or $\dot{m}_{ji}$) terms possible in Equation (1) when agglomeration alone is considered. Here, the convention is that mass transfers from size class j into size class i. The converse is true for $\dot{m}_{ji}$, such that mass transfers from size class i into size class j. Droplets transfer from smaller size classes to larger size classes when agglomerating, and therefore droplet size class j is always smaller than droplet size class i for the inter-phase mass-transfer term $\dot{m}_{ij}$. Once again, the converse is true for $\dot{m}_{ji}$, so that droplet size class i is always smaller than droplet size class j for agglomeration. No inter-phase mass transfer is allowed for any other combinations of i and j, and therefore $\dot{m}_{ij}$ and $\dot{m}_{ji}$ are set to zero for those cases. Note that, for evaporation alone, droplets become progressively smaller, and therefore droplet size class j is always larger than droplet size class i for the inter-phase mass-transfer term $\dot{m}_{ij}$, which is the reverse of the case for agglomeration.

The inter-phase mass-transfer equations $\dot{m}_{ij}$ for every allowable combination of i and j are determined by first expanding the summation terms in the discretised form of the population balance for agglomeration (Equation 3). Matching pairs of identical terms are then identified in the resultant set of N_P equations. One term within a matching pair represents the mass flow out of size class i into size class j, while the other term is conversely the mass flow into size class j from size class i. Each matching pair represents one of the allowable inter-phase mass-transfer terms given in Equation (1). The following set of equations, which represent every inter-phase mass-transfer combination possible, has thus been derived:

$$\dot{m}_{i+1,i} = \sum_{j=1}^{i} 2^{j-i}\,\beta_{i,j} N_i N_j (\bar{v}_i \rho) \qquad i = 1 \rightarrow (N_P - 1) \tag{4}$$

$$\dot{m}_{i+1,j} = \beta_{i,j} N_i N_j (\bar{v}_j \rho) \qquad i = (j+1) \rightarrow (N_P - 1), \quad j = 1 \rightarrow (N_P - 2) \tag{5}$$

where the inter-phase mass-flow $\dot{m}$ of droplets is calculated from the inter-phase number flowrate by multiplying it with the density ρ and volume $\bar{v}$ of the droplet in the given size class. The number density N_i of droplets within droplet size class i is equal to the volume fraction r_i divided by the droplet volume $\bar{v}_i$ of that size class.

Khain and Pinsky (1997) have shown that the agglomeration kernel β has the following form:

$$\beta = \beta_o (D_i + D_j)^2 u_r \tag{6}$$

where u_r is the instantaneous relative velocity between colliding droplets, which has both mean and fluctuating components. Here, we assume that u_r is given by the expression:

$$u_r = \sqrt{(U_i - U_j)^2 + (2k_i + 2k_j - 2\overline{u_i' u_j'})} \tag{7}$$

We also assume that the correlation between fluctuating droplet velocities $\overline{u_i' u_j'}$ is zero, since this effect cannot be incorporated into the Lagrangian approach using the simple droplet turbulence model adopted in this work (described below). The constant β_o is essentially a fitting parameter, which we use to match the predictions of the Lagrangian and Eulerian approaches for one set of spray conditions, holding it constant for all subsequent agglomeration predictions that use different sets of spray conditions.

Lagrangian Agglomeration Model

The Lagrangian agglomeration model is a modification of the O'Rourke model (1981), 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 Ioannides (1983). When considering a collision between two parcels, the parcel containing the larger number of droplets (N_j) is called the 'contributor', while the parcel containing fewer droplets (N_i) is called the 'collector'. Rüger *et al*. (2000) have shown that the collision frequency ν between the collector and contributor parcels is proportional to the mean number density, a collision cross-sectional area, and a relative velocity, as follows:

$$\nu = \frac{N_j}{V}\frac{\pi}{4}(D_i + D_j)^2 u_r \tag{8}$$

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 Equation (8) becomes

$$\nu = \frac{N_j}{b_1 l^3}(D_i + D_j)^2 u_r \qquad (9)$$

where b_1 is an empirical constant. A "proximity" function is derived from Equation (9), as follows:

$$P = \frac{N_j}{l^3}\Delta t(D_i + D_j)^2 u_r \qquad (10)$$

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,

$$P \geq P_c \equiv -\frac{b_1 \log 0.5}{1.5} \qquad (11)$$

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:

$$D^3 = D_i^3 + D_j^3 \qquad (12)$$

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

RESULTS AND DISCUSSION

No Agglomeration Case

Figure 2 compares the Lagrangian and Eulerian predictions of the axial mean velocity profiles of the droplets at various axial locations downstream of the nozzle. Clearly, both models predict similar decay rates for the axial mean velocity at the centre-line. Figure 3 shows that the spreading rates of droplets of different sizes are also similarly predicted by both models. Figure 3 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 Eulerian model has already been validated using experimental data of a spray with similar boundary conditions to those tested here (Nijdam *et al*., 2003). Thus, both Lagrangian and Eulerian approaches are able to predict the main features of a turbulent spray, including the decay of centreline velocity and the radial dispersion of droplets with axial distance from the nozzle.

