Development of an efficient statistical volumes of fluid–Lagrangian particle tracking coupling method

H. Grosshans*,†, R.-Z. Szász and L. Fuchs

Division of Fluid Mechanics, Lund University, Box 118, 22100 Lund, Sweden

SUMMARY

The breakup of a liquid jet into irregular liquid structures and droplets leading to the formation of a dilute spray has been simulated numerically. To overcome the shortcomings of certain numerical methods in specific flow regimes, a combined approach has been chosen. The intact liquid core, its primary breakup and the dense spray regime are simulated using the volumes of fluid (VOF) method in combination with LES, whereas the Lagrangian particle tracking (LPT) approach in the LES context is applied to the dilute spray regime and the secondary breakup of droplets. A method has been developed to couple both simulation types on a statistical basis. This statistical coupling approach (SCA) reflects the dominating physical mechanisms of the two-phase flow in each regime to a high degree. The main benefit of the SCA is computational efficiency as compared with the more straightforward approach where one follows each structure, denoted here as the direct coupling approach. The computational benefits stem from the reduction of computational time since the VOF simulation is run only until statistical convergence and not during the whole spray development. A second benefit using the SCA is the possibility to use the stochastic parcel method in the LPT simulation whereby a large number of droplets may be handled. The coupling approach is applied to the atomization of a fuel jet in a high pressure chamber, demonstrating the gain of efficiency of the SCA as compared with direct coupling approach. Copyright © 2014 The Authors. International Journal for Numerical Methods in Fluids published by John Wiley & Sons Ltd.

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1. INTRODUCTION

A typical atomizing two-phase flow, developed from an injection nozzle, passes through various flow regimes. At the nozzle, the intact core of the liquid jet can be observed. Turbulence in the liquid jet and instability mechanisms, dominantly cavitation in the injection nozzle and aerodynamic instabilities, causes the primary breakup of the jet [1]. The region where the jet is completely disintegrated but the liquid volume fraction is still high is called the dense spray region. Because of turbulent dispersion, the spacing between the droplets increases, and the liquid volume fraction decreases. Secondary breakups lead to decreasing droplet sizes and an enhancement of the evaporation of the droplets. This is called the dilute spray region.

The primary breakup, the dense spray region and the structure of dilute sprays have been studied experimentally (e.g. in [2–5]), but as this region is optically dense, it is difficult to measure. Measurements are limited to identifying rather large liquid structures or global parameters of the spray. Thus, to obtain a higher spatial and temporal resolution, numerical simulations need to be performed.

*Correspondence to: H. Grosshans, Division of Fluid Mechanics, Lund University, Box 118, 22100 Lund, Sweden
†E-mail: holger.grosshans@energy.lth.se

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Because of different phenomena that dominate and have to be covered in simulations in the different flow regimes, different numerical methods show to be the most appropriate. The intact liquid core and the dense spray region are often simulated by applying an interface resolving technique, such as the volumes of fluid (VOF) method [6, 7], the level set method [8] or a combination of both [9–11]. In the VOF method, both phases are described in Eulerian framework, and an additional equation is solved for the liquid volume fraction to track the position of the gas–liquid interface. The main advantage is that it can handle liquid structures of any shape, and also, that the wakes caused by droplets are resolved on the computational grid. This limits the use of models in the simulation to a minimum and therefore leads to a high accuracy. Drawback is the high computational cost, as a fine resolution is required to achieve this high accuracy.

The dilute spray region is usually simulated by applying the Lagrangian particle tracking (LPT) method, for example, in [12, 13]. In this region, the liquid phase is dispersed, the droplets are small, and the surface tension tends to give the droplets a spherical shape. Thus, each droplet can be tracked individually in Lagrangian framework, and models can be applied to describe the droplet behaviour such as secondary breakup, aerodynamic drag or evaporation. The advantage of this method over the VOF method is that the required grid resolution is several orders lower, and therefore, the computational speed is higher. The drawback is that the droplets models are established for a certain validity range which, when violated, decreases the accuracy of the method.

The aim of this paper is to simulate two-phase flows in various flow regimes. Therefore, a coupling approach is developed, which links the VOF method for the dense spray region and the LPT method for the dilute spray region. To study the flow time resolved and to capture the dynamic effects of the spray breakup, an LES is performed.

Previous VOF–LPT coupling approaches apply the direct coupling approach (DCA) [14–17]. Here, each droplet that leaves the VOF domain is injected individually in the LPT domain. This is straightforward and gives a clear and accurate description of the complete development of the liquid phase.

The major aim of this work is to develop a coupling method of a high computational efficiency and at the same time to reflect the physical principles of the flow to a high degree. Thus, a method is developed to couple both simulations on a statistical basis and is consequently named statistical coupling approach (SCA). Here, only the statistical distribution of the droplet field properties is transferred from VOF to LPT instead of transferring each droplet individually. Compared with the aforementioned approach, this leads for two reasons to a computational significantly faster method: first, the VOF simulation has to be run only until statistical convergence and not during the whole spray development. And second, in the LPT simulation, the stochastic parcel method can be applied, which is much more efficient when applied to the huge number of droplets in a spray, than tracking each droplet individually as in other coupling approaches. For statistically stationary sprays, the accuracy of the proposed approach is only marginally lower than that of the straightforward coupling approach. For time-dependent injection, one may use the proposed approach, with similar high efficiency as for the stationary case, if one is interested in phase averaged data.

A test case is simulated to compare the performance of SCA and DCA.

