Transition model from the VOF method to Lagrangian modelling for molten metal atomisation

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1 Abstract

Atomisation processes of liquids occur in many applications, mostly to increase the specific surface area of the liquid (as in engine injection processes or evaporative cooling by sprays). In other applications a fine spray itself is the target of an atomisation process, as in powder production from molten metals for additive manufacturing or the generation of fine paint droplets in painting processes.
If one wants to model such a process by flow simulations, one is confronted with a complex multi-phase system. When liquids are atomised in a gas, different transport mechanisms occur, from jet breakup to spray, for which different modelling theorems are usually used in the flow simulation:
If the liquid or the resulting lamellae is still largely coherent, surface tracking methods such as the Volume of Fluid (VOF) method are used to model the processes at the interface between liquid and gas, in particular the decay of the surface. Once a lamella has formed from which droplets emerge in the ongoing decay process, the resulting droplets are usually so small that they cannot be resolved locally efficiently over several cells even with adaptive grids. To describe the further transport of the spray, a different approach must be used here. Usually, the resulting spray is then described with a Lagrangian approach. In order to model the entire process from liquid breakup to the spray, a transition model from the Euler approach with surface tracking methods (Volume of Fluid, VOF) to the discrete Lagrangian approach of the dispersed particles must be realised. This transition poses special challenges to the modelling, e.g. to ensure mass conservation or to consistently represent the interaction effects between droplets and gas.
The implementation of such a transition model based on the open-source CFD toolbox OpenFOAM is presented. Besides the pure implementation of the decay modelling, performance optimisations are crucial both for the adaptive grids in the VOF domain and for efficient load balancing in Lagrangian particle transport. Good agreement with experimental results is achieved both for the resulting particle size and for the deformation of the liquid jet in the fuel jet in cross flow benchmark.

2 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

2.1 VOF modelling with adaptive mesh refinement

For the application of VOF-to-Lagrangian modelling, the isoAdvector method developed by Roenby [1] and available in the ESI releases of OpenFOAM is used in the VOF domain. 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 most of the gas and liquid flow is simulated on a rather coarse grid. Figure 1 shows the local mesh refinement along the VOF interface.

2.2 Transition region from VOF to Lagrangian modelling

By converting coherent VOF phases in droplet form 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 height. This allows regions of intense collisions of VOF lamellae and droplets to be resolved with the interfacial effects using surface tracking techniques, see Figure 2. 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, as shown in Figure 3.

