Hybrid VOF to Lagrangian CFD Model for Jet Breakup and Spray Transport

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Abstract
This study presents the implementation of a hybrid Volume of Fluid (VoF) to Euler–Lagrange model for simulating jet breakup phenomena using the open-source CFD toolbox OpenFOAM. In the near-nozzle region, primary breakup is resolved via a VoF approach combined with adaptive mesh refinement (AMR). The transition to Lagrangian droplets within the spray is governed by local cell properties, specifically the size and sphericity of liquid-filled regions. Secondary breakup processes within the spray are also taken into account, and two-way coupling effects between Lagrangian droplets and the continuous gas phase are modelled via source terms.

The model's applicability is demonstrated for a range of atomization scenarios. Accurate predictions are achieved for a fuel injection benchmark involving twin fluid atomization, particularly with respect to jet deflection and droplet size distribution. For single fluid atomization from a hole-type nozzle, droplet sizes and velocities show good agreement with experimental measurements. Furthermore, the model successfully captures key physical effects in the transonic gas-assisted atomization of molten metals.

To ensure robust and computationally efficient performance in industrial applications, special emphasis is placed on the numerical treatment of droplet identification, AMR load balancing, and seamless integration into OpenFOAM's modular architecture.

Keywords: OpenFOAM, Volume of Fluid (VOF), Lagrangian, atomization, liquid jet in crossflow, CFD

Introduction
Due to increasing computing resources and continuous improvements in the development of modelling methods, flow simulations (CFD) are increasingly being used to model complex applications. In industrial settings such as spray cooling, fuel injection, and paint or metal atomization, the ability to model the entire jet breakup and spray formation process with sufficient physical accuracy and within realistic computational limits is essential. However, existing CFD models often struggle to meet these demands, particularly when transitioning from interface-resolving multiphase models to particle-based spray descriptions within a unified computational framework.
In typical multiphase CFD simulations of atomization, two main flow regimes are considered: the near-nozzle region, where the liquid phase undergoes instabilities, ligament formation, and primary breakup; and the far-field region, in which dispersed droplets dominate. Accurate modelling of the full process chain requires hybrid approaches that combine Eulerian interface-resolving methods -such as the Volume of Fluid (VoF) technique- with Lagrangian particle tracking (LPT) in the developed spray. Transition models must identify suitable liquid structures for conversion from an Eulerian to a Lagrangian representation while maintaining mass, momentum, and spatial consistency.
Early applications of the hybrid approach can be found in the work of Tomar [1], which employs a Volume-of-Fluid-based method, and in Kim et al. [2], who use a Level-set-based strategy. Different approaches are used to identify the droplet: Tomar et al. define such separated liquid structures based on a single condition: the volume of a liquid element must fall below a specified threshold. In contrast, Kim et al. apply two criteria: the liquid structure must not only be smaller than a given volume threshold, but also approximately spherical in shape. Herrmann [3] developed a parallel coupling between, which recognizes liquid structures and transfers them from the Eulerian phase to a Lagrangian description while maintaining position, mass and momentum. For this he used the Refined Level-Set Grid method and conducted grid convergence analyses of droplet size distributions.

Various authors have also integrated transition models from VOF to LPT into the open-source CFD toolbox OpenFOAM used here. In the work of Heinrich and Schwarze [4] the isoAdvector interface tracking method is used in the VOF approach of OpenFOAM and secondary break-up and statistical particle-particle collisions in the spray are also taken into account.
Janodet [5] extends in his thesis the solver Yales2 to efficiently calculate disintegration processes when injecting liquid kerosene. Here, too, it was shown that the resolution of the phase boundary is of particular importance and that libraries for parallelization in adaptive grid refinement on unstructured grids are being expanded. He validated his transition model of the Eulerian to the Lagrangian droplet modelling with experiments as well as theoretical and numerical reference solutions.
Although these studies demonstrate the feasibility of Eulerian–Lagrangian methods for spray modelling, most are limited to low or moderate Reynolds and Weber numbers. More recently, Kuo and Trujillo [6] extended the approach to complex, high-Re and high-We scenarios, including a diesel spray–based configuration under non-evaporating conditions. They also proposed a novel secondary atomization model based on maximum entropy principles.
Trautner [7] uses in his work an extended surface tension model in which, similar to the eddy viscosity approach, the surface tension is adjusted by turbulence variables. He examines the resulting structure of the jet break-up and compares the calculated droplet sizes with experiments.
Despite the progress made, many existing approaches remain constrained by limited scalability or reliance on simplified physical assumptions. Most studies focus on specific atomisation applications in which special effects such as gas-phase compressibility, heat transfer with phase transitions or non-Newtonian fluid behaviour can usually be neglected. In contrast, the objective of the present work is to implement a robust and flexible transition framework within the OpenFOAM solver architecture that is applicable to a broad range of industrially relevant atomization scenarios. To this end, the model supports the integration of compressible gas dynamics, temperature-dependent fluid properties including solidification effects, and complex rheology, enabling the simulation of highly customized processes such as molten metal atomization or paint spraying.
The current work addresses these gaps by presenting a VoF-to-Lagrangian transition model that combines interface-resolving accuracy in the primary breakup zone with an efficient Lagrangian treatment of the dispersed spray. By leveraging adaptive mesh refinement (AMR), parallelized droplet detection algorithms, and full OpenFOAM integration, the model offers a practical solution suitable for engineering use cases that demand both fidelity and efficiency.
Special emphasis is placed on achieving computational efficiency and robustness, making the approach suitable for simulations on dual-CPU workstation systems with runtimes of just a few days. This allows the method to be used in real-world industrial applications without the need for high-performance computing infrastructure.