2. GOVERNING EQUATIONS AND NUMERICAL METHODS

2.1. Primary breakup and dense spray region

The VOF method is used to handle the liquid and gaseous phases. The flow field is described in Eulerian framework by the incompressible, isothermal Navier–Stokes equations for multiphase flows without phase changes. The equations are non-dimensional, normalised by the nozzle diameter ($d_{\text{noz}}$) the injection velocity ($U_{\text{inj}}$), the liquid density ($\rho_l$) and the liquid viscosity ($\mu_l$). Evaporation takes place at the liquid surface, but as the liquid surface to mass ratio in this flow regime is low, evaporation can be neglected [2]. Thus, it is reasonable to assume constant temperature. As the Mach number of the liquid flow is approximately 0.3, it is reasonable to assume incompressibility for the liquid. However, the Mach number of the gaseous phase is in a region very close to the nozzle up to 0.7, hence, there might be small errors introduced. Mass conservation is given by
Equation (1a) and momentum conservation by Equation (1b).

\[ \frac{\partial u_i}{\partial x_i} = 0, \quad (1a) \]

\[ \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re_{jet}} \frac{\partial}{\partial x_j} \mu \frac{\partial u_i}{\partial x_j} + \frac{\kappa \delta n_i}{We_{jet}}. \quad (1b) \]

The last term on the right-hand side of the momentum equation represents the effect of the surface tension of the liquid at the phase interfaces, where \( \kappa \) is the non-dimensional interface curvature, \( \delta \) is the Dirac function and \( n_i \) a unit vector normal to the interface. The jet Reynolds number \( (Re_{jet}) \) and Weber number \( (We_{jet}) \) are defined as

\[ Re_{jet} = \frac{U_{inj} d_{noz}}{v_l}, \quad (2) \]

\[ We_{jet} = \frac{\rho U_{inj}^2 d_{noz}}{\sigma}. \quad (3) \]

To compute the phase interface, in addition, a transport equation for the liquid volume fraction \( \alpha \) in a computational cell is solved

\[ \frac{\partial \alpha}{\partial t} + \frac{\partial u_i \alpha}{\partial x_i} = 0, \quad (4) \]

where \( \alpha = 1 \) represents a computational cell which is fully filled by liquid, and \( \alpha = 0 \) represents a computational cell which is fully filled by gas. The viscosity \( \mu \) and density \( \rho \) in the momentum equation are non-dimensional parameters, relating to 1 for cells completely filled with liquid and to the gas–liquid viscosity and density ratio for cells completely filled with gas. For cells that contain an interface, \( \mu \) and \( \rho \) obtain a value between 1 and the gas–liquid viscosity and density ratio assuming a linear dependency on \( \alpha \).

The surface tension term in the momentum conservation equation is modelled as described in [18], where the product of the Dirac function and the interface unit normal is in non-dimensional quantities expressed by

\[ \delta n_i = \frac{\partial \alpha}{\partial x_i}. \quad (5) \]

The interface curvature is estimated from the \( \alpha \) field using the direction averaged curvature model [19]. To reduce the computational effort, the curvature is calculated in the direction of the largest normal component. The interface capturing method has shown second-order global accuracy when applied to a transient rising bubble [20]. The maximum error in the curvature for a droplet under static equilibrium using this method has been investigated in [21]. It has been shown that, if the droplet is resolved by ten cells over the diameter, the maximum error for \( \kappa \) is approximately 4%. As the Weber numbers in engines are usually large, the surface tension term is small compared with the other terms in the momentum equation, and the influence of the mentioned error on the solution is small as well.

The governing equations are discretized by the finite difference method. The convective terms are approximated by a third-order accurate scheme, the diffusive and pressure terms by fourth-order schemes and the time derivatives by an implicit second-order backward scheme. The large scale structures in the flow field are simulated by LES, where the discretization scheme applied on a grid acts as a low-pass filter. The grid size, \( h \), is considerably smaller than the largest scale, but it is as well much larger than the Kolmogorov eddies \( (l_0 \gg \eta \gg h) \) for large Reynolds numbers. Therefore, the large scale structures are captured, whereas the small scale structures are filtered out. When applying any spatial filtering to the governing equations, new terms appear, these are called sub-grid-scale (SGS) terms. LES is based on Kolmogorov’s hypothesis: the large scale structures are dependent on the specific flow situation, whereas the behaviour of the small scale structures is
isotropic and geometry independent, that is, universal. If the scales that are filtered out are small enough to be considered as universal, the SGS terms can be closed by a turbulence model. As an indicator for the definition of an appropriate grid size, the size of the Taylor scale eddies can be used, as they are defined to be located between large scale and Kolmogorov scale eddies. In general, it can be stated that the smaller the filter size is, the smaller is the contribution of the SGS terms and the more accurate will be the solution. If the grid is fine enough, the contribution of SGS terms even diminishes and can therefore be neglected. However, the SGS terms also have a function of dissipating energy that is transferred by the energy cascade. To account for dissipation, in this work, the ‘implicit turbulence model’ [22, 23] with no explicit SGS expression is used. By not including explicit dissipation, the overall dissipative properties of the discrete system are reduced. It must be emphasised that one may rely on such a model only if the resolution is fine enough to allow a clear separation of scales of the integral and the dissipative scales. This is reasonable if a considerable part of the turbulence energy spectrum is resolved, that is, the computational grid is fine enough. In that case, the implicit turbulence model is also accurate for the liquid gas interface of droplets: droplets are small, thus, to distort a droplet, the turbulence spectrum needs to contain a significant amount of energy in the small scales. As the largest part of the turbulence energy is transported by large scales, the effect of the small scale motions on the liquid gas interface can be neglected.

In this case, the grid is chosen to be approximately three times finer than the size of Taylor scale eddies.