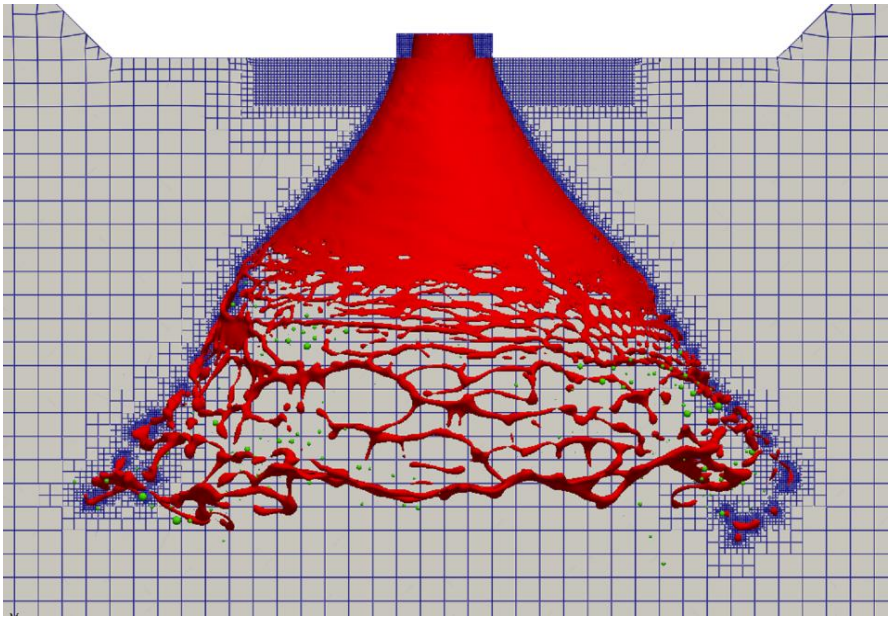


Figure 1 - adaptive mesh refinement for the VOF phase

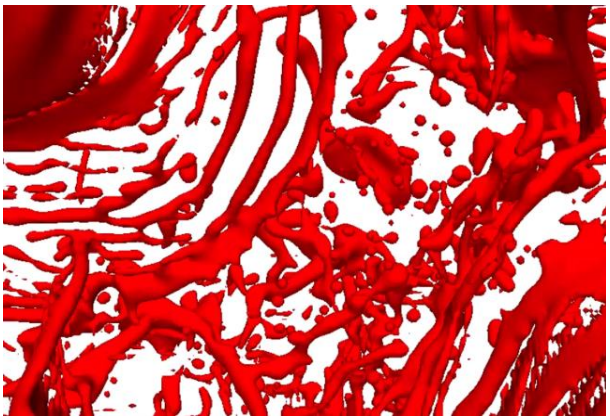


Figure 2 - region with collisions of droplets and lamella

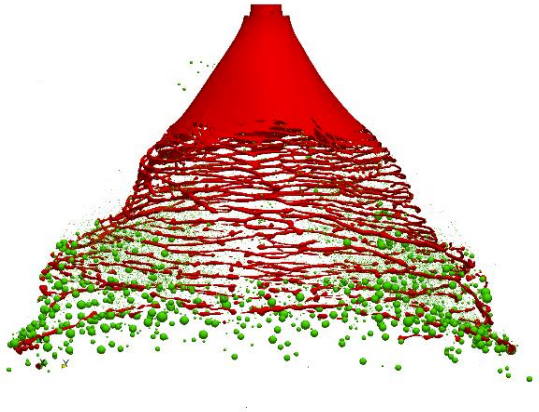


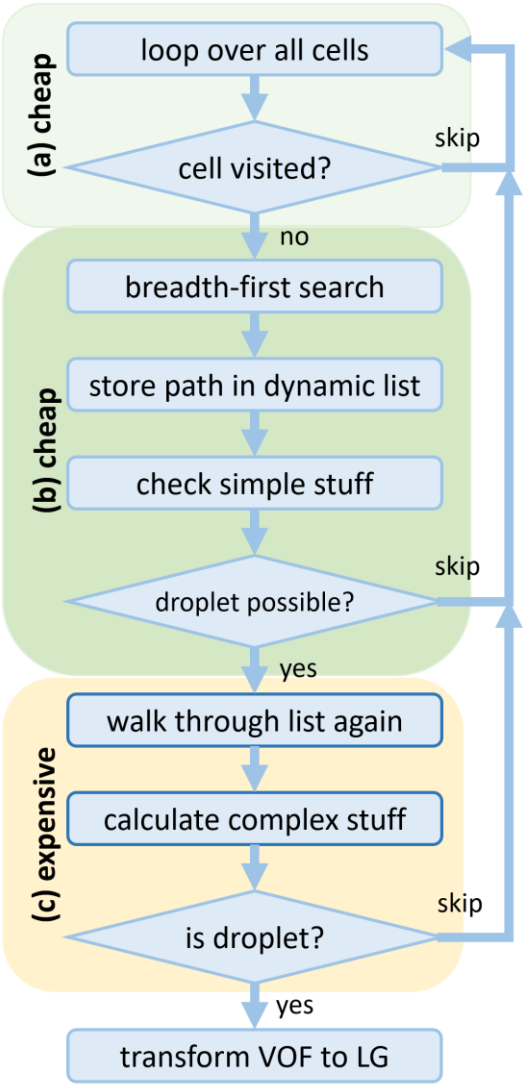
Figure 3 - lower regions without further droplet collisions

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.
The VOF-to-Lagrangian conversion from VOF droplet to Lagrangian particle is basically mass conserving. The accuracy in the simulation of the phase fractions depends only on the quality of the VOF method used in combination with the interface tracking and in particular its resolution, i.e., above

all the number of grid refinement levels used. It is also taken into account that partially filled VOF cells also contribute to the mass of a Lagrangian particle according to their degree of filling and the cell size.

