Lagrangian and Eulerian models for simulating turbulent dispersion and coalescence of droplets within a spray

Justin J. Nijdam, Baoyu Guo, David F. Fletcher *, Tim A.G. Langrish

Department of Chemical Engineering, University of Sydney, NSW 2006, Australia

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Abstract

Lagrangian and Eulerian modelling approaches are compared for simulating turbulent dispersion and coalescence of droplets within a spray. Both models predict similar droplet dispersion rates and shifts in droplet size distribution due to coalescence 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 coalescence 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.

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1. 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 coalescence 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
<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>$b_1$</td>
<td>Lagrangian model constant</td>
</tr>
<tr>
<td>$c_{oi}^{(d)}$</td>
<td>Local instantaneous inter-phase drag coefficient</td>
</tr>
<tr>
<td>$C$</td>
<td>Constant for turbulence or cross-trajectory model</td>
</tr>
<tr>
<td>$C_D$</td>
<td>Droplet drag coefficient</td>
</tr>
<tr>
<td>$D$</td>
<td>Droplet diameter or nozzle diameter</td>
</tr>
<tr>
<td>$D_{oi}$</td>
<td>Gas–droplet turbulent dispersion coefficient</td>
</tr>
<tr>
<td>$G$</td>
<td>Production term in turbulence transport equation</td>
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<tr>
<td>$k$</td>
<td>Turbulent kinetic energy</td>
</tr>
<tr>
<td>$l$</td>
<td>Inter-parcel distance</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>Intra-phase mass-transfer rate</td>
</tr>
<tr>
<td>$N$</td>
<td>Droplet number density, or droplet number in a tracked parcel</td>
</tr>
<tr>
<td>$N_p$</td>
<td>Number of droplet phases</td>
</tr>
<tr>
<td>$P$</td>
<td>Proximity function (Lagrangian model) or pressure</td>
</tr>
<tr>
<td>$q_{oi}$</td>
<td>Gas–droplet fluctuating velocity correlation</td>
</tr>
<tr>
<td>$r$</td>
<td>Volume fraction, or radial distance</td>
</tr>
<tr>
<td>$R$</td>
<td>Radial distance (mm)</td>
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<tr>
<td>$R_{1/2}$</td>
<td>Half radius (mm)</td>
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<td>$Re$</td>
<td>Reynolds number</td>
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<tr>
<td>$S_{TD}$</td>
<td>Turbulence modulation term in turbulence transport equations</td>
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<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$u'$</td>
<td>Fluctuating velocity</td>
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<tr>
<td>$\overline{u'u'}$</td>
<td>Axial kinetic stress</td>
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<td>$\overline{u'v'}$</td>
<td>Turbulent shear stress</td>
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<tr>
<td>$u_t$</td>
<td>Instantaneous relative velocity between two droplets</td>
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<tr>
<td>$U$</td>
<td>Mean velocity or axial mean velocity</td>
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<td>$v$</td>
<td>Droplet volume</td>
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<td>$\overline{v'v'}$</td>
<td>Radial kinetic stress</td>
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<tr>
<td>$V$</td>
<td>Radial mean velocity</td>
</tr>
<tr>
<td>$V_{R_o}$</td>
<td>Local instantaneous relative velocity between the droplet and gas phases</td>
</tr>
<tr>
<td>$V_d$</td>
<td>Eddy-droplet drift velocity</td>
</tr>
<tr>
<td>$\langle</td>
<td>V'</td>
</tr>
<tr>
<td>$X$</td>
<td>Axial distance</td>
</tr>
<tr>
<td>$Z$</td>
<td>Ratio of axial distance from nozzle and nozzle diameter</td>
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**Greek symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>$\beta$</td>
<td>Coalescence kernel (Eulerian model)</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Turbulent dissipation rate</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Laminar or turbulent viscosity</td>
</tr>
<tr>
<td>$\nu_0'$</td>
<td>Turbulent kinematic viscosity of gas</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density (kg/m$^3$)</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Turbulent Prandtl or Schmidt ($Sc$) number</td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>Eddy lifetime</td>
</tr>
<tr>
<td>$\tau_{0i}$</td>
<td>Droplet relaxation time</td>
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<tr>
<td>$\tau_{0i}'$</td>
<td>Eddy-droplet interaction time</td>
</tr>
<tr>
<td>$\zeta_r$</td>
<td>Relative velocity in cross-trajectory model</td>
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</tbody>
</table>
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. [1] and Berlemont et al. [2] have used Lagrangian calculations in their analyses. In the Eulerian approach, the airflow and droplet phases are both treated as interpenetrating, interacting continua. 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 [3] and Issa et al. [4]. The gas-flow turbulence is treated similarly in both the Eulerian and Lagrangian approaches.