2.2. Dilute spray region

The continuous gaseous phase is described in Eulerian framework by the Navier–Stokes equations with constant diffusivities and coupled to the liquid phase by two-way coupling [24]. As the spray is dispersed and its droplets are small, the isothermal assumption taken in the dense spray region does not suit any longer, and temperature changes are taken into account. Low Mach number flow is assumed, which means that the density is a function of the temperature only. The continuous phase volume fraction is assumed to be unity. Mass, momentum, energy and mixture fraction conservation are given in dimensional form by Equations (6a)–(6d).

\[
\frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g u_j}{\partial x_j} = \dot{\rho}_{gs}, \tag{6a}
\]

\[
\frac{\partial \rho_g u_i}{\partial t} + \frac{\partial \rho_g u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \mu_g \frac{\partial u_i}{\partial x_j} + \rho_g F_{s,i}. \tag{6b}
\]

\[
\frac{\partial \rho_g T_g}{\partial t} + \frac{\partial \rho_g u_j T_g}{\partial x_j} = \frac{\partial}{\partial x_j} \rho_g D_{th} \frac{\partial T_g}{\partial x_j} + \dot{Q}_s. \tag{6c}
\]

\[
\frac{\partial \rho_g Z}{\partial t} + \frac{\partial \rho_g u_j Z}{\partial x_j} = \frac{\partial}{\partial x_j} \rho_g D_m \frac{\partial Z}{\partial x_j} + \dot{Z}_s. \tag{6d}
\]

\(D_{th}\) and \(D_m\) denote the thermal and mass diffusion coefficients. Source terms for mass, momentum, energy and mixture fraction, \(\dot{\rho}_{gs}, \rho_g F_{s,i}, \dot{Q}_s\) and \(\dot{Z}_s\) are introduced, which account for the coupling from the liquid to the gaseous phase.

The system of equations is closed by the equation of state,

\[
\rho_g = \frac{\rho_{g,in} T_{g,in}}{T_g} = \frac{p_{in}}{R T_g}, \tag{7}
\]

where \(R\) is the specific gas constant, and the subscript ‘\(in\)’ denotes the inlet conditions. Thus, the gas density is only depending on the temperature and is independent of the pressure.
The convective terms are approximated by an up to fifth-order Weighted Essentially Non Oscillatory (WENO) scheme, the diffusive and pressure terms by fourth-order central differences and the time derivatives by an implicit second-order backward scheme. The large scale structures in the flow field are simulated by an LES. The residual stresses are modelled by the ‘implicit’ SGS modelling [22, 23], as discussed in Section 2.1.

The dispersed phase is described by stochastic parcels, which are tracked individually in Lagrangian framework. The number of droplets at a position between \( x \) and \( x + dx \), a velocity between \( u_d \) and \( u_d + d u_d \), a diameter between \( d_d \) and \( d_d + dd_d \), a temperature between \( T_d \) and \( T_d + dT_d \), a distortion parameter between \( y \) and \( y + dy \) and a distortion rate between \( \dot{y} \) and \( \dot{y} + d\dot{y} \) is given by

\[
f(x, u_d, d_d, T_d, y, \dot{y}) dx d u_d dd_d dT_d dy d\dot{y}.
\]

This droplet distribution function is used to express the source terms according to [25] as follows.

\[
\rho_g s = -\frac{\pi}{2} \int f \rho_l d_d^2 d d d d u_d d d d dT d dy d\dot{y}.
\]

\[
\rho_g F_{s,t} = -\frac{\pi}{6} \int f \rho_l \left( d_d^3 \frac{d u_d}{dt} + 3d_d^2 \frac{d d_d}{dt} \right) dx d u_d dd_d dT d dy d\dot{y}.
\]

\[
\dot{Q}_s = -\frac{\pi}{6} \int f \rho_l \left( d_d^3 c_p l dT d dt + 3d_d^2 \frac{d d_d}{dt} h_{lat} \right) dx d u_d dd_d dT d dy d\dot{y}.
\]

\[
\dot{Z}_s = -\frac{\pi}{2} \int f \rho_l d_d^2 d d_d dx d u_d dd_d dT d dy d\dot{y}.
\]

Aerodynamic drag forces are taken into account for the momentum exchange between the gaseous and liquid phases. The acceleration of an isolated, rigid, spherical droplet is according to Newton’s second law of motion given by

\[
\frac{d u_d}{dt} = -\frac{3\rho_g}{4\rho_l d_d} C_w |u_{rel}| u_{rel},
\]

where \( C_w \) is the drag coefficient of the droplet, and \( u_{rel} \) is the velocity of the droplet relative to the air. Following [26], \( C_w \) is defined depending on the droplet Reynolds number, \( Re_d \), as

\[
C_w = \begin{cases} 
\frac{24}{Re_d} \left( 1 + \frac{1}{6} Re_d^{2/3} \right) & \text{for } Re_d \leq 1000. \\
0.424 & \text{for } Re_d > 1000.
\end{cases}
\]

The influence of droplet deformation on the drag and resulting lift forces is not taken into account. The droplet Reynolds number is defined as

\[
Re_d = \frac{u_{rel} d_d}{v_g}.
\]

The virtual mass force accounts for the acceleration of the surrounding gas when a droplet is accelerated. It is shown in [27] that the virtual mass force can be neglected in the dilute spray regime for low gas–liquid density ratios. Faxen forces account for the non-uniform flow around a droplet. As stated earlier, we expect the turbulent scales in the dilute spray regime to be one order larger than the droplet diameters, thus, the flow around droplets can be considered uniform, and Faxen forces can
be neglected. Saffman forces are caused by the rotation of droplets which is caused by velocity gradients in shear flows. In the case considered in this work, the distance between the droplets and the walls is quite large, therefore, the droplets will not be affected by a shear layer and Saffman forces can be neglected. There are no other sources that cause strong rotational forces of the droplets, thus, also Magnus forces are neglected.

For secondary breakup, the bag breakup and the stripping breakup regimes are assumed to be dominant. They are modelled according to [28], which combines the wave breakup model and the Taylor analogy breakup model. The evaporation of liquid mass is taken into account by an evaporation model, which assumes that the droplet is composed of a single component and has a spherical shape with uniform properties [29].

3. COUPLING OF VOLUMES OF FLUID AND LAGRANGIAN PARTICLE TRACKING

In the VOF approach, all liquid structures are resolved by the computational grid, therefore, no additional models are needed besides the modelling of the surface tension term and the SGS terms. This makes the method adequate to simulate a two-phase flow in different regimes. The main drawback of this approach is related to the need for adequate grid resolution of each droplet. In the dilute spray regime, where the droplets are small, high spatial resolution is required, which implies longer computational time with limited gain in accuracy. Thus, the computational costs may be too high to simulate a complete spray using only the VOF method.