1 Modelling approach

The modelling of the jet breakup is done in 3 steps:

- Volume of Fluid (VOF) modelling with adaptive mesh refinement
- transition range VOF to Lagrangian representation
- droplet transport with Lagrangian method

The underlying equations for modelling with the VOF approach are given by:

1.1 The Eulerian approach with Volume-of-Fluid (VOF) modelling

In the volume of fluid modelling a continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0 \tag{1}$$

and the momentum transport

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \rho g + \nabla \cdot (\mu \nabla \boldsymbol{u}) + \boldsymbol{F}_{\sigma} - \boldsymbol{F}_{\boldsymbol{p}} \tag{2}$$

are solved. To capture the liquid-gas interface an additional transport for the volume fraction is used:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \boldsymbol{u}) = 0, \qquad \alpha = \begin{cases} 0 \rightarrow phase\ 1, e.g. liquid \\ 1 \rightarrow\ phase\ 2, e.g. gas \end{cases} \tag{3}$$

Based on the volume the fluid properties are estimated as followed:

$$\rho = \alpha \rho_l + (1 - \alpha)\rho_g \tag{4}$$

$$\mu = \alpha \mu_l + (1 - \alpha)\mu_g \tag{5}$$

For the application of VOF-to-Lagrangian modelling, the isoAdvector method developed by Roenby [8] and available in the ESI releases of OpenFOAM is used in the VOF domain. Two implementations were realised: Firstly, incompressible modelling based on the conservation equations described above. In OpenFOAM, the interIsoFoam was selected as the basis for this and extended by the Lagrangian transformation of the droplets. Furthermore, a compressible implementation was realised in which the energy equation is solved additionally. The compressible version is based on the compressibleInterIsoFoam. To reduce computational time, only the primary break-up of the VOF phase is detailed and modelled using local adaptive mesh refinement near the VOF interface, while the Lagrangian particles are transported on a coarser grid.

1.2 The Euler-Lagrangian formulation

The Lagrangian-Particle-Tracking (LPT) approach simulates the motion of Lagrangian parcels across the computational domain. In the parcel approach, each parcel stands for a group of droplets sharing the same characteristics, such as size and velocity. Treated as point masses, they are considered to have no volume. Their position and velocity are updated at every time step using differential equations governing trajectory and momentum:

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p \tag{6}$$

$$m_p \frac{d\boldsymbol{u}_p}{dt} = \boldsymbol{F}_D + \boldsymbol{F}_G \tag{7}$$

In the implementation of the VOF to LPT approach, each transferred droplet corresponds to exactly one parcel. This means that parcel modelling as a clustered drop packet would not be necessary for the initial conversion. However, the parcel approach makes it possible to consider a secondary break-up according to Reitz-Diwakar, in which, for example, the diameter is reduced and a parcel with multiple droplets is transported instead of a single physical droplet. The interaction of the parcels with the continuous phase is modelled via momentum source terms. In principle, it is also possible to take particle-particle interaction into account using a statistical collision model. For the atomization cases investigated here, the droplet-droplet interaction could be neglected due to the low volume loading with droplets.

1.3 Transition region from VOF to Lagrangian modelling

The modelling of the transition from droplets to the Lagrangian view using the adaptive mesh refinement method is shown schematically in Figure 1.
By converting coherent VOF phases in droplet shape into equally sized Lagrangian droplets, the time required for modelling the spray dispersion can be significantly reduced compared to the pure VOF approach, or it even makes the simulation of the disintegration with subsequent spray dispersion possible at all. Particularly in the case of breakup into a fine spray, this is necessary because, on the one hand, the droplets produced during atomisation are so small and numerous that they cannot be resolved over several cells with free surface modelling. On the other hand, the mesh for the Lagrangian particles can be much coarser than for a continuous VOF phase with a finely resolved interface. This makes it possible to calculate the further spray propagation over a longer distance and also to efficiently model effects such as secondary breakup (breakup of round droplets into several small droplets).
Typically, the transformation from VOF to Lagrangian starts at a certain predefined height. This allows regions of intense collisions of VOF lamellae and droplets to be resolved with the interfacial effects using