Mostafa and Mongia [5] have shown that both the Eulerian and the 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 coalescence 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 confidence in future simulations, (2) to determine whether each approach predicts similar droplet turbulent dispersion and coalescence 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.

2. Model description

2.1. Eulerian model

In this approach, the gaseous and droplet phases are treated as separate interpenetrating continua, with the transport of both phases being modelled within an Eulerian framework. The two-fluid model of Simonin [3] is used to simulate the turbulent dispersion of the droplet phase, while the standard $k–\varepsilon$ turbulence model [6] is employed to predict the turbulent motion of the gas phase. We use a steady, two-dimensional (axisymmetric, cylindrical coordinate system) form of the Eulerian model to predict the turbulent dispersion and coalescence of droplets within the spray.
2.2. Mass balance

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 steady-state continuity equation takes the general form:

\[
\nabla \cdot (\rho U_i) = \sum_{j=1}^{N_p} \left( \dot{m}_{ij} - \dot{m}_{ji} \right).
\]

(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 Eq. (1) represents inter-phase mass-transfer as droplets move from one size group into another due to coalescence, 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.

2.3. Momentum balance

The steady-state momentum equations for the gaseous and droplet phases are, respectively,

\[
\nabla \cdot (\rho \rho_0 U_0 U_0) = -r_0 \nabla P + \nabla \cdot \left( r_0 \rho_0 \left( \nabla U_0 + (U_0)^T \right) \right) - \frac{2}{3} \nabla (r_0 \rho_0 \mu_0) - \frac{2}{3} \nabla (r_0 \mu_0 \nabla \cdot U_0) + \sum_{j=1}^{N_p} c_{0j}^{(d)} V^R_{0j},
\]

(2)

\[
\nabla \cdot (r_i \rho_0 U_i U_i) = -r_i \nabla P + \nabla \cdot \left( r_i \mu_0 \left( \nabla U_i + (U_i)^T \right) \right) - \frac{2}{3} \nabla (r_i \rho_0 k_i) - \frac{2}{3} \nabla (r_i \mu_0 \nabla \cdot U_i) - c_{0i}^{(d)} V^R_{0i}
\]

\[
+ \sum_{j=1}^{N_p} (\dot{m}_{ij} U_j - \dot{m}_{ji} U_i),
\]

(3)

where \(N_p\) momentum equations are required to represent a range of droplet-size classes, given that different velocities are known to develop among droplets of different sizes for the jet flows investigated here. The first terms on the left- and right-hand sides of these equations appear in the conventional momentum transport equations, and represent the convective- and pressure-gradient components of momentum transport, respectively. The second, third, and fourth terms on the right-hand side of these equations come from the closure model of the turbulent Reynolds stresses (based on the eddy–viscosity hypothesis) to describe the turbulent diffusion of momentum, as explained by Simonin [3]. The fifth term in both momentum equations represents the inter-phase drag force, which develops when a relative velocity \(V^R_{0i}\) emerges between the gaseous phase and the droplet phases. The inter-phase drag term appears in the gaseous phase momentum equation as a sum of all drag contributions from each of the droplet-size classes. The last term in the droplet momentum equation describes the inter-phase transfer of momentum between phases \(i\) and \(j\) due to coalescence.