In the LPT approach, the volumes of the computational cells are assumed to be much larger than the volume of the droplets. The droplets are assumed not to displace ambient fluid and are considered as mathematical particles, which allows one to track the droplets individually in the Lagrangian framework. This makes the method computationally efficient. However, one must supplement models for certain processes such as secondary breakup, evaporation, aerodynamic interaction with the surrounding gas or droplet–droplet interaction. Such models are usually derived from experiments or analytically for simplified flow situations. The simplifying assumptions that are taken when deriving such models include that the droplets are spherical and they do not interact with each other. Thus, the droplets in the dilute spray regime are assumed to be small (i.e. the droplet–droplet spacing is large as compared with the droplet size and surface tension tends to give the droplets a spherical shape). In such regimes, the LPT is a good approximation. In the intact liquid core and dense spray regime, where primary breakup occurs, the liquid structures are of irregular shape and collisions and aerodynamic interaction among liquid structures are frequent. Therefore, the physical processes in the injection region of the flow are poorly reflected by the LPT method, as shown in [30].

To overcome the drawbacks of both methods, coupling approaches have been developed, linking a VOF simulation of the liquid core and the dense spray regime to an LPT simulation of the dilute spray regime. The DCA, where the physical domain of both simulations overlap, as shown in Figure 1(a), has been developed in the past (c.f. [14–17]). Because of overlapping, it is possible to determine for each liquid structure whether it is adequately described by the VOF or by the LPT framework.

Compared with a full VOF simulation, the physical applicability is only slightly reduced by this coupling approach, as a droplet is only tracked in the LPT frame if it is judged to be within the validity range of the used droplet models. At some downstream point, the spray is diluted and the droplets spherical, the whole spray in downstream direction is described by the LPT method. Compared with the total size of the domain, this downstream point is close to the injection nozzle, therefore, the physical size of the VOF domain is significantly smaller than the one of the LPT domain. This leads as well to a significantly better computational efficiency, as compared with the pure VOF method. The first drawback of the DCA is that each droplet that is injected in the LPT part has to cross the VOF domain first. By nature of the numerical methods, the timestep and the grid size of the VOF simulation are at least one order of magnitude smaller than the ones of the LPT simulation. Thus, the computational time of a droplet travelling a certain distance in the VOF domain is several orders of magnitude larger than in the LPT domain. The second drawback of the DCA is that each droplet in the particle cloud in the LPT simulation is tracked individually.
The large number of droplets in a practical spray cannot be handled on individual bases. Therefore, most LPT approaches use also the parcel model whereby each parcel represents a large number of small droplets.

The coupling approach developed in this work is on a statistical basis and is hence named SCA: a layer, called the statistical coupling layer (CL), is introduced close to the outlet of the VOF simulation where the liquid mass, which passes by, is analysed. This layer has to be positioned far enough downstream from the injector, so the spray is diluted enough to be simulated with an LPT approach. At this layer, the statistical parameters of the droplet distributions are extracted and used as starting conditions for the LPT simulation.

The first major advantage of the SCA is that the VOF simulations only need to run until the statistical convergence of the droplet distributions. This can be used in the LPT simulation as starting condition for much larger time spans. Thus, in the SCA, the LPT part does not have to ‘wait’ for the VOF part, and the coupling method shows a higher computational efficiency compared with the DCA. The second advantage of the SCA is that the droplets can be tracked in the LPT simulation using the stochastic parcel method. Here, a number of droplets is grouped in one parcel. All the droplets within the parcel are assumed to be of the same properties, that is, same size, position, diameter, distortion, velocity and temperature. Using the stochastic parcel method makes the description of a complete spray feasible in Lagrangian framework.

The drawback of the SCA compared with the DCA is that the CL is fixed in space. Therefore, it cannot be at the ideal position for all liquid structures to be transferred from the VOF to the LPT simulation, which reduces the physical applicability of the method. This can be observed in Figure 2, which shows a snapshot of the penetrating jet and the schematic location of the CL: already in an early stage, there are small droplets sheared away from the jet surface. These are small enough to be tracked in the LPT framework, but as they have not reached the CL yet, they are handled in the
VOF framework. On the other hand, one can see larger liquid structures close to the centreline of the jet that will reach the CL and will therefore be transferred to the LPT framework, but analysing their size and shape, it might be more appropriate to track them further in the VOF framework until they experience further breakups. Another drawback of the SCA is that, in its present form, it cannot handle transient sprays.

3.1. Extraction of the liquid phase from volumes of fluid

Primary breakup creates a large number of droplets of different scales and shapes. The CL is introduced close to the outlet where the liquid droplets pass through. The CL is considered to be far enough downstream from the injector where the spray is diluted enough to comply with the assumptions of the LPT approach. The downstream position of the CL is defined depending on the maximum liquid volume fraction in a plane. The liquid volume fraction is a result of the VOF simulation, thus, the location of the CL is defined afterwards. But as the storage requirement is too high, it is not possible to store 3D data for each timestep. Thus, there are many CLs introduced in the domain, and depending on the average liquid volume fraction, one plane is chosen to be suitable. In this case, it has been decided after the initial simulation to choose a plane in which the liquid volume...
fraction at the jet centre line reaches 0.25. It shall be emphasised that this is the maximum value for one cell, hence, all the other cells contain less liquid. Also, as the cells in the LPT simulation are several orders of magnitude larger in volume than the VOF cells, the liquid volume fraction on the LPT side will be smaller.

To identify the surface area of a liquid structure that passes the layer at a certain moment in time, the algorithm shown in Figure 3 is used. This algorithm is similar to the one described in [31] and is extended to time-dependent problems.