surface tracking techniques. Below the primary decay and collision region, the transformation to Lagrangian particles can be performed, as the droplets can now no longer interact with each other.
The VOF-to-Lagrangian algorithm transforms coherent VOF phases below a certain diameter limit so that very large Lagrangian droplets are avoided, and they continue to be modelled with VOF methods and accurate interface tracking. In addition, a shape factor for sphericity must be defined so that only approximately spherical droplets are converted into spherical Lagrangian particles and ligaments are further tracked with a VOF method until they actually break down into small droplets.
Various criteria can be defined for the conversion from the VOF phase to Lagrangian particles, for example minimum and maximum droplet size, minimum or maximum number of cells, required sphericity, etc. Control options for spatially delayed conversion are also available: This allows regions where droplet-droplet collisions are to be expected, or areas with additional gas jets during twin fluid atomisation, to be excluded from droplet conversion until primary decomposition is complete.

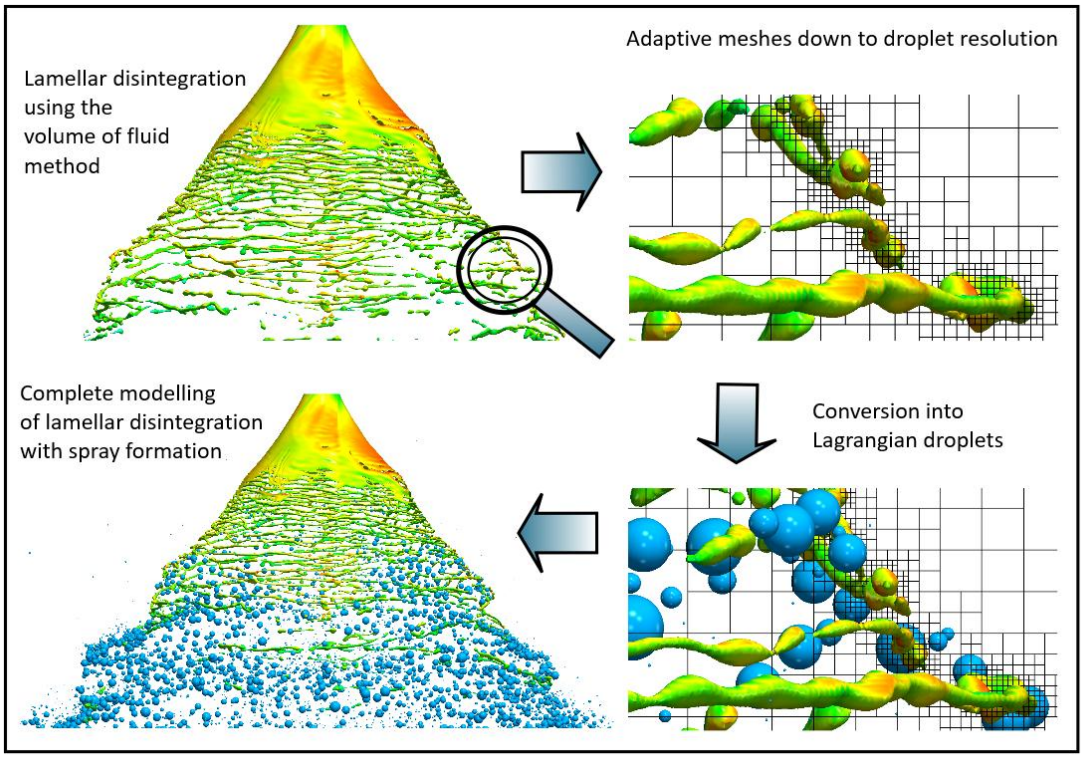

Figure 1. *Transition Modelling VOF to Euler-Lagrange in detail. The local grid refinement around the coherent VOF phase, and the coarsened grid around the transformed Lagrangian particle are shown.*

1.4 The VOF-to-Lagrangian droplet identification algorithm

The general performance advantage of the VOF-to-Lagrangian method is that the VOF interface is resolved accurately using dynamic grid refinement as long as the lamellae are connected, or the droplets are very large. If a droplet with sufficient size and appropriate spherical shape detaches, it is converted into a Lagrangian particle, and the local grid is unblocked for un-refinement. If un-refinement occurs, the local number of cells is reduced by several orders of magnitude and the calculation times for the Eulerian simulation decrease significantly.
The transport of the droplets as Lagrangian particles is possible on the coarser grid and requires only a small amount of computational effort compared to detailed VOF modelling.
The implementation of droplet conversion used here is based on a connected-component labelling (CCL) approach. For this, the storage of cells and the management of their connectivity used by OpenFOAM is very advantageous. On the one hand, the entire computational domain can be managed very efficiently by a field over the grid cells, in which it is directly noted whether a cell has already been visited and evaluated for droplet conversion. In addition, when traversing the algorithms described below, in each cell it is possible to directly address all neighbouring cells, as pointers to these cells are stored and provided by OpenFOAM in the polyMesh grid data structure. Only the processor boundaries