The local instantaneous relative velocity \(V^R_{0i}\) between the droplet phases and the gaseous phase is given by equation:

\[
V^R_{0i} = (U_i - U_0 - V^d_i),
\]

(4)

where \(V^d_i\) is the turbulent drift velocity, which accounts for the dispersion of droplets by the turbulent motion of the gaseous phase. The inter-phase drag coefficient \(c_{0i}^{(d)}\), which is a local instantaneous value accounting for both the mean and fluctuating components of the relative velocity, is defined by the following expression:

\[
c_{0i}^{(d)} = \frac{3}{4} \frac{C_D}{d} r_i \rho_0 ||V_i||,
\]

(5)

where \(C_D\) is the drag coefficient, given by the well-known empirical correlation:

\[
C_D = \frac{24}{Re} (1 + 0.15Re^{0.87}), \quad Re = \frac{\rho_0 ||V_i|| d}{\mu_0} \quad (Re < 1000).
\]

(6)
The local instantaneous slip velocity \( \langle |V_i| \rangle \) is given by equation:

\[
\langle |V_i| \rangle = \sqrt{V_{i0}^2 + \left( 2k_i + 2k_0 - 2g_0 \right)}.
\]  

(7)

The term inside the bracket of Eq. (7) represents the fluctuating component of the relative velocity. The turbulent kinetic energy \( k \) and the correlation between gas–droplet fluctuating velocities \( q_{0i} \) are defined by the following expressions:

\[
k = \frac{1}{2}(u'u' + v'v' + w'w'), \quad q_{0i} = \left( u'_{0i}u'_{0i} + v'_{0i}v'_{0i} + w'_{0i}w'_{0i} \right).
\]  

(8a, b)

Simonin [3] has derived an expression for the turbulent drift velocity \( V_i^d \) by investigating the limiting case, when the droplets are small enough to follow the turbulent motion of the gas flow exactly, so that a diffusion mechanism alone is sufficient to describe the transport of droplet volume fraction by the turbulent gas flow. The equation thus derived for the drift velocity \( V_i^d \) is

\[
V_i^d = -D_{0i}^l \left( \frac{1}{r_i} \nabla r_i - \frac{1}{r_0} \nabla r_0 \right).
\]  

(9)

Deutsch and Simonin [7] have demonstrated theoretically that the gas–droplet turbulent dispersion coefficient \( D_{0i}^l \) can be adjusted from the value adopted in the limiting case (when small droplets disperse in a turbulent flow) to take into account reduced dispersion rates for larger droplets, which have greater inertia and are therefore unable to follow exactly the turbulent motion of the gas flow. They have shown that the gas–droplet turbulent dispersion coefficient \( D_{0i}^l \) is related to two turbulent characteristics of the gas and droplet phases: the gas–droplet fluctuating velocity correlation \( q_{0i} \), and an eddy-droplet interaction time \( \tau_{0i}^e \), as follows:

\[
D_{0i}^l = \frac{1}{3} q_{0i} \tau_{0i}^e.
\]  

(10)

Small droplets have relatively high values of \( D_{0i}^l \) because they have low inertia and are able to follow the gas flow turbulent motions closely. Therefore, the droplet and gas fluctuating velocities are highly correlated, and the time that a droplet and an eddy interact \( \tau_{0i}^e \) is only limited by the characteristic life span of the eddy \( \tau_{0i}^e \) within which the droplet resides. However, large droplets attain relatively low values of \( D_{0i}^l \) because they have greater inertia, and therefore their motion is not correlated closely with the turbulent motion of the gas flow. In addition, the interaction time \( \tau_{0i}^e \) of large droplets is shorter than the characteristic eddy life span \( \tau_{0i}^e \), because the relatively high inertia of large droplets assists them in passing through eddies, a phenomenon otherwise known as the cross-trajectory effect [8].

### 2.4. Turbulence model

The \( k-\varepsilon \) turbulence model described by Launder and Sharma [6] is used to model the transport of turbulence in the gas phase, with additional terms included in the equations to model the attenuation of gas-phase turbulence (or turbulence damping) by the presence of the fine droplets, a phenomenon discussed by Gore and Crowe [9]:

\[
\nabla \cdot \left( r_0 \rho U_0 k_0 \right) = \nabla \cdot \left( r_0 \frac{\mu_0}{\sigma_k} (\nabla k_0) \right) + r_0 (G - \rho_0 e_0) + S_{TD},
\]  

(11)

\[
\nabla \cdot \left( r_0 \rho U_0 e_0 \right) = \nabla \cdot \left( r_0 \frac{\mu_0}{\sigma_0} (\nabla e_0) \right) + r_0 \frac{e_0}{k_0} (C_1 G - C_2 \rho_0 e_0) + \frac{e_0}{k_0} C_3 S_{TD}.
\]  