2.3 Droplet identification algorithm

Special emphasis was placed on the implementation of the droplet identification algorithm. An essential feature should be that the identification should take place independently of predefined cutting planes at any position in the calculation space in order to ensure maximum flexibility. In addition, it should be possible to specifically omit regions of particular interest.
These requirements necessitate very efficient processing since the transformation of a droplet could in principle start in any cell of the grid.



First, the search for potential VOF cells eligible for conversion is started on a field of all cells in the simulation domain, starting at step (a) in the flow chart in Figure 4.
If a cell has already been visited, the processing of the cell can be stopped immediately. If there is a cell that has not been processed, a breadth-first search is carried out in the direction of the neighbouring cells that have not been visited. These are stored in a dynamic list and can in turn add to other cells in the current search path (step (b) in the flowchart).
Cells that are included in the search path are considered visited and are not otherwise considered as starting cells or in the width search. The computational steps up to this point consist of memory accesses, integer operations and simple floating point number comparisons, so they are hardly computationally intensive. In addition, these operations can be performed on all processors simultaneously, which leads to very good efficiency on a well-balanced load distribution.
At the end of the width search, a preselection for the drop conversion is already made: if, for example, one of the cells lies in an area that is locked for conversion, all cells in the list are marked as locked and not pursued further.
After these pre-processing steps (a) and (b), a list with contiguous cells containing a sufficiently high VOF phase fraction is available. The cells in the list are also surrounded by at least one cell containing only air, thus representing a potential drop.
Only now is the cell list examined with the calculation-intensive operations (step (c) in the flow chart).

Figure 4 - algorithm of droplet identification

Droplet volume, centre of mass and droplet shape are calculated, and other criteria such as minimum and maximum size are checked. This computationally intensive part of the algorithm is thus only used on a very small residual set of all cells. If all requirements are met, a Lagrangian particle is created as a droplet and the plenty of cells involved are replaced again by a few large cells in the next grid coarsening step.
The VOF-to-Lagrangian function is called at freely definable times. This makes it possible to convert the droplets into Lagrangian particles for a fully developed pure VOF simulation at a late stage, for example for evaluation purposes. A conversion after each calculation step is also possible, as the time required is negligible compared to the other solver tasks. A synchronisation with the grid redefinition or un-refinement is advantageous. The computationally expensive adaptive grid refinement is ideally not performed in every time step but depending on the time step width or the resulting interface Courant number in an interval that prevents an uncontrolled crossing of the VOF interface across unrefined cells. If a grid refinement is pending, cells that were transferred into a Lagrangian particle by the VOF-to-Lagrangian algorithm can be combined again directly afterwards into a few large cells.

Figure 5 shows the embedding of the VOF-to-Lagrangian algorithm in the solver structure.
A time step of the simulation first starts with the transport of all already identified droplets through the managing LagrangianCloud instance. Following the particle movement, the cloud checks whether new droplets can be added. For this purpose, the VOF-to-Lagrangian conversion is started. New droplets are then added to the cloud and the cells previously occupied with VOF phase are released. The source terms for momentum and, if applicable, energy equations are provided for the following systems of equations in the Eulerian calculations.
The solver then solves the equations of the VOF phase, now reduced by the converted droplets, as well as the equation for momentum, pressure and turbulence variables.
Numerous variables for process control are already provided at runtime. These include, for example, the current particle size distribution in the entire cloud and in the evaluation planes. Efficiency variables such as processor utilisation in the context of load distribution are also determined here and can be monitored by users at runtime. With the runtime monitoring tool RunGui, the data is immediately graphically processed and displayed.
Within the scope of the solver read processes carried out here, there is the possibility for the user to adjust process parameters during the simulation, e.g., the number of grid refinement levels, time step widths or tolerances of individual equation system solvers.