represent a limitation here, which either require more complex and time-consuming treatment, or can be neglected for the application cases and target computer architectures.
The identification of connected VOF cells that can be converted into Lagrangian particles is done with a parallel breadth-first search algorithm on the scalar field of the liquid phase. Each processor starts independently with an arbitrary cell in its local computational domain. Each cell is a starting cell for a search at most once. A cell that has already been visited and processed is skipped directly. From the starting cell, the neighbouring cells are then traversed and, if they have not yet been marked as processed, evaluated with a first level of processing steps. Here, only simple marking operations and list operations are performed, which run quickly ("(a) cheap" level in Figure 3). Successful searches that can lead to a droplet are stored in dynamic lists so that a renewed traversal of the VOF cells belonging to the droplet can take place directly along the stored path. This approach saves computation time and memory, as only relevant VOF areas are evaluated in greater detail on smaller subset of cells in a second level analysis with slightly higher computational effort ("(b) cheap" in Figure 3). If the required criteria for droplet conversion are actually met, another traversal through the dynamic list is performed to calculate the computationally intensive final properties of the droplet ("(c) expensive" in Figure 3). The VOF phase is set to zero in the cells of the final phase, a Lagrangian particle with the calculated droplet properties is newly created in the cell of the calculated droplet centre. To avoid numerical instabilities, a damping term for the momentum equation of the cells involved in the droplet conversion is used. In particular, the newly formed droplet regularly has a larger volume than the cell in which it was newly inserted. Only with the following grid un-refinements are the cells of the droplet environment merged and enlarged, and droplet volume and cell volume are again in a suitable ratio to each other with a much larger cell space against a rather small droplet diameter.

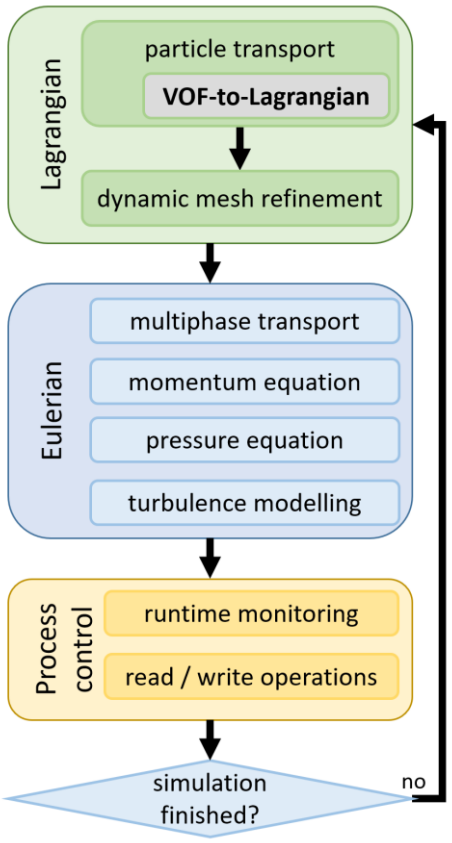

Figure 2. *CFD solving process. The VOF-to-Lagrangian algorithm precedes the dynamic mesh refinement, so that un-refinements can be done early.*

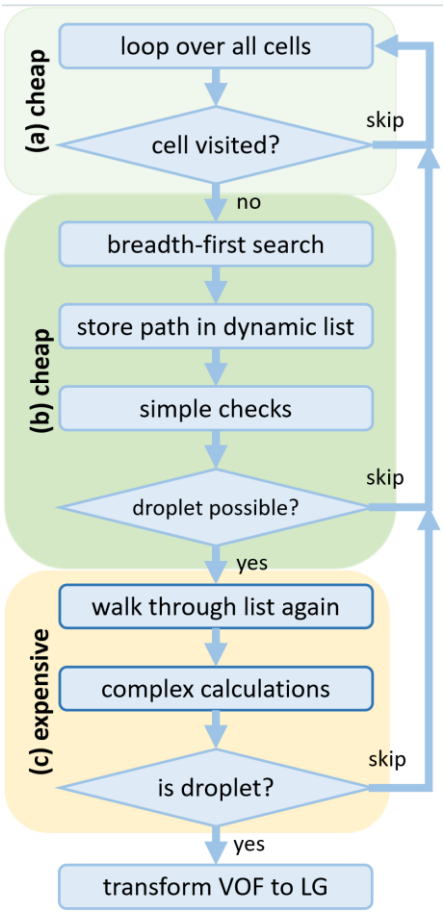

Figure 3. *Droplet identification. A three-level approach to handle different levels of computational complexity is used.*