(12)

The first terms on the left- and right-hand sides of these equations appear in the standard scalar transport equations and represent the convective and diffusive components of scalar transport, respectively. The second term on the right-hand side represents both the production of turbulence by shear (or mean velocity gradients) and the dissipation of turbulent energy by viscous action at the smallest (Kolmogorov) turbulence scales, where \( G \) is the production term calculated as follows:

\[
G = \mu_0 U \cdot \left( \nabla U_0 + (\nabla U_0)^T \right) - \frac{2}{3} \nabla \cdot U_0 (\mu_0 \nabla \cdot U_0 + \rho_0 k_0)
\]  

(13)
and $\varepsilon$ is the turbulent dissipation rate. The third term on the right-hand side of Eqs. (11) and (12) represents the damping or destruction of turbulence by the presence of the droplets, where the source term $S_{TD}$ is defined as

$$S_{TD} = \sum_{j=1}^{N_p} c_{ij}^{(d)} \left[ \left( q_{ij} - 2 k_0 \right) + \nu_j^d \cdot \nu_j^R \right],$$

(14)

Eq. (14) is derived directly from the instantaneous fluid momentum equations [3]. The constants $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{\kappa}$, and $C_{\sigma}$ take on values of 1.6, 1.92, 1.0, and 1.3, respectively, which were determined by Launder and Sharma [6] and retuned by McGuirk and Rodi [10] for a turbulent round jet. Simonin [3] has found a value for $C_{3\kappa}$ of 1.2.

The droplet-phase turbulence $k_i$ is not modelled using a transport equation. Rather, an analytical expression based on Tchen’s theory [11] of the dispersion of discrete particles by steady, homogeneous turbulent fluid motions is employed to relate droplet-phase turbulence $k_i$ to the gas-phase turbulence $k_0$, as follows:

$$k_i = \frac{\tau_{0i}}{\sigma^T_i} \frac{q_{0i}}{\sigma_0} k_0,$$

(15)

where $\tau_{0i}$ is the eddy-droplet interaction time, and $\sigma_{0i}$ is the droplet relaxation time, which is a measure of the inertial effects acting on the droplet. The droplet–gas fluctuating velocity covariance $q_{0i}$ is modelled using the following analytical expression:

$$q_{0i} = 2 k_i,$$

(16)

which is also derived within the framework of Tchen’s theory.

### 2.5. Characteristic time scales

Three time-scales have been adopted above in order to characterise the droplet flow. The characteristic time or lifespan of the energetic turbulent eddies $\tau_{0i}$ and the droplet relaxation time $\tau_{0i}^F$ are given, respectively, by

$$\tau_{0i} = \frac{3}{2} C_{\mu} \frac{k_0}{\varepsilon_0}, \quad \tau_{0i}^F = \frac{4}{3} \frac{\rho_i}{\rho_0} \frac{d}{C_D \langle |V_R| \rangle},$$

(17a, b)

where the constant $C_{\mu}$ takes a value of 0.09. The eddy-droplet interaction time is written as

$$\tau_{0i} = \frac{\tau_{0i}}{\sigma_0^T} \left[ 1 + C_{i} \tilde{\varepsilon} \right]^{-\frac{1}{2}}, \quad \tilde{\varepsilon} = \frac{\langle |V_R| \rangle}{\sqrt{\frac{k_0}{3} \varepsilon_0}}.$$  

(18)

The bracketed term of Eq. (18), which was first developed by Csanady [8], accounts for the cross-trajectory effect when large droplets pass through turbulent eddies due to their high relative inertia. According to Deutsch and Simonin [7], the parameter $C_i$ takes values of 0.45 in the direction parallel to the mean relative velocity and 1.8 in the orthogonal directions. However, we calculate the eddy-droplet interaction time using the radial value for $C_i$ of 1.8, because a sensitivity analysis has shown that the axial turbulence dispersion force is relatively unimportant for the spray investigated in this work, since it is swamped by the mean drag force in the axial momentum equation. The turbulent Schmidt number $\sigma_0^T$ for turbulent scalar diffusion in an axisymmetric round jet has been measured experimentally by Antonia and Bilger [12] and takes an average value of approximately 0.67.