First, the IDs (identifiers) of the cells of the CL are initialized with a zero field (Figure 4(a)) and a ‘new droplet ID’ = 1 is created. Next, there is a loop over all cells (here, the indices $i$ and $j$ are used for cells in $x$-direction and $y$-direction, whereas $ii$ and $jj$ indicate the last cells) as long as their ID is still zero. If the liquid volume fraction of these cells is zero, the cell ID is set to $-1$.

![Figure 4. Algorithm to identify connected liquid structures at the coupling layer.](image)

![Figure 5. Algorithm to identify connected liquid structures over several timesteps.](image)
(Figure 4(b)) and the loop is continued. If the liquid volume fraction is larger than zero, the cell ID is set to the new droplet ID (Figure 4(c)). In this case, a loop over all neighbouring cells is conducted. If their liquid volume fraction is zero, their ID is set to −1, and the loop is continued at the previous cell checking another neighbour. If it is larger than zero, its ID is also set to the new droplet ID and a loop is conducted over its neighbouring cells (Figure 4(d)). When all neighbours and their neighbours are checked, the complete connected liquid structure is identified and the pointer will be set back to the cell which was first identified as part of the drop. At this point, a new droplet ID is created and the loop is continued over all cells whose ID is still zero (Figure 4(e)). When this loop is finished, the cells with the same droplet identifier represent a connected liquid structure.

By identifying the connected liquid masses that pass the CL per timestep, the total volume of each liquid structure is determined (Figure 5). Figure 5(a) visualises the cut of the CL to show the location of the views in Figure 5(b,c). Figure 5(b) shows the connected volume passing the CL during the current timestep, which is given by

$$V_t = \sum_{n=1}^{N_t} u_{str,n,t} \cdot \Delta t \cdot \alpha_{n,t} \cdot h_x \cdot h_y,$$

where $N_t$ is equal to the number of cells connected to one droplet in the current timestep $t$. $h_x$ and $h_y$ are the cell sizes in $x$-direction and $y$-direction, which are constant for the equidistant grid used in this work. Figure 5(c) shows the situation at the next timestep: the volume that passed the layer in the preceding timestep has propagated further downstream and new gas and liquid volumes are passing the layer in the current timestep. The connection between the droplet identified in the last timestep and the liquid volumes of the current timestep is established analogue to the previously described algorithm. The volume of the current timestep is added to the volume obtained in the last timestep. After the complete liquid structure has passed this layer, its complete volume is obtained by

![Figure 6. Accuracy test of the coupling layer.](image-url)
\[ V_{\Delta t} = \sum_{t=T_0}^{T_1} \sum_{n=1}^{N_t} u_{str,n,t} \cdot \Delta t \cdot a_{n,t} \cdot h_x \cdot h_y, \]  

(15)

where \( T_0 \) and \( T_1 \) are the first and last timestep at which the droplet passes the CL. From this, an equivalent radius of a spherical droplet, as well as its centre of gravity and droplet velocity vector is calculated.

Three test cases (Figure 6(a)) have been run in [32] on different grid resolutions to test the accuracy of the extraction method applied at the CL. A single liquid structure has been introduced in the domain and accelerated towards the outlet through the CL. Test case (1) represents the ideal case of a spherical droplet; for test case (2), an ellipsoid has been introduced, which represents a distorted droplet; and in test case (3), the distorted droplet is rotating around one of its axes. The results of the test cases can be seen in Figure 6(b). The ordinate shows the grid resolution as the ratio of the diameter \( d \) of the introduced droplet to the cell size \( h \). For the ellipsoid cases, the diameter represents the equivalent diameter of a spherical droplet, that is, \( V_{d,\text{equi}} = V_{\text{ell}} \) leads to

\[ d = \frac{3}{2} \sqrt{\frac{d_{\text{ell1}}}{d_{\text{ell2}}}}. \]  

(16)

The abscissa shows the ratio of the volume of the droplet as it has been identified by the CL, \( V_{\text{coupl}} \), to the droplet volume injected to the simulation, \( V_{\text{inj}} \). The CL uses a threshold for the volume fraction to define if a cell contains a droplet or not. If a droplet occupies only a small part of a cell, the volume fraction for this cell can be lower than the threshold. In this case, the droplet volume identified by the CL is smaller than the real value. Hence, all testcases in Figure 6(b) show a value of less than 1 for the ratio between identified droplet volume and simulated droplet volume. But if the droplet diameter is resolved by at least 3 cells \( (d/h > 3) \), the test cases show an error of a maximum of 30% and a minimum of 10% in the identified droplet volume. Hence, if most of the liquid mass is transported in liquid structures that are larger than 3 grid cells, the results produced by the CL are considered to be accurate.

The same procedure for calculating the equivalent droplet volume is applied to obtain the equivalent droplet velocity components and its position of the centre of gravity.

3.2. Starting conditions for the Lagrangian particle tracking calculations

As the timescales of the VOF simulation are much smaller than the ones required for the LPT simulation, it is not practical to synchronise both calculations and to inject each droplet that has
been extracted from VOF into LPT. Instead, on the VOF side, statistical data is extracted and used to perform Monte Carlo simulations on the LPT side. When a droplet is injected on the LPT side, the droplet diameter, velocity vector, density, temperature and the droplet position vector must be given. The rotational symmetry of the spray at the position of the CL is checked as shown in Figure 7 for the average streamwise velocities. The symmetry is checked concerning four lines of the angles $\psi = 0^\circ, 45^\circ, 90^\circ$ and $135^\circ$. For each line, the points on one side are compared with their corresponding mirrored point on the other side to obtain a measure for the average non-symmetry, $\Upsilon$, given by

$$
\Upsilon(u_{str}) = \sum_{i=1}^{ii} \sum_{j=1}^{jj} |(u'_{str} - u''_{str})_{i,j}|/(ii \cdot jj).
$$

(17)