The special treatment of processor boundaries mentioned above is as follows. For a fully parallel implementation of droplet identification, the processors would have to exchange and compare their

marked lists with each other during the search for connected areas as soon as a processor boundary patch is reached. A droplet across multiple processor boundaries and back to the first processor is also possible here. With increasing processor count and large droplets with many cells, this probability increases, with a large computational domain, a high number of cells and small droplets, the probability decreases. In the application areas investigated by the authors and the computer architectures currently used, it turns out that the complex parallel droplet identification would only be used for a few droplets. So, if a processor boundary is hit during droplet identification, the conversion is initially postponed, and the droplet is further transported as a VOF phase. The hit of a processor boundary patch belongs to the level (b) of the droplet identification algorithm and is therefore still of low complexity. After a few iterations, the droplet is then exclusively located within a single processor domain and is converted regularly. A careful selection of a specialized decomposition strategy matching the current applications lamella and spray form further supports this approach of postponed droplet transition.
The realized implementation of droplet conversion typically requires less than three percent of the total computation time. Since the Lagrangian particles can be tracked on a significantly coarser grid, the total computation time of the simulation is drastically reduced. Increased memory consumption for the Lagrangian particles is not a challenge for modern HPC systems. The VOF-to-Lagrangian transition algorithm implemented here concentrates on stability and can simplify the parallel handling without a relevant performance loss.
In general, droplets must be completely surrounded by a layer of empty cells for their transformation. For numerical reasons, it is necessary to define a lower threshold for this, as the transport of the VOF phase can lead to values other than zero, depending on the simulation parameters selected, which are not significant in terms of mass, but which can influence the droplet identification. A further limit for a minimum number of cells to form a droplet is available to avoid too small droplets of insignificant mass and size. The letter criteria triggers in the first level of the VOF to Lagrangian algorithm already. The maximum droplet size can also be limited. This ensures that large droplets continue to be tracked using the VOF method and continue to disintegrate accurately until they reach an acceptable size for further transport as Lagrangian particles. The criterion of sphericity is similar, whereby only sufficiently spherical droplets are converted, while ligaments without a spherical shape continue to be modelled as a VOF phase until final disintegration. These droplet formation criteria require the most expensive level (c) of the conversion algorithm in Figure 3.
For many applications, it is necessary to exclude certain areas from the early conversion of VOF phase into Lagrangian particles. This is the case, for example, in the proximity of the inflow surface of the liquid, where a coherent region with lamella decay must first build up. With colliding liquid jets or colliding sprays with complex droplet-droplet interaction, too early a transfer into the Lagrangian phase is undesirable, as the collision might be better resolved with a VOF modelling approach, than with stochastic particle collision models. Or in the case of twin fluid atomization with secondary gas jets, the large droplets should first be atomized by the jets in a VOF approach and only then be tracked further as Lagrangian particles with secondary decay models. If the criteria of excluded region triggers, an early exit of the VOF-to-Lagrangian algorithm directly after the level (a) occurs, skipping all the more complex calculations as early as possible (Figure 3).
The VOF-to-Lagrangian conversion itself is mass-conserving. The overall accuracy of mass conservation in the simulation is only limited due to the quality of the selected VOF method and interface tracking algorithm. Depending on the droplet conversion criteria, very small fractions of VOF phase might be transported as VOF phase through the entire domain, although with appropriate mesh refinement settings these cells will not be refined and therefor will not require additional computational effort. These stranded VOF fraction can however be evaluated in collector planes or at domain boundaries to keep track of their total fraction of mass and overall significance.

2 Validation cases

2.2 Benchmark “fuel injection”

Validation includes a fuel jet injection benchmark, showing good agreement with experimental data for droplet sizes. The fuel jet in cross flow benchmark is used for validation [9][4][10]. Here, aviation fuel is injected into a channel via a nozzle and atomised by the cross-flowing air. In the experimental investigations, both the deflection of the liquid jet is determined, and the particle sizes are measured in two planes downstream. In addition to the decay of the lamella into droplets, a secondary breakup also comes into play due to the Weber numbers. The secondary breakup was modelled with a Reitz-Diwakar model. The turbulence modelling was carried out with an LES model.