### 2.6. Turbulent viscosity

The turbulent viscosity of the gas phase $\mu_0$ in the $k-\varepsilon$ turbulence model is defined by the following expression [6]:

$$\mu_0^T = \frac{2}{3} \rho_0 k_0 \tau_{0i} = C_{\mu} \rho_0 \frac{k_0^2}{\varepsilon_0}.$$  

(19)
Simonin [3] has developed an expression for the turbulent viscosity of the droplet phase \( \mu_i \), which is consistent with Tchen's theory:

\[
\mu_i = \rho_i \left( \frac{\tau_0 \sigma_0}{3} d_{0i} + \frac{1}{2} \frac{\tau_0^E}{3} k_i \right).
\]

(20)

2.7. Coalescence model

Coalescence of droplets in a poly-disperse spray can be mathematically described by the population balance equation [13], 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 coalescence. Hounslow et al. [13] have produced a discretised form of the population balance for coalescence 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:

\[
\frac{v_{i+1}}{v_i} = 2.
\]

(21)

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 Fig. 1.

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. [13] have derived the following discretised form of the population balance for coalescence:

\[
\frac{dN_i}{dt}_{\text{agg}} = \sum_{j=1}^{i-2} 2^{j-i+1} \beta_{i-1,j} N_{i-1} N_j + \frac{1}{2} \beta_{i-1,i-1} N_i^2 - N_i \sum_{j=1}^{i-1} 2^{j-i} \beta_{i,j} N_j - N_i \sum_{j=i}^{N_p} \beta_{i,j} N_j.
\]

(22)

Here \( N_i \) is the number of droplets per unit volume in the \( i \)th droplet-size class, and \( \beta_{i,j} \) is the coalescence 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 Eq. (22) represents the birth of a droplet in the \( i \)th size class due to coalescence 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 coalescence 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 coalescence 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 coalescence 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 Eq. (22) 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 Eq. (22) 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 coalescence 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 Eq. (1) when coalescence 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 coalescence. 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 coalescence.

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 coalescence (Eq. (22)). 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 Eq. (1). The following set of equations, which represent every inter-phase mass-transfer combination possible, has thus been derived:

\[
\dot{m}_{i+1,j} = \sum_{j=1}^{i} 2^{-i} \beta_{i,j} N_i N_j (\bar{v}_i \rho), \quad i = 1 \rightarrow (N_p - 1),
\]

\[
\dot{m}_{i+1,j} = \beta_{i,j} N_i N_j (\bar{v}_j \rho), \quad i = (j + 1) \rightarrow (N_p - 1), \quad j = 1 \rightarrow (N_p - 2),
\]

where the inter-phase mass-flow \( \dot{m} \) of droplets is calculated from the inter-phase number flowrate by multiplying it with the density \( \rho \) 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 [14] have shown that the coalescence kernel \( \beta \) has the following form:

\[
\beta = \beta_0 (D_i + D_j)^2 u_t,
\]

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

\[
u_t = \sqrt{(U_i - U_j)^2 + (2k_t + 2k_j - 2\overline{u_i' u_j'})}.
\]

We also assume that the correlation between fluctuating droplet velocities (or correlated 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). Thus, this paper is only able to demonstrate whether coalescence due to average-droplet velocity differences and non-correlated droplet turbulence are modelled similarly using the Lagrangian and Eulerian approaches. As a starting point, we have chosen an arbitrary value for the coalescence efficiency \( \beta_0 \), which has the same order of magnitude as the coalescence efficiency measured by other workers, such as Beard et al. [15] for water droplets.

### 2.8. Lagrangian model

Details of the Lagrangian modelling approach have been reported elsewhere [16] and only a brief description is provided here. The Reynolds-averaged Navier–Stokes equations together with the \( k-\varepsilon \) turbulence
model are used to simulate the airflow patterns. Parcels of droplets are tracked simultaneously in three-dimensional space and with time by solving Newton’s law of motion, with drag and added mass forces (a very small effect) being accounted for in the simulations. Note that a transient, three-dimensional simulation is required in order to properly model the interaction of droplet parcels throughout time and space. The turbulent effect is included within the droplet-parcel transport model using the eddy-lifetime method of Gosman and Ioannides [17]. The gas/discrete-phase coupling is accounted for via the drag force term, which is added to the gas momentum equation as a source.

