LES MODELING OF LIQUID ATOMIZATION IN OPENFOAM USING A SURFACE DENSITY FUNCTION

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Spray atomization is often encountered in industry. It is used to coat, cool, paint a large variety of device or feed a combustion chamber with a liquid fuel that needs to be dispersed and vaporized before reactions take place. Thus, atomization is one of the most widely used process in industry and it needs to be controlled and optimized to improve the technical and economical output of the considered device. Moreover, even if the atomization process represents a small fraction of the complete physical chain in the system, it will affect anyway the evolution and the characteristics of all the other processes. For example, atomization of a liquid fuel at the inlet of a combustion chamber has a direct impact on droplets formation, dispersion and vaporization but its aftermath affects considerably heat transfers, vapor mixing, combustion process and pollutant formation. It is thus necessary to deeply understand the mechanisms of destabilization, breakup and dispersion of the liquid phase in the atomization process to improve the considered devices by developing adapted and accurate models. However, to do so, detailed information on the flow characteristics at the outlet of the atomizer is necessary.
Experimental measurements could be a way to obtain this information but standard techniques such as PDA (Phase Doppler Analyzer) or Mie scattering are not applicable to dense flows. Some of these difficulties may be overcome by using direct numerical simulation (DNS) or large eddy simulation (LES). DNS resolves all relevant space and time scales but it is presently restricted to simple flows at low or moderate Reynolds numbers due to the wide range of scales present in turbulent flows and the corresponding immense numerical resolution requirements [1]. In the LES approach, only the large scales are resolved, while the effect of the small fluctuations is accounted for by a subgrid turbulence model. Computationally, LES can be much less expensive than DNS enabling also the simulation of turbulent flows at high Reynolds numbers. However, LES alone is not able to tackle a complete industrial atomization system several models have to be introduced to be able to capture the whole process from the first liquid sheet destabilization to the vaporizing (and possibly reacting) dispersed spray.

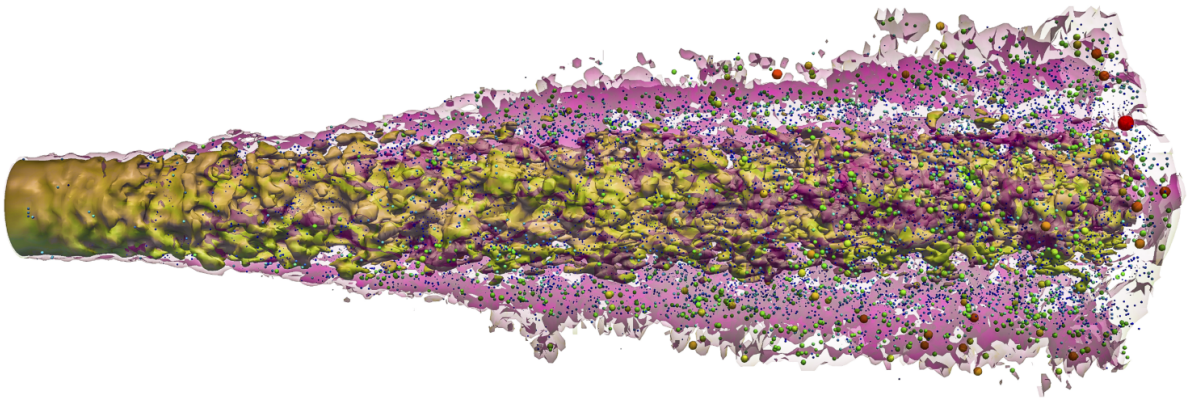

Figure 1: OpenFOAM simulation a liquid jet atomization

One of the main stumblingblock of the LES of interfacial flows is to capture properly the liquid phase atomized from the main liquid core. Indeed thin ligaments and small droplets are forming from the destabilized interface and they need to be characterized at a subgrid level. Several techniques exists to address this problem. It is possible, for example, to refine

the mesh where needed [2, 3] but, in the end, the computational cost is skyrocketing and a complete simulation involving all the processes from the atomization down to dispersed spray evolution is impossible. Another solution s to switch from a front tracking method to a discrete Lagrangian description when any droplet enters into the subgrid level. Then, the small subgrid liquid entities are considered as a set of spherical droplets [4, 5] that are dispersing following individual or group tracking [6]. However, many physical properties are not conserved (for example, the geometry of the liquid structure is far from being typicaly spherical, gas mass is added to the simulation, etc). The solution proposed in this work is to use the general notion of surface density in the secondary atomization area before switching to a Lagrangian description only in the dispersed zone where all droplets are nearly self-similar to a sphere. the amount of liquid-gas surface area per unit of volume : Σ. The liquid-gas flow at the exit of the injector is considered as a global mixture defined by a liquid volume fraction and a surface density. This approach, developed by Vallet and Borghi [7] has been called ELSA for Eulerian Lagrangian Spray Atomization [8]. The ELSA approach in turbulent flows [9] is particularly suited for complex geometry and can be applied to vaporizing sprays with colliding droplets [10] (cavitation can be considered also). On the other hand, this formalism may be applied to the study of bubbles within liquid and aerated liquid for example could be tackled by the method.
The transport equations for Σ and the liquid mass fraction is developed in the LES framework and models are proposed for the unclosed terms. The turbulent diffusion flux of liquid is closed using a gradient law while the production and destruction of liquid surface due to mean flow and turbulence stretching, collision and coalescence are accounted for with source terms developed over the years primilarily in a RANS context. Since there is no geometrical constraint compared to a direct Eulerian to Lagrangian substitution, information issued from these equations allows to determine the local drop size, drop number and drop distributions. Encouraging results demonstrate that the known advantages of the ELSA model in the RANS framework (quick computation, reconstruction of the subgrid spray properties, application in complex geometries, etc) are present in the LES framework. Note that this is an open development that will be made available to anybody interested by the method.

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