V-liq (m/s)	32
$\dot{m}_{liq}$ (kg/s)	0.004
D_{liq} (mm)	0.458
$Density_{liq}$ (kg/m³)	780
$Density_{Air}$ (kg/m³)	5.88
Surface Tension (N/m)	0.0197
Weber Number (-)	1500
Momentum Ration (-)	10

Table 1. *Simulation parameter.*

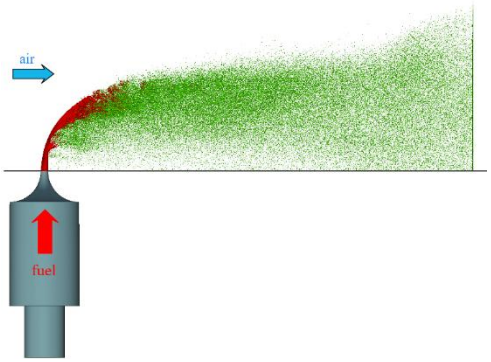

Figure 4. *Injection nozzle used.*

Figure 5 shows the deflection of the injected liquid phase by the air in comparison with experimental measurements.
For the measurements, the mean, minimum and maximum position of the jet contour are shown as blue spheres.
The simulation results are given in transparent red. The fluctuations result from the turbulent jet decay.
The mean deflection of the simulated liquid phase in the red VOF area coincides very well with the mean measured positions.

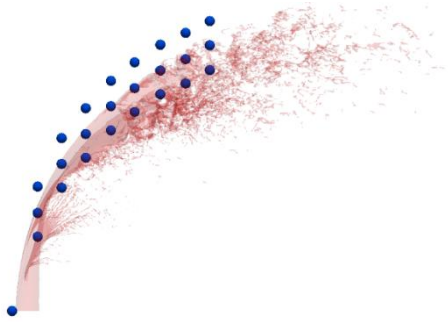

Figure 5. *Jet penetration trajectory, experiment (blue dots) vs simulation (red).*

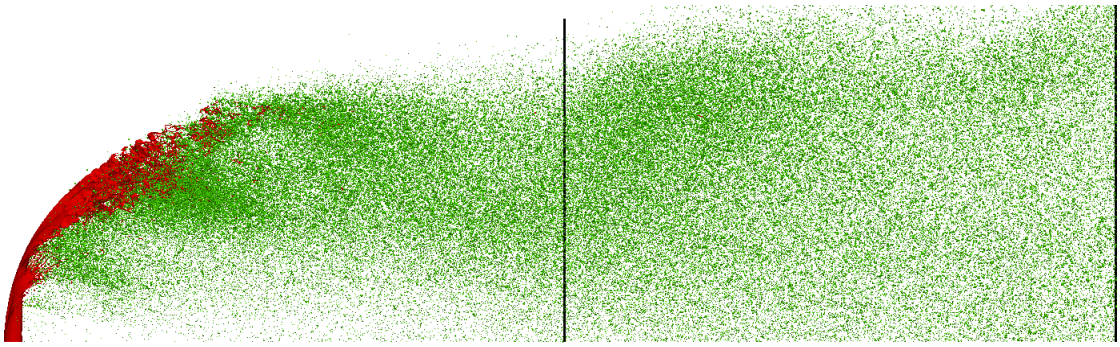

Figure 6. *Fluid phase modelled as VOF is coloured red, Lagrangian particles are coloured green. The collector planes are show as black lines.*

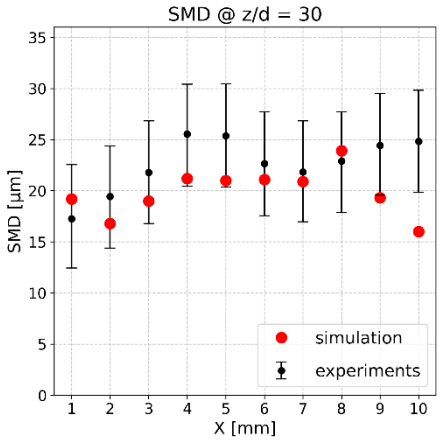

Figure 7. *Fuel injection benchmark. Sauter mean diameter for simulation and experiments at distance z/d=30.*

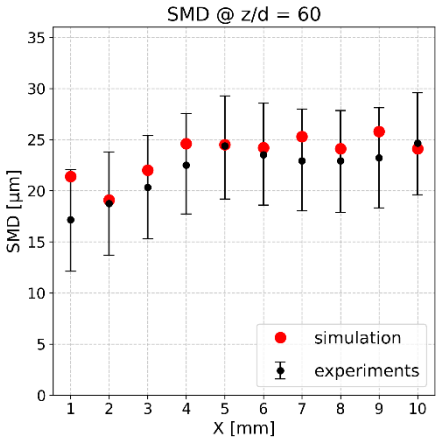

Figure 8. *Fuel injection benchmark. Sauter mean diameter for simulation and experiments at distance z/d=60.*

Figure 7 and Figure 8 show the measured and simulated particle sizes for two different measurement planes from the nozzle outlet at different distances above the ground. Here, too, there is good agreement between simulation and experiment for the resulting particle sizes.