Agglomeration Case

The Lagrangian and Eulerian models are first fitted to each other for one set of spray conditions by arbitrarily choosing a value for the Lagrangian parameter b_1 of 3.2,

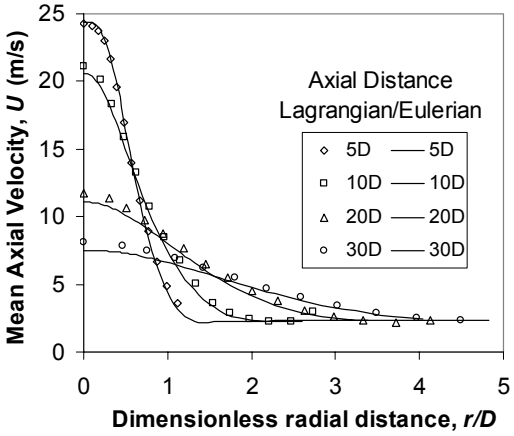

Figure 2: Mean axial velocity U (mean of all droplet size classes) verses dimensionless radial distance at various axial locations from the nozzle exit.

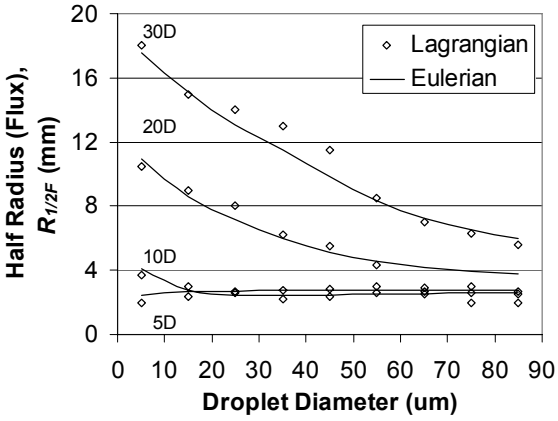

Figure 3: The half-radii $R_{1/2F}$ of the radial profiles of droplet volume flux for different droplet size classes at various axial locations from the nozzle exit.

and adjusting the Eulerian parameter β_o, which takes a value of 4.18, to match the predicted Sauter mean diameter D_{32} at 30 nozzle diameters from the nozzle exit. All subsequent simulations involving different droplet flows, gas flows, or droplet size distributions adopt the same values for these parameters. A second set of parameters - double the Lagrangian parameter (b_1=6.4) and half the Eulerian parameter (β_o=2.09) - is also tested over a range of droplet flows. This test gives an indication of the compatibility of both approaches for predicting droplet-droplet interactions with different agglomeration efficiencies. Here, the agglomeration efficiency is a number that multiplies the agglomeration kernel (Equation 6) or critical agglomeration probability (Equation 11), 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. Note that the Lagrangian agglomeration parameter b_1 is inversely proportional to the Eulerian agglomeration parameter β_o.

Figure 5 shows a comparison between the Lagrangian and Eulerian predictions of the Sauter-mean diameter D_{32} for sprays having the same normalised droplet volume distribution, and air velocity and turbulence profiles at the nozzle exit, but having different total droplet flows. Both models predict 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 the validity of the Lagrangian and Eulerian numerical codes, so that they 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 Eulerian and Lagrangian approaches, respectively, to ensure that the solution is independent of these quantities. Additionally, the discretisation of the droplet size distribution used in the Eulerian approach (given by Equation 2) is sufficiently fine, and the time-step (0.0004 seconds) used in the Lagrangian model is small enough so that further refinement would not affect the solution significantly. Finally, this result shows that both models predict similar agglomeration rates 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 very similar for both the Lagrangian and Eulerian models, as shown in Figure 6. Similar agreement is also found when simulating the downstream development of a mono-size (36μm) droplet dispersion, as shown in Figure 7. Thus, both models also similarly predict agglomeration of droplets in sprays with different droplet-size distributions at the nozzle exit.