The small values for $\Upsilon$ for the four symmetry lines, given in Table I, allow to assume rotational symmetry of the spray. The droplet temperature and density are fixed, as the spray is assumed to be isothermal and incompressible on the VOF side. Thus, and because the streamwise position is defined by the location of the CL, the number of needed parameters reduces to four: the droplet diameter $d$, streamwise velocity $u_{str}$, spanwise velocity $u_{spa}$ and spanwise position $r_{spa}$. If there exists a statistical dependence between two or more of these parameters, this information shall not get lost in the coupling procedure. Therefore, the correlation coefficient is evaluated for all combinations. The correlation coefficient $\chi_{i,j}$ for a pair of parameters $(x_i, y_i)$ is defined as

$$
\chi_{i,j} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \cdot \sum_{i=1}^{n}(y_i - \bar{y})^2}},
$$

(18)

where $\bar{x}$ and $\bar{y}$ are defined as

$$
\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \quad \text{and} \quad \bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i.
$$

(19)

For those parameters that show only a minor correlation to the other parameters, independent Monte Carlo simulations are performed to create time histories for the droplet injection. For those that show a strong correlation to another parameter, a linear relation between both is derived. This relation is used to create the time history of the dependent parameter from the result of the Monte Carlo simulation of the correlated parameter.

The method to perform a Monte Carlo simulation to choose the droplet diameter time history is explained in the succeeding text. The choice of the streamwise and spanwise velocities is analogous. The method is based on the one presented in [29].

The result of the extraction procedure of the previous chapter is the PDF of the droplet diameter distribution, $f(d_d)$. For the injection of droplets, the stochastic parcel method [33] is used. Here, the best resolution of the diameter distribution function is obtained for those droplet diameters, where the ratio of the number of droplets to the number of parcel is the lowest. As the most interesting processes, droplet evaporation and gas–liquid momentum exchange, depend on the mass of the droplets, the resolution is chosen to be the highest for those droplet diameters that represent the largest liquid mass. Therefore, $f(d_d)$ is scaled to $g(d_d)$, which gives the droplet diameter PDF proportional to the injected droplet mass.

| $\psi$ | $\Upsilon(u_{str})$ |
|-------|---------------------|
| 0     | 0.0297              |
| 45    | 0.0328              |
| 90    | 0.0292              |
| 135   | 0.0343              |
\[ g(d_d) = d_d^3 f(d_d) . \]  

(20)

\(g(d_d)\) is integrated to find its cumulative distribution, \(h^*(d_d)\),

\[ h^*(d_d) = \int_0^{d_d} g(\Psi) d\Psi . \]  

(21)

The maximum droplet diameter to be injected is defined as \(d_{d,max}\). In order not to lose the mass for the larger droplets at injection, \(h^*(d_d)\) is scaled to \(h(d_d)\) so that \(h(d_{d,max})\) equal to 1

\[ h(d_d) = \frac{1}{h^*(d_{d,max})} h^*(d_d). \]  

(22)

If the values of \(h(d_d)\) are called \(\xi\), the inverse function of \(h(d_d)\) is written as

\[ h^{-1}(\xi) = d_d . \]  

(23)

This result is used to perform the actual Monte Carlo simulation. A random number generator creates a series of numbers uniformly distributed between 0 and 1 which are assigned to the variable \(\xi\). When this numbers are applied to Equation (23), a time history of droplet diameters is established. The distribution of this time history will converge at a large number of injected droplets to \(f(d_d)\).

The number of droplets per parcel follows from the assumption that the mass per parcel is constant. The same procedure as the one described earlier is followed for the streamwise and spanwise velocities. For those parameters, instead of the droplet diameter distribution, \(f(d_d)\), the streamwise, \(f(u_{str})\), and spanwise, \(f(u_{spa})\), velocity distributions are used.

For a simple case where the droplet diameter distribution, \(f(d_d)\), is assumed to be uniform, this method is visualised in Figure (8).

![Figure 8. Example for the droplet diameters produced by a Monte Carlo simulation.](image)

Table II. Resulting droplet diameters and droplet numbers.

| \(\xi\) | \(d_d\) | \(N_d\) |
|-------|--------|--------|
| 0.2   | 0.67   | \(m_p \times 3.32\) |
| 0.4   | 0.795  | \(m_p \times 1.99\) |
| 0.6   | 0.88   | \(m_p \times 1.47\) |
| 0.8   | 0.95   | \(m_p \times 1.17\) |
| 1.0   | 1.0    | \(m_p \times 1.00\) |
The functions of \( g(d_d) \), \( h(d_d) \) and \( h^{-1}(\xi) \), obtained by using Equations (20), (22) and (23) are shown as well in Figure 8. A random number, \( \xi \), is applied to the inverse function to obtain the diameter of the injected parcels. To use a simple example, the random number generator creates discrete values uniformly distributed between 0 and 1, with a stepping of 0.2. The random numbers and resulting droplet diameters are shown as black dots in Figure 8 and tabulated in Table II.

If the mass for each parcel \( (m_p) \) is fixed at injection, the number of droplets per parcel is \( N_d = m_p \times d_d^{-3} \), also tabulated in Table II. It can be seen that more parcels are injected at a higher droplet radius, which satisfies the aforementioned desire to better resolve the droplet distribution function, where the mass is higher. However, the number of droplets per parcel is higher for parcels of a lower mass. Therefore, if the stepping of the random number is small enough, the injected droplet distribution will converge to \( f(d_d) \). The step size used in the current work is of the order of the numerical round-off error.

3.3. Coupling of the gaseous phase

The CL is also used to link the gaseous phase of the VOF to the LPT simulation. As the time and length scales of the continuous phase in the LPT simulation are of an order larger than in the VOF simulation, there will be interpolation in space and time to be done when applying the field to the LPT simulation. The fluctuations of the small scale structures will be filtered out during the coupling of both simulations. Therefore, the average velocities are used as a steady gas inlet condition in the LPT simulation.

4. CASE SET-UP

A test case of a liquid spray is simulated applying the previously developed SCA.