2.3 Benchmark “Deux-B”

Additional applications, such as pressure atomization from hole-type nozzles, also yield accurate results for droplet sizes and velocities, see Figure 10 and Figure 11.
The comparison is made here with experimental data from the thesis of E. Deux [11]. The simulation in OpenFOAM is also carried out with an LES approach with the dynamic-k subgrid model.

Atomised Fluid	Water
Exit diameter	0.5 mm
Flowrate	34,66 l/h
Re	27356
Oh	0.0047

Table 2. *Simulation parameter.*

In comparison to the twin fluid atomisation in the fuel injection benchmark, a single-component atomisation is used. For this reason, the secondary break-up (also modelled with the model according to Reitz-Diwakar) is of minor importance.

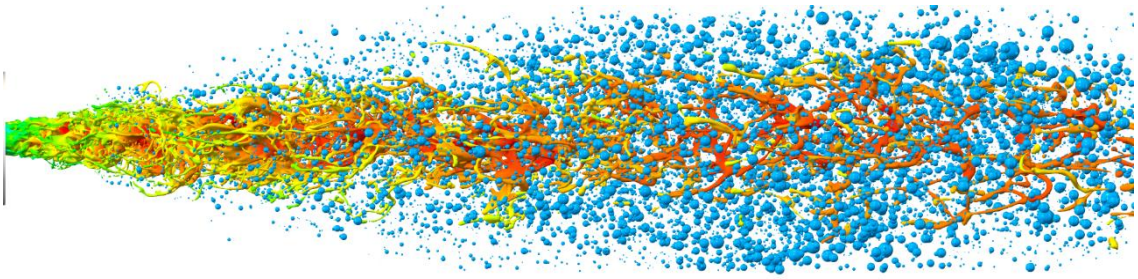

Figure 9. *Deux-B benchmark, Lagrangian particles shown in blue, ligaments with a velocity colouring.*

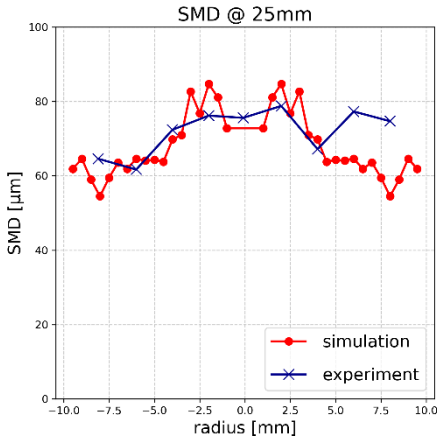

Figure 10. *Deux-B benchmark: droplet sizes for a single-component atomisation at 25mm from the nozzle exit.*

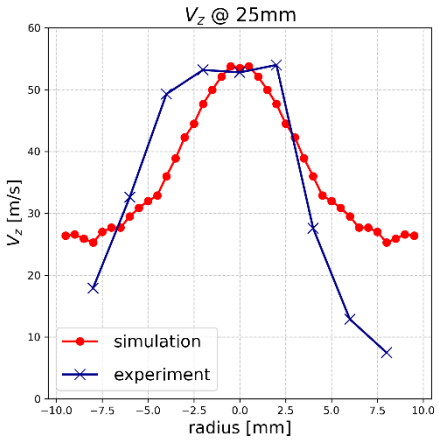

Figure 11. *Deux-B benchmark: z-component of droplet velocities at 25mm from the nozzle exit.*

2.4 Application for molten metal atomization

The model developed in this way is used to explain processes in the atomisation of metal melts during powder production. In this process, a pressure swirl atomiser is first applied to the molten metal, which causes the lamella to primarily disintegrate.
Due to the high-speed gas jet a compressible formulation is applied. For turbulence modelling again the LES approach with the dynamic k-equation model is used.