2.9. Coalescence model

The Lagrangian coalescence model is a modification of the O’Rourke model [18], for which parcels of droplets are tracked simultaneously in three-dimensional space and with time. 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. [1] have shown that the collision frequency $\nu$ between the collector and contributor parcels is proportional to the mean number density, a collision cross-sectional area, and a relative velocity, as follows:

$$\nu \propto \frac{N_j \pi}{V} (D_i + D_j)^2 u_r,$$

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 Eq. (27) becomes

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

where $b_1$ is an empirical proportionality constant, which is inversely proportional to the constant $\beta_0$ in the Eulerian approach. A “proximity” function is derived from Eq. (28), as follows:

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

which effectively represents the probability of collision between two parcels over a given time interval $\Delta t$. 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 $P_c$:

$$P \geq P_c \equiv \frac{b_1 \log 0.5}{1.5}.$$

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:

$$D^3 = D_i^3 + D_j^3.$$

Note that we use the empirical constant $b_1$ to match the predictions of the Lagrangian and Eulerian approaches for one set of spray conditions, holding it constant for all subsequent coalescence predictions that use different sets of spray conditions. Both models should predict the same amount of coalescence for a given set of constants ($\beta_0$ for the Eulerian approach and $b_1$ for the Lagrangian approach), irrespective of the droplet number density and jet velocity.

3. Boundary conditions

The round jet spray investigated experimentally by Nijdam et al. [19] is used here as a case study. The experimental apparatus consisted of a wind tunnel and a nozzle (a long thin tube, 9.8 mm in diameter, located
centrally at the exit plane of wind tunnel), which generated a round air jet within a co-flow of air with velocities of approximately 23 m/s and 2.4 m/s, respectively. The co-flow had a turbulence intensity of 1.4%. The nozzle configuration is shown in Fig. 2. The air jet was laden with a dispersion of non-evaporating turpentine droplets ($\rho = 810 \text{ kg/m}^3$) in the size range from 1 to 90 mm, which were produced by an ultrasonic nebulizer located upstream of the nozzle. A phase-Doppler anemometer (PDA) was used to measure the axial velocity and volume fraction of the droplets within the jet at various locations downstream of the nozzle. The gas mean velocity and turbulence profiles were taken to be the same as the corresponding profiles for the 5 $\mu$m droplets, since the Stokes number for these droplets, which is defined as the ratio of the droplet relaxation time $s_F$ to the eddy-droplet interaction time $s_t$, was typically of order 0.01 [19]. Mathematical expressions fitted to the experimental inlet boundary profiles for gas turbulent kinetic energy $k$, droplet axial and radial mean velocities $U$ and $V$, and droplet volume fraction $r$ are given in Table 1. The gas turbulent energy dissipation $\varepsilon$ was extracted from the measured gas turbulent kinetic energy, gas turbulent shear stress, and gas axial velocity gradient profiles using the turbulent viscosity and the Boussinesq hypothesis for shear stress. The total droplet flow for this base case was approximately 2 ml/min. Note that the droplet-size distribution is discretised according to Eq. (21), as indicated by the droplet diameters given in the peak volume fraction $r_0$ column of Table 1, so that the population balance discretisation of Hounslow et al. [14] can be adopted in the Eulerian coalescence model.

4. Numerical simulations

A commercially available computational fluid dynamics (CFD) program called ANSYS CFX4 is used to solve the equation sets for the Eulerian and Lagrangian approaches described above. This program employs Fig. 2. Spray nozzle configuration (not to scale).
Table 1