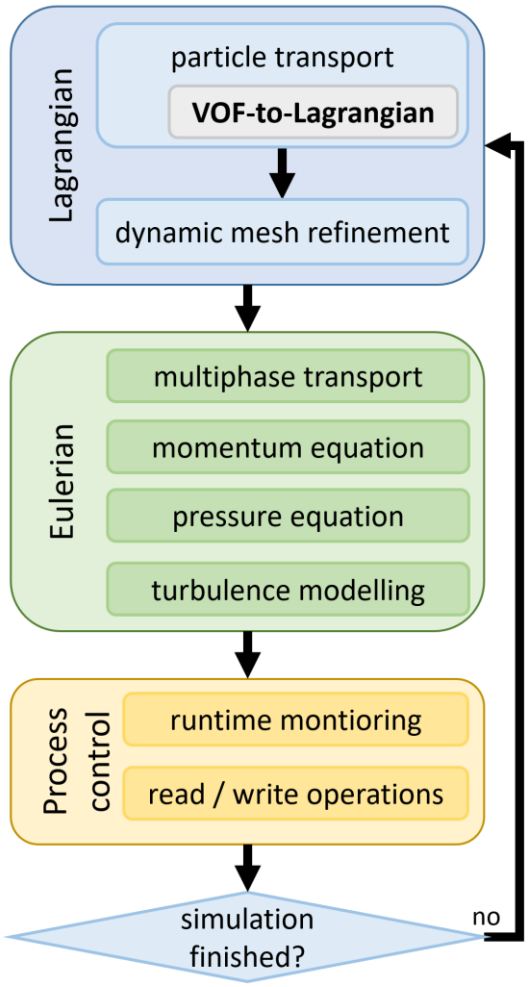


Figure 5 - solver flow chart

2.4 Droplet transport with a Lagrangian approach

In the further course of the modelling, the spray is modelled with a Lagrangian approach. In Lagrangian modelling, it is then particularly easy to consider secondary breakup processes, i.e., the further decay of the droplets into smaller droplets. This can be realised via the parcel approach: While in the transition from VOF to Lagrangian each VOF droplet is still transformed to exactly one Lagrangian particle, secondary decay can be realised by the parcel approach, where each modelled Lagrangian particle represents several droplets. For example, once a critical Weber number is reached for a droplet, this unstable droplet decays by updating the parcel diameter and the number of transported droplets per parcel. The secondary breakup process itself is thus only an internal process in the management of the parcel properties, which in the following, however, takes influence on the transport process of the parcel (such as a changed resistance or inertia due to the changed diameter) and changes the interaction with the continuous flow. It is also possible to divide the parcel into a limited number of new parcels, in which many small droplets in a representative parcel are then tracked separately from the largest parcel. This is possible because particle transport is much cheaper in terms of calculation than the much more complex VOF method with its fine interface resolution.

2.5 Implementation

In OpenFOAM, the VOF-to-Lagrangian method is embedded in a framework of libraries, utilities, and solvers, see Figure 6. OpenFOAM provides powerful particle management tools (so-called cloud functions) for this purpose, which have been extended and expanded for this application.
In addition to the eponymous VOF-to-Lagrangian cloudFunctionObject, there are further cloudFunctionObjects for runtime monitoring and post-processing of the particles, e.g., planes that generate size and mass statistics for particles flying through and that can also remove them from the simulation if required (collectivePlanes).