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 ml/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 45 μm 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

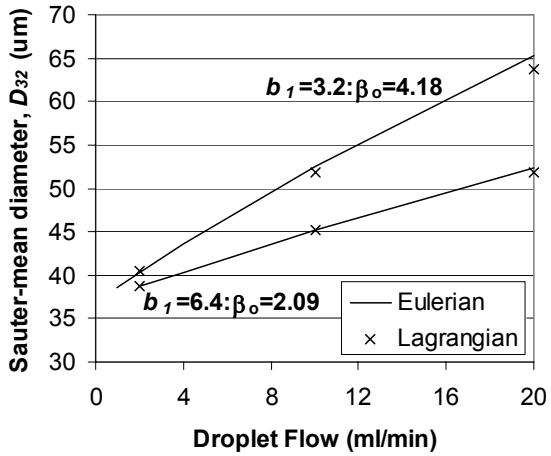

Figure 5: Comparison of Lagrangian and Eulerian predictions of the integral Sauter-mean diameter D_{32} at an axial location of 30D for sprays with different droplet flows, and with different agglomeration efficiencies.

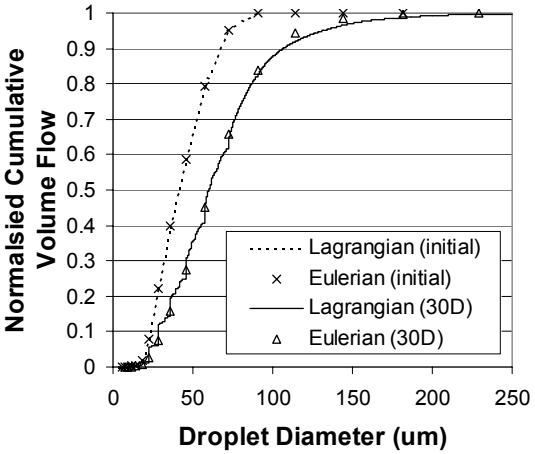

Figure 6: Comparison of Lagrangian and Eulerian predictions of the droplet size distribution at an axial location of 30D for a spray with a poly-disperse droplet size distribution (droplet flow is 10 ml/min, b_1 is 3.2).

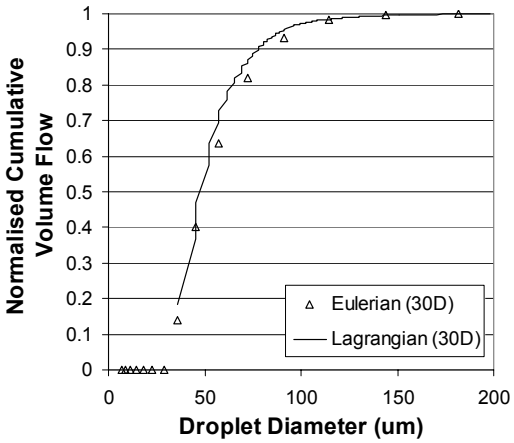

Figure 7: Comparison of Lagrangian and Eulerian predictions of the droplet size distribution at an axial location of 30D for a spray with an initial mono-sized distribution with 36 μm droplets (droplet flow is 10 ml/min, b_1 is 3.2).

Table 1: Sauter-mean diameter D_{32} at an axial location of 30D for poly-disperse sprays with different air velocities and droplet flows: comparison between Lagrangian and Eulerian predictions (b_1 is 3.2).

Droplet Flow (ml/min)	Velocity	D_{32} @ 30D (μm)	
		Lagrangian	Eulerian
10	1x	51.8	52.5
10	2x	45.4	45.5
20	2x	52.5	52.7

agglomeration. Table 1 shows that both the Eulerian and Lagrangian models predict similar trends.

We have found that the computation time required to complete an agglomeration simulation is of similar order of magnitude in both approaches. However, the Eulerian approach is probably limited in practice to two-dimensional calculations using computer hardware currently available, because a great number of transport equations are needed in order to properly discretise the droplet size distribution. On the other hand, a three-dimensional calculation is realistically possible for the Lagrangian approach, so that it is more applicable for a wider range of different flows. In addition, the effort required to code the turbulent dispersion model used for the Eulerian approach together with limitations inherent in the model, which cannot be used for sprays with high turbulence intensities at the nozzle exit as discussed by Nijdam *et al*. (2003), make it less appealing than the Lagrangian approach, which uses a relatively simple but effective turbulent dispersion model. Finally, the Eulerian model is limited for practical use even if a three-dimensional calculation is realistically possible, because impinging sprays can never be simulated properly using this approach. Droplets in the same size class originating from different nozzles that point towards each other, cannot pass by each other and cross-over the central axis of the impinging spray system in an Eulerian simulation, because of the inherent flaw in the assumption that each droplet size class is represented by a continuum. 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.

CONCLUSIONS

Both Lagrangian and Eulerian approaches are 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 similar order of magnitude for both these approaches. However, the Eulerian approach is more limited than the Lagrangian approach with regards to the range of applicability and ease of implementation.

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