The characteristics of the simulations are oriented on a Diesel spray. The injection speed \( U_{inj} \) of the simulated spray is 500 m/s and follows a top hat profile, the nozzle diameter \( d_{noz} \) is \( 10^{-4} \) m, the results are normalised to these values. The jet Reynolds number is equal to 15 000, the jet Weber number is \( 1.2 \times 10^6 \), the liquid–gas density ratio is 10 and the liquid–gas viscosity ratio is 46. The ambient gas density is 14.8 kg/m\(^3\), the ambient gas temperature is 1150 K.

A VOF simulation with a domain size of \( 8 \times 8 \times 42 \) \( d_{noz} \) is run to determine the position of the CL. As it is the position where the average liquid volume fraction is lower than 0.25 at the centreline (Figure 9), \( z = 29.6 \) is chosen to be the location of the CL. The averaging time relates to the jet crossing the domain 15 times.

To compare, the droplet diameter and streamwise velocity distributions for various downstream planes are shown in Figure 10. It can be seen in Figure 10(a) that the most small droplets are identified at the first plane, \( z = 15.6 \). As one can conclude from the average liquid volume fraction
at this position, the liquid, yet, is not jet fully broken up. Thus, only small droplets are stripped away from the surface. These small droplets are highly sensitive to turbulent eddies. Thus, their streamwise velocity is lowered as can be observed in Figure 10(b). The further downstream planes, where the jet is broken up, show larger droplets and higher streamwise velocities. It can also be noted that after the jet is broken up, the statistical droplet distributions are in a certain range not very sensitive to the position of the position of the CL.

The decision about the position of the CL at $z = 29.6$ leads to the arrangement of the computational domain for the coupling case as schematically shown in Figure 11.

For the VOF simulation, this domain is of a size of $8 \times 8 \times 29.6 \, d_{noz}$. A Cartesian equidistant grid of the cell size $h = 0.05 \, d_{noz}$ is used, forming altogether a mesh of $1.6 \times 10^7$ grid points. A grid resolution study has been performed as shown in Figure 12. A difference of less than 4% is observed between $h = 0.1 \, d_{noz}$ and $h = 0.05 \, d_{noz}$; therefore, the grid resolution of $h = 0.05 \, d_{noz}$ is considered to be adequate. The VOF domain is followed by the LPT domain, which is of a size of $30 \times 30 \times 11 \, d_{noz}$. A Cartesian equidistant grid of the cell size $h = 0.25 \, d_{noz}$ is used. This set-up results in $6.3 \times 10^5$ grid points.

The accuracy of the VOF simulation alone has been shown in [19, 20], the accuracy of the LPT simulation alone has been shown in [34].

To assess the developed SCA, a simulation for the same case but applying the DCA is simulated. Here, for simplicity, the DCA is applied in the same way as the SCA, without overlapping of the domains. Thus, both simulations use the same simulation in the VOF domain. Therefore, if the DCA is applied using overlapping domains, the computational advantage of the SCA will be larger as the one shown in the following figures.
5. RESULTS

The droplet diameter, streamwise velocity, spanwise velocity and spanwise position are extracted from the VOF simulation at the CL. The averaging time of the results in the VOF domain corresponds to the jet crossing the domain 15 times. The scatter plots and the correlation coefficients of the four parameters against each other are shown in Figure 13.

The correlation coefficients show that there is a strong correlation between the streamwise velocity and the spanwise position of the droplets, whereas all combinations of other parameters show a weaker correlation, which is, therefore, neglected in the injection procedure. Following this finding, for the SCA, three independent Monte Carlo simulations are performed, for the
droplet radius, the streamwise velocity and spanwise velocity. The spanwise position, $r_{spa}$, is determined by a relationship from the streamwise velocity, $u_{str}$. For the case shown in Figure 13, this relationship is

$$|r_{spa}| = \max(0, -5 \cdot u_{str} + 4). \tag{24}$$

The droplet diameter distribution resulting from the VOF simulation, Figure 14(a), shows a peak at $d_d/d_{noz} \approx 0.08$. Very small droplets are badly resolved in the VOF approach; however, the contribution of these underresolved droplets to the total liquid mass in the system is very small. The droplets smaller than 0.075 $d_{noz}$ contain 0.87% of the total mass and the related error is therefore considered to be negligible.

The distribution of the streamwise velocity component seen in Figure 14(b) shows a peak at $u_{str}/u_{inj} \approx 0.1$ and an approximately linear decreasing curve until the point where the streamwise velocity is equal to the droplet injection velocity. The spanwise velocities in Figure 14(c) show a peak at $u_{spa}/u_{inj} \approx 0.05$, but the gradient of the curve towards the higher velocities is much steeper than the one for the streamwise velocities. This is caused by the fact that the spanwise velocities are not related to the momentum given to the droplet at injection, but it is purely caused by turbulent dispersion, that is, the trajectory of the droplets is changed because of aerodynamic interaction with turbulent eddies in the surrounding gas.

The LPT simulations using the SCA are started with the previously described statistical distributions, by performing Monte Carlo simulations. The results of these Monte Carlo simulations are shown as well in Figure 14(a,c). The distributions resulting from the Monte Carlo simulations converge to the distributions from the VOF simulation, which demonstrates the accuracy of the developed statistical coupling algorithm. However, it can be seen in Figure 14(a) that the

![Droplet diameter distribution.](image1)

![Stream wise velocity distribution.](image2)

![Span wise velocity distribution.](image3)

Figure 14. Droplet distributions extracted from the volumes of fluid (VOF) and injected in the Lagrangian particle tracking (LPT) simulations applying the statistical coupling approach (SCA) and direct coupling approach (DCA).
distributions converge better for larger droplets than for smaller droplets. This relates to the fact that the stochastic parcel method is used to track the droplets, that is, the droplet distributions are best resolved for those droplet diameters that carry the highest mass, as described in Section 3.2. Thus, the droplet distributions, as injected in the SCA, does converge slow for very small droplets.

Figure 15. Snapshot of the simulations coupled with the statistical coupling approach at $t = 16$. Blue phase is tracked in volumes of fluid, and red mass is tracked in Lagrangian particle tracking framework.