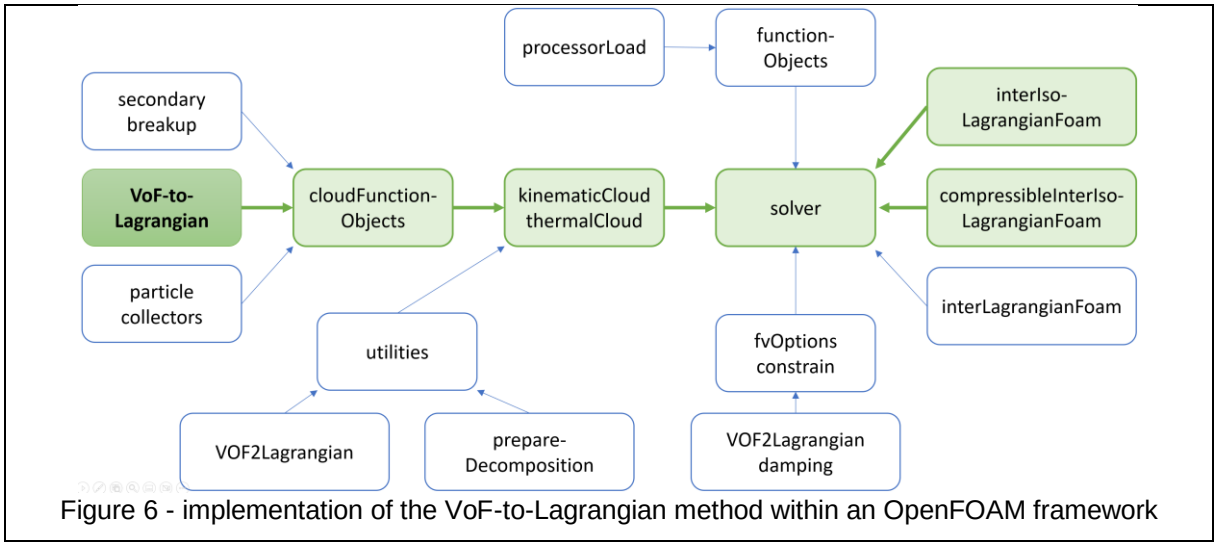


Figure 6 - implementation of the VoF-to-Lagrangian method within an OpenFOAM framework

A secondary breakup of the already transformed droplets can also be modelled as a cloudFunctionObject using Reitz-Diwakar or Pilch-Erdman approaches. Solvers for compressible and incompressible simulations are available; in addition, the isoAdvector method and the MULES method for tracking the interface in the VOF range are supported. The evenly utilisation of the processor cores, the load balancing, is optionally monitored with the help of functionObjects, utilities generate graphics for the uniformity measures of the particle cloud. Pre-processing tools support the efficient distribution of the grid to the processors (decomposition), post-processing tools enable the tracking of converted particles to the final deposition location.

3 Fuel jet in cross flow benchmark

The fuel jet in cross flow benchmark is used for validation [2] [3] [4]. 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

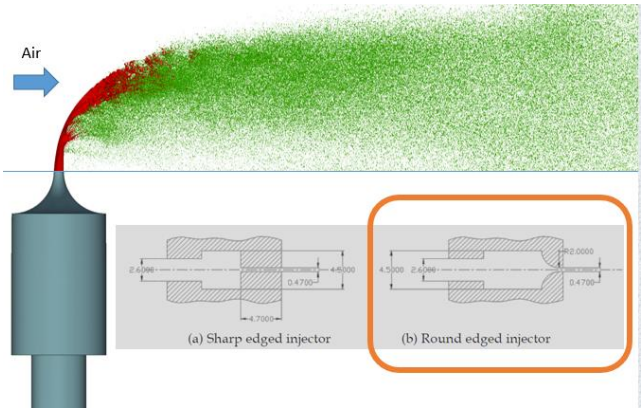


Figure 7 - injection nozzle used

Figure 8 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.

