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An efficient VoF-to-Lagrangian extension for spray breakup simulations

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The atomisation of liquids into a spray is a widely used process to increase the specific surface area of the fluid. Typical applications are the injection of fuel in combustion processes, the atomisation of water for cooling processes by droplet evaporation or the atomisation of molten metals for powder production.

In the exit region of the nozzle the liquid film sheet is modelled with the Volume of Fluid (VoF) method on a grid with adaptive mesh refinement. The interfaces of the ligament and droplet formation are resolved with either the IsoAdvector or the MULES approach. After the primary breakup the forming droplets are transformed into Lagrangian particles. Without the necessity to resolve the interface accurately any longer the grid can be unrefined, hereby saving an essential amount of memory and computational time. The Lagrangian particles are further tracked and might face secondary breakup effects, modelled with Pilch-Erdman or Reitz-Diwakar breakup models.

OpenFOAM provides many of the required models, however some of them needed some extensions, modifications, or improvements to fit our projects needs. In particular, the VoF-to-Lagrangian transformation was re-implemented with a focus on very high computational performance, independency from predefined planes, and integration into different solver types like compressible (e.g., liquid metal atomization) and incompressible (e.g., SCR applications) solvers. For performance reasons the VoF-to-Lagrangian transformation should be performed as soon as the droplets reach an approximate sphere shape. In case of secondary gas injection for further atomization of the spray, specific regions of particular interest can be excluded from the transformation, so that the disruption of large droplets is further evaluated with the more accurate VoF method, and the shift to the Lagrangian tracking method starts immediately afterwards. To simplify the integration of the VoF-to-Lagrangian method into the different solvers, it was implemented as a cloudFunctionObject. The same is true for the secondary break up models, which were reimplemented as cloudFunctionObjects as well. Finally, a collection of postprocessing tools in the form of cloudFunctionObjects and functionObjects completes the extension package.

In the presentation the validation of the implementation is shown against a benchmark for a fuel jet in a cross flow. Furthermore, the results of the implemented extensions are shown for simulations from liquid metal atomization and SCR applications.