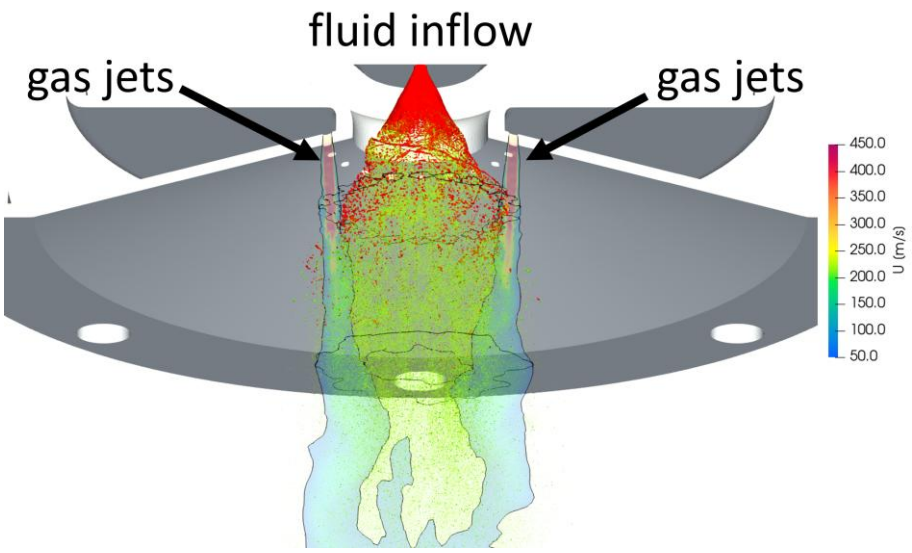

Figure 12. *Molten metal atomisation.*

Subsequently, the droplets are atomised into small particles by gas jets at high speed, see Figure 12.

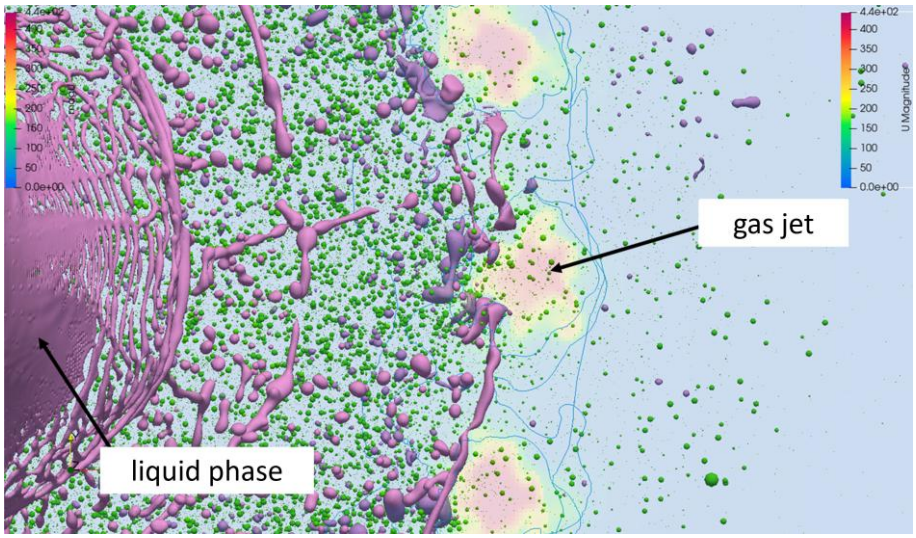

Figure 13. *Interaction of ligaments with gas jets during molten metal atomisation.*

With this model, significant effects on the breakup processes could be better understood. In particular, the interaction of the gas jets with the ligaments and effects on the particle size could be analysed, see Figure 13.

Conclusions and outlook

A conversion model from an interface-tracking approach (VOF) to a Lagrangian particle-based modelling framework has been presented. This model is well-suited for closed-loop simulations of jet break-up processes, including subsequent spray formation. The results show good agreement with experimental data across the entire breakup process, from the primary disintegration of ligaments to the secondary breakup into microparticles. The simulation tool is also already being used for various technical atomization configurations, such as AdBlue injection, liquid metal disintegration or paint atomization.

However, the wide range of atomization applications often necessitates individual adaptations and extensions of the simulation process to accurately capture the physically relevant effects. For example, in the simulation of paint atomization, a shear-thinning viscosity model was implemented for the liquid phase, which can be coupled with a compressible flow model on the gas side. In the simulation of metal melt atomization, temperature-dependent material properties in combination with extensions to the heat transfer equation were implemented in the melt model to consistently represent both the solidification of ligaments in the VoF phase and the solidification of Lagrangian particles within the thermal energy balance. Other applications that have already been realised include atomising liquids from flat spray nozzles. These are characterized by a lamellar structure that poses a particular challenge from a

computational perspective, as the characteristic film surface dimensions often exceed the resolvable lamella thickness by several orders of magnitude. This, in turn, requires specialized meshing strategies-such as the use of highly anisotropic cells within adaptive mesh refinement-to avoid excessively high computational costs for technically relevant problems.
Despite the promising agreement, further model refinement remains necessary. Current research highlights several areas that deserve further investigation. These include, for example, proposed models that incorporate turbulence-induced modifications to surface tension during atomisation [7].
Additionally, it is essential to assess whether the interaction between Lagrangian particles in the spray and the turbulent gas phase is captured with sufficient accuracy, and to determine the corresponding grid resolution requirements necessary to resolve these interactions effectively. It is also planned to integrate further models for the secondary break-up in the Lagrangian spray and to check them for different atomization applications. New investigations [6] show promising approaches here.
An ongoing area of research involves the development of decomposition strategies that anticipate the evolving shape of the spray in both the VOF and Lagrangian phases. The goal is to optimize computational efficiency by minimizing the need for costly load balancing while maintaining accuracy.

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