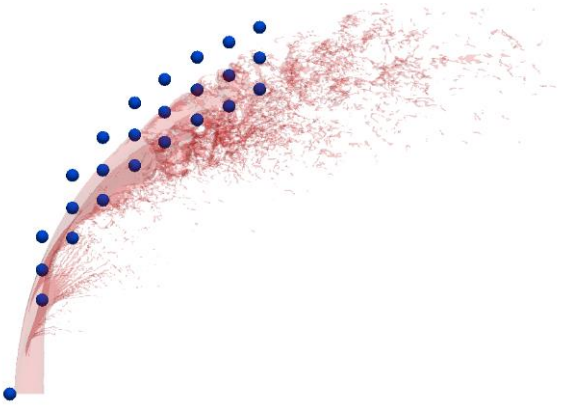
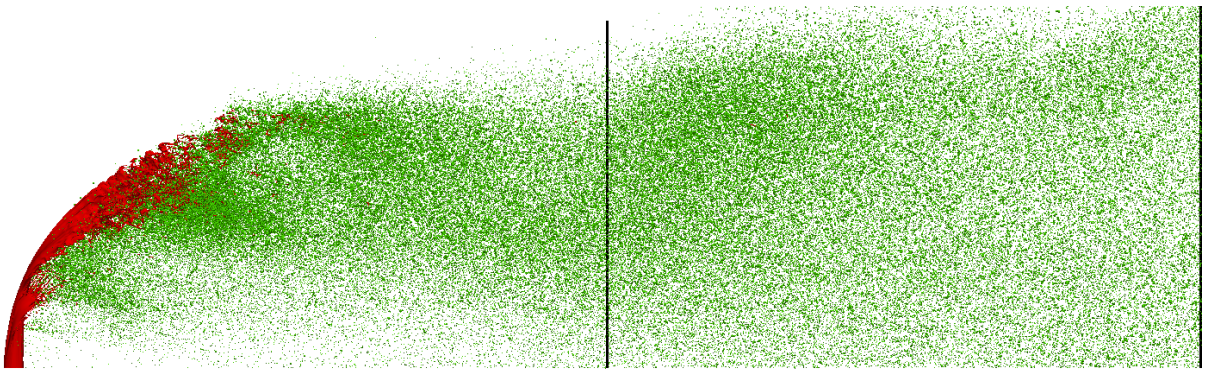


Figure 8 - jet penetration trajectory, experiment (blue dots) vs simulation (red)



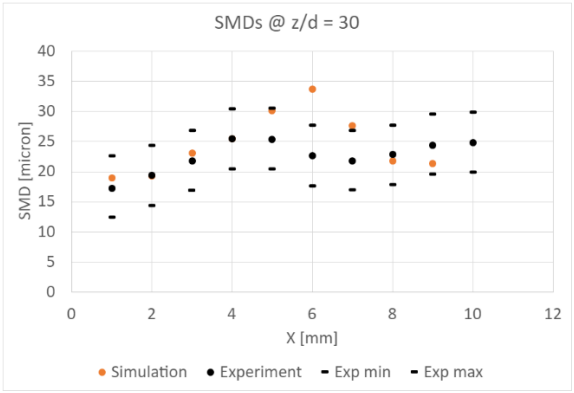


Figure 9 - monitoring section 1: particle sizes (sauter mean diameter), comparison simulation (orange) and experiment (black)

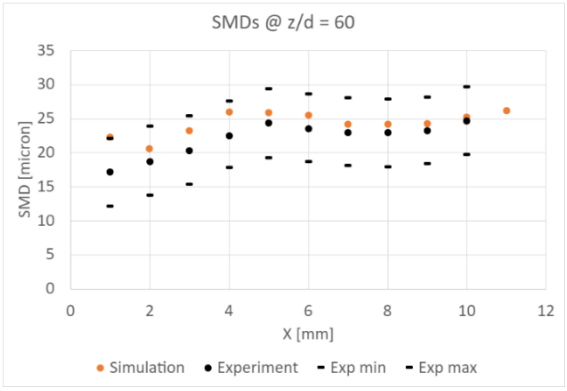


Figure 10 - monitoring section 2: particle sizes of simulation (orange) and experiment (black)

Figure 9 and Figure 10 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.

4 Application

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.
Subsequently, the droplets are atomised into small particles by gas jets at high speed, see Figure 11.