Figure 16. Results of the Lagrangian particle tracking simulation, statistical coupling approach (SCA) compared with direct coupling approach (DCA).

(a) Average streamwise gas velocity at $z = 28d_{noz}$.  
(b) Average streamwise gas velocity at $z = 33d_{noz}$.

(c) Average streamwise velocity SCA.  
(d) Average streamwise velocity DCA.
However, as stated before, this region of the droplet diameter distribution is anyhow underresolved in the VOF simulations and contains a neglectable part of the liquid mass. The same effect contaminates the droplet velocity distributions.

The distributions of the droplets injected with the DCA approach are shown in the same figures. As the injected droplet time history is produced from the time history extracted from the VOF simulation, the distributions converge very well.

A snapshot at $t = 16$ of the spray simulated with the SCA is shown in Figure 15. The liquid mass that is described by the VOF method is coloured blue, and the droplets tracked in Lagrangian framework are coloured red. As noted earlier, in the SCA, there is only a statistical relationship between the VOF and the LPT simulation. Thus, Figure 15 does not show one consistent realisation of the spray but one realisation in the VOF and one realisation in the LPT domain.

The average streamwise velocity of the LPT simulations is shown in Figure 16. Although the profiles in Figure 16(a,b) show a good agreement between SCA and DCA, the profiles of the SCA are smoother. One reason is the application of the stochastic parcel method in the SCA. This gives in general a better representation of the droplet distribution function for those diameters which transport the most liquid mass, compared with the discrete approach of the DCA. As the droplets with large mass influence the gas phase more than very small droplets [35], the profiles are more smooth for the SCA. Another possible reason is that the supply of droplets from the VOF simulation is due to finite simulation time not unlimited in the DCA. Thus, the properties of injected droplets are repeated at some point in time, which is not necessary when applying the SCA. A difference between the two methods is the capturing of the beginning of the spray development: the DCA accounts naturally for the properties of the first droplets that reach the LPT domain, whereas the statistics in the SCA are not time resolved. But as Figure 16 shows time-averaged figures, this does not effect the results.

6. COMPUTATIONAL EFFICIENCY

The relative computational costs for the simulated case are given in Table III. The computational time for the VOF simulation, $t_{VOF}$, is the sum of all 16 involved processors in the DCA and SCA. It is not applicable for the pure LPT approach. The SCA is significantly less expensive than the DCA, as it is only run until statistical convergence, whereas the DCA has to follow the generated droplets during the VOF and LPT simulations. The computational time for the LPT simulation, $t_{LPT}$, is identical for all LPT simulations, with a given number of droplets, independently how the initial droplet set-up is determined. However, the LPT simulation time using the DCA is larger because the stochastic parcel method cannot be used and each droplet is tracked individually. The total computation times shows that the SCA is about four times faster than the DCA. For a spray that is simulated until evaporation, the domain size covering the dispersed spray may be larger, and thus, more droplets are needed to be provided from the VOF simulation if the DCA is applied. Therefore, the VOF simulation has to be carried out for a longer period. In the SCA, the VOF simulation is only carried out until a statistical convergence, whereby the computational time is not affected by the size of the LPT domain. For such a case, the computational benefits of the SCA over the DCA are expected to be larger.

|                  | $t_{VOF}$ | $t_{LPT}$ | $t_{tot}$ | $t_{tot}$/$t_{SCA,tot}$ |
|------------------|-----------|-----------|-----------|-------------------------|
| Pure LPT         | —         | 96        | 96        | 0.0056                  |
| DCA              | $6.9 \times 10^4$ | 105       | $6.9 \times 10^4$ | 4.1                     |
| SCA              | $1.6 \times 10^4$ | 96        | $1.7 \times 10^4$ | 1                       |

LPT, Lagrangian particle tracking; DCA, direct coupling approach; SCA, statistical coupling approach.
7. SUMMARY AND CONCLUSIONS

The initial and secondary breakup of a liquid jet into a spray has been simulated using LES. The dense and dilute spray regimes have been simulated using a combination of the VOF and LPT approaches, respectively. The disintegration of the liquid core into ligaments and droplets due to aerodynamic instabilities has been studied. By introducing a so-called CL close to the outlet, a method has been developed to identify droplets, their radius, position and velocity. The extracted data were used to build up data sets, which can be used as an initial condition of droplet properties in the simulation of a dilute spray using the LPT approach. The statistics of the droplets injected in the LPT simulation were shown to converge to the statistics extracted from the VOF method, thus, the injection models accurately the extracted statistics. The results of the SCA showed were accurate when compared with the results obtained by the DCA.

The strongest benefit of the proposed approach is its computational efficiency. For the analysed case, the SCA shows to be four times faster to produce converged spray results than the DCA, while the benefit is expected to be higher if a complete spray is simulated.

The major disadvantage of the SCA compared with the DCA is that in the here presented version, it is not able to handle sprays for which the droplet time history is not stationary. Two proposals shall be given to handle the transient behaviour: the first proposal is to create ensemble average distributions instead of averaging droplet diameter distributions in time. Starting from that, a transient spray could be modelled in the LPT simulation. Drawback of this proposal is that a large amount of VOF simulations are needed to build ensemble averages. Thus, the computational efficiency, which is the actual benefit of the SCA, is compromised. The second proposal is to combine the DCA and SCA. If one identifies those phases of the time histories of the spray which are statistically non-stationary, the DCA can be applied to the transient phases and the SCA to the statistical stationary phases.

A shortcoming of the presented test case of the SCA is that droplet distortions are not yet coupled between VOF and LPT. This relates to the assumption that most droplets are small and spherical when reaching the CL. However, the distortion parameters for each droplet are extracted at the CL and can be given as a starting parameter for the LPT simulation in future works.

The position of the CL in this work is based on the liquid volume fraction at the jet centre line. This can be improved in future works, by, for example, also taking into account the droplet distortion. Also, the shape of the CL, which is here a plane, can be arbitrary and be adapted to the local droplet properties.

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