<table>
<thead>
<tr>
<th>Variable</th>
<th>Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Excess axial mean velocity (m/s) ( \dot{U}_e )</td>
<td>(1) Peak excess axial mean velocity, ( \dot{U}<em>{e0} ), ( \dot{U}</em>{e0} = -0.02951d + 22.3676 )</td>
</tr>
<tr>
<td>Radial mean velocity (m/s) ( V = 0 )</td>
<td>where ( d ) is droplet diameter (( \mu )m) ( \equiv n_1 ) = 4.4466, ( n_2 ) = 2.0400, ( R_{U2U} ) = 5.095</td>
</tr>
<tr>
<td>Volume fraction ( r = r_0 \exp[-A(R/R_{U2VF})^n] )</td>
<td>(2) ( A = 0.6942 ), ( n = 2.1543 ), ( R_{U2VF} ) = 2.8058</td>
</tr>
<tr>
<td>Gas turbulent kinetic energy (m(^2)/s(^2)) ( k )</td>
<td>(1) ( A = 2.192 ), ( B = 4.973 ), ( C = 0.220 ), ( D = 30.0 ), ( n = 1.438 )</td>
</tr>
<tr>
<td>Gas turbulent energy dissipation (m(^2)/s(^3)) ( \varepsilon )</td>
<td>(1) ( D = 0.0098 ) m</td>
</tr>
</tbody>
</table>

A structured mesh and a finite volume formulation to solve the partial differential equations. A value for the turbulence constant \( C_{1e} = 1.55 \) is chosen in both the Eulerian and Lagrangian gas turbulence equations, even though McGuirk and Rodi [10] have found a value of 1.6 for a turbulent round jet, because Nijdam et al. [20] have shown that this new value produces better agreement between the predicted and experimental gas axial mean velocity decay.

4.1. Eulerian model

An axisymmetric cylindrical coordinate system is chosen to represent the jet in order to reduce the problem to two dimensions. A second-order upwind differencing scheme is used to discretise the convection terms in the momentum equations, while the Van Leer differencing scheme is employed to discretise the convection terms in the volume fraction and turbulence equations. In addition to under-relaxing the momentum and turbulence equations, the drift velocities and the fourth and fifth terms of the momentum equations (Eqs. (2) and (3)) are also under-relaxed to reduce instabilities in the solution. Finally, false time steps of 0.001 s are required on every momentum equation and double precision is necessary in all calculations in order to achieve convergence. Details of the numerical techniques employed are found in the ANSYS CFX4 user manual [21].

The droplet-size distribution is discretised into 15 size classes, so that 15 sets of continuity and momentum equations are solved for the droplet phase. The grid has 10 evenly spaced nodes across the half-width of the nozzle. The distance between nodes gradually expands in the cross-stream direction towards the edge of the flow domain, which computational tests have shown is sufficiently far from the nozzle to not affect the solution significantly. The distance between nodes in the axial direction also expands away from the nozzle. The grid has approximately 2500 nodes, and the converged solution does not change significantly when the number of nodes is quadrupled. Convergence of the solution is achieved within 1000 iterations using the grid and numerical scheme described above. Here, the convergence criterion is satisfied when the total sum of the mass residuals for the control volumes falls below the tolerance value of \( 10^{-10} \) kg/s, which is approximately \( 10^{-4} \% \) of the total droplet inflow.

4.2. Lagrangian model

Droplet parcel trajectories are calculated using a three-dimensional simulation. The droplet parcels are introduced at the inlet in the form of a round spray, with the velocity and size distribution specified according to the measured radial profiles given in Table 1. A fully coupled gas–droplet calculation is computationally expensive; therefore, a steady sequential droplet tracking simulation without coalescence is conducted initially in order to determine the gas flow-field. This fixed gas flow-field is subsequently used in the time-dependent droplet coalescence calculation. Through a case study, we found that this simplification does not affect the predicted droplet-size distribution at the domain outlet. There are approximately 20,000 droplet parcels within
the flow domain at any given moment. The time step of 0.0004 s is approximately two orders of magnitude smaller than the minimum droplet residence time within the flow domain. The droplet size, velocity, and number at various locations throughout the spray are averaged over a sufficient number of time steps that a quasi-steady state of the droplet flow is established.

The three-dimensional grid has approximately 120,000 nodes, and the predictions do not change significantly when a grid of 370,000 nodes is used. The grid spacing, which is similar to the Eulerian grid, is finest at the nozzle exit and becomes gradually coarser away from the nozzle. Further details of the Lagrangian numerical procedure can be found in Guo et al. [16].

5. Results and discussion

5.1. No coalescence case

Fig. 3 compares the Lagrangian and Eulerian predictions of the axial mean velocity profiles of the droplets at various axial locations downstream of the nozzle for the base case droplet flow of 2 ml/min. Clearly, both models predict similar decay rates for the axial mean velocity at the centre-line. Fig. 4 shows that the spreading rates of droplets of different sizes are also similarly predicted by both models. Fig. 4 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 [20]. Thus, both Lagrangian and Eulerian approaches are able to predict the main features of a turbulent spray, including the decay of centre-line velocity and the radial dispersion of droplets with axial distance from the nozzle.