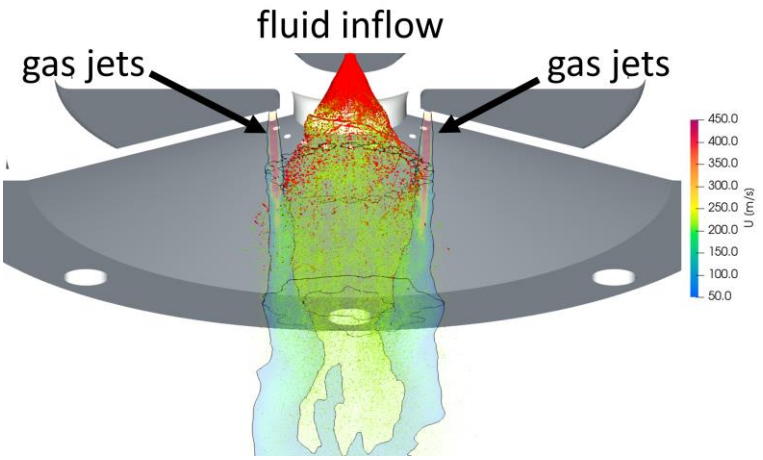


Figure 11 - molten metal atomisation

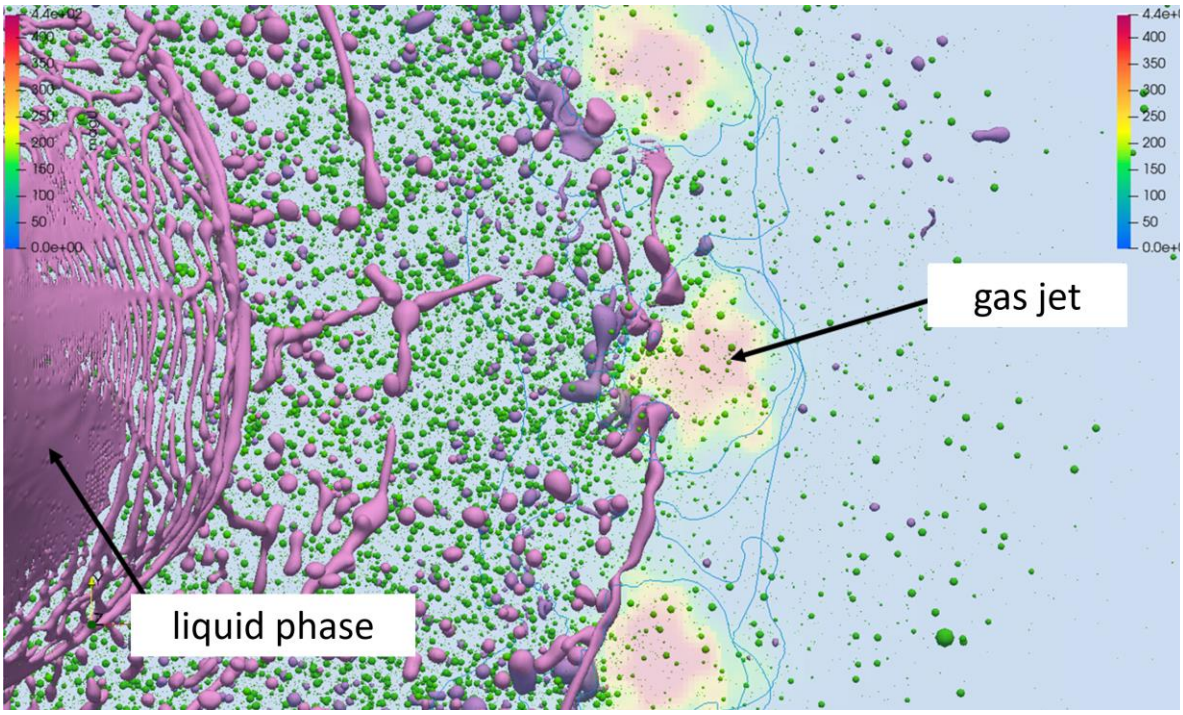


Figure 12 - interaction of ligaments with gas jets during molten metal atomisation

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 12.

5 Conclusion

A conversion model from a free surface view (VOF) to a Lagrangian modelling approach of the particles was presented. This model is suitable for closed-loop modelling of jet decay processes with subsequent spray modelling. Good agreement was obtained compared to experimental data for the entire breakup process from primary decay of the ligaments to secondary breakup into microparticles.

6 Acknowledgements

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7 References

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