5.2. Coalescence case

The Lagrangian and Eulerian models have first been fitted to each other for one set of spray conditions (with a total droplet flow of 2 ml/min) by arbitrarily choosing a value for the Eulerian parameter $b_0$ of 4.18, and adjusting the Lagrangian parameter $b_1$, which takes a value of 3.2, 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 ($b_0 = 2.09$) – has also been 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 coalescence efficiencies. Here, the coalescence efficiency is a number that multiplies the coalescence kernel (Eq. (25)) or critical coalescence probability (Eq. (30)), 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 coalescence parameter $b_1$ is inversely proportional to the Eulerian coalescence parameter $b_0$.

Fig. 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 coalescence parameters ($b_1$ and $b_0$). 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 coalescence calculations. Secondly, this result implies that a sufficient number of droplet-size classes (15 droplet-size classes) and parcels (about 20,000 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 Eq. (21)) is sufficiently fine, and the time step (0.0004 s) 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 coalescence rates over a wide range of droplet flows and for different coalescence efficiencies.

![Graph showing comparison between Lagrangian and Eulerian predictions of the Sauter-mean diameter $D_{32}$](image_url)

Fig. 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 coalescence 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 Fig. 6. Similar agreement is also found when simulating the downstream development of a mono-size (36 μm) droplet dispersion, as shown in Fig. 7. Thus, both models also similarly predict coalescence of droplets in sprays with different droplet-size distributions at the nozzle exit. Indeed, Nijdam et al. [22] have confirmed that both the Lagrangian and Eulerian approaches are consistent with each other by comparing the predictions of these models with two sets of experimental coalescence data, each set having different droplet-size distributions and velocity profiles at the nozzle exit.

Fig. 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).

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 Fig. 6. Similar agreement is also found when simulating the downstream development of a mono-size (36 μm) droplet dispersion, as shown in Fig. 7. Thus, both models also similarly predict coalescence of droplets in sprays with different droplet-size distributions at the nozzle exit. Indeed, Nijdam et al. [22] have confirmed that both the Lagrangian and Eulerian approaches are consistent with each other by comparing the predictions of these models with two sets of experimental coalescence data, each set having different droplet-size distributions and velocity profiles at the nozzle exit.

![Graph showing comparison of Lagrangian and Eulerian predictions of droplet-size distribution](image1)

![Graph showing comparison of Lagrangian and Eulerian predictions of droplet-size distribution](image2)

Fig. 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 2

<table>
<thead>
<tr>
<th>Droplet flow (ml/min)</th>
<th>Velocity</th>
<th>$D_{32}$ @ 30D (μm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Lagrangian</td>
</tr>
<tr>
<td>10</td>
<td>1×</td>
<td>51.8</td>
</tr>
<tr>
<td>10</td>
<td>2×</td>
<td>45.5</td>
</tr>
<tr>
<td>20</td>
<td>2×</td>
<td>52.5</td>
</tr>
</tbody>
</table>
The effect of the gas-flow velocity and turbulence on the extent of coalescence is shown in Table 2. 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 coalescence within the spray, so that $D_{32}$ at 30 nozzle diameters reduces from 52 $\mu$m to 45 $\mu$m. When the droplet flow is doubled from 10 ml/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 $\mu$m to 53 $\mu$m. According to the Lagrangian predictions, $D_{32}$ at 30 nozzle diameters only increases marginally from 51.8 $\mu$m to 52.5 $\mu$m when the gas velocity is doubled while keeping the droplet number density constant. Thus, according to a CFD sensitivity analysis, the extent of coalescence 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 industrial 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 coalescence. Table 2 shows that both the Eulerian and Lagrangian models predict similar trends.

We have found that the computational time required to complete a coalescence 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. [22], 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 as a continuum, with a single velocity at any point in space. 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.

6. Conclusions

Both Lagrangian and Eulerian approaches are able to simulate droplet turbulent dispersion and coalescence 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 coalescence 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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References