Hybrid treatment of small droplets in atomized jet

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Résumé :

L'atomisation de combustible a un impact direct sur l'émission de polluants dans l'atmosphère. Face au besoin de caractériser l'atomisation primaire, l'étude numérique de l'intéraction liquide-gaz croît dans le but de maîtriser la création de particules polluantes et de la réduire. Elle est effectuée sur l'ensemble du spray, de son injection dans la chambre de combustion jusqu'à l'évaporation des gouttes créées suite au *secondary breakup*. Notre but est d'augmenter la précision du transport des gouttes au sein des jets atomisés, typiquement, une goutte est 100 fois plus petite que le diamètre d'injection.

Cette différence d'échelle rend la définition de l'interface liquide-gaz complexe et créeer des zones sous résolues. Pour résoudre ce probleme d'échelle, un coupling entre un suivi Eulérien et un suivi Lagrangian a été proposé, voir Hermann, [1]. Cette communication se concentre sur les critères de transformation d'une goutte eulérienne en particule lagrangienne et les modifications physiques et numériques entourant cette transformation. L'implémentation d'une méthode de suivi de particule polydisperse basée sur des critères géometriques est présentée. Ils sont finalement appliqués sur l'étude d'un jet atomisé.

Abstract :

Atomization of liquid fuel has a direct impact on the production of pollutant emission in engineering propulsion devices. Due to the multiple challenges in experimental investigations, motivation for numerical study is increasing on liquid/gas interaction from injection till dispersed spray zone. Our purpose is to increase the accuracy of the treatment of droplets in atomized jet, which are typically 100 times smaller than the injection size. As the size of the droplets reduces with the primary breakup of liquid fuel, it is increasingly challenging to track the interface of the droplets accurately. To solve this multiscale issue, a coupled tracking Eulerian-Lagrangian Method is proposed, see Hermann, [1]. This communication focuses on the criteria of transformation of this coupling from interface captured droplets to Lagrangian particles and numerical/physical reconstruction during this process. From the literature, interaction criteria of transformation are all geometric, implementation of physical parameter is made in this communication. Those criteria are finally applied on a liquid jet atomization.

Key Words : Numerical simulation, DNS, Two-phase flow, Atomization, Multiscale, Particles, Droplets

Introduction

Atomization is a multiphase and a multiscale flow phenomenon which is still far from being understood. Direct Numerical Simulation (DNS) is an important tool to interpret the experimental results and go further into the atomization understanding. Due to the wide range of scale, centimeter for the liquid jet to micrometer for droplets in the dispersed spray area, it is challenging to model this process. In the past few years, numerical schemes of Interface Capturing Method (ICM) have been improved. However, ICM schemes are still not sufficient to go further in the dispersed spray area with DNS. Two strategies have been then developed, an Adaptive Mesh Refinement (AMR) technique, which consists of refining only the needed area and a coupling between ICM and Particles Tracking Method (PTM), Hermann [1]. It used criteria and transformation hypotheses for small droplets to validate the assumption that a small droplet is transported such as a particle. This validation is an important step to go from ICM to PTM. Different strategies for the PTM are proposed in the literature to cover th particles with diameter smaller than the mesh size, Δx, until that ICM becomes accurate. Ling et al. [2] improved the Lagrangian Point Particle (LPP) method adding another PTM, which increases the number of mesh inside of the diameter of a droplet. In Zuzio et al. [3], in addition to the implementation of a second PTM, they enhanced the accuracy of the ICM implementing AMR in their code. The goal of our communication is to discuss transformation hypothesis and new developed criteria and the reconstruction of the surrouding flow during a transformation. Then test them on engineering applications.

Numerical Methods

Our in-house multiphase code, *ARCHER*, is a DNS code which has strong experience in interface treatment and atomization process, Osmar et al. [4]. It solves incompressible Navier Stokes equation on a cubic staggered grid where the pressure and the velocity are decoupled. Interface is tracked with CLSVOF, *Coupled Level-set Volume of Fluid method*, Ménard et al. [5], coupling a *Level-set* distance function [6] and a *Volume of Fluid* (VOF) method. The *Level-set* function ϕ describes the interface at its zero level curve of a continuous function defined by the signed distance to the interface.

The in-house coupling strategy is based on various PTM used when the inconsistency of the ICM is shown. A classical LPP method is used for small particles, and for the larger ones, Immersed Boundary Method (IBM), based on the work of Uhlamn [7] with the extension of Breugem [8], is considered.

To take advantage of PTM when ICM is not enough accurate, the droplet must validate some physical hypothesis before to be transformed and then considered as a particle. We will then highlight existing parameters which are implemented in our in-house code to compare and discuss their sufficiency.

Hypothesis of Transformation

The transformation process from droplet to particle is quite similar in both ways, but does not occur in similar situations. First, from ICM to PTM, four main hypotheses have been introduced in the literature. The first hypothesis introduced in Tomar et al.[9], focuses on the size of the droplet, with respect to the mesh size ; if the size is below a given size limit, the transformation occurs. The second hypothesis is a distance parameter, a droplet has to be isolated enough from any other interface. This parameter evolved from Tomar et al. [9] who set it with a tagging process, see Hermann [1], to Zuzio [3] who defines the distance criteria to the diameter of the studied droplet. The first geometric parameter concerning the

shape of the droplet is implemented in Hermann [1], it compares the volume of the droplet to a maximal volume that cannot overcome a particle. Overcoming this *cut-off* volume will create instability on the PTM. The fourth parameter has firstly be implemented in Ling et al. [2], it considers the sphericity of the droplet, figure 1. It is calculated by different ways in the literature, Ling et al. [2] quantified it on an aspect ratio, calculated with *VOF*, while Zuzio et al. [3] calculated this criteria with a Level-Set function. All of those parameters have been implemented in our in-house code and have been analyzed in Chéron

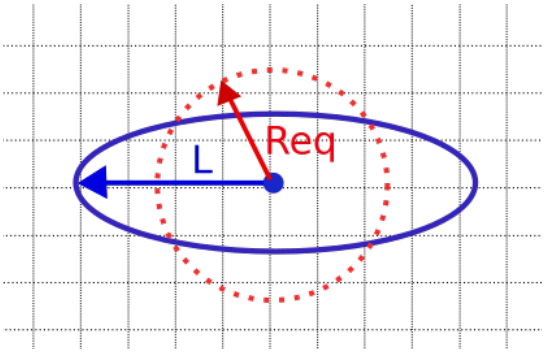

FIGURE 1 – Sphericity criteria for droplets transformation. Blue line : Interface Structure, Red dashed : Equivalent Particle.

et al. [10]. Focusing on the geometric state of the atomized droplets is not sufficient, it can be spherical during an iteration even if it does not have any physical property of a convertible droplet.

To straighten the hypothesis of transformation, the non dimensional Weber number of the droplet can be a solution.

$$We = \frac{\rho_{droplet} dV_{slip}^2}{\sigma} \tag{1}$$

It is calculated with the density ρ and diameter d of the object, surface tension σ and the slip velocity between the object and surrounding gas flow. The main concern in this non dimensionless parameter is the definition of the slip velocity. According to Cisse et al. [11], the slip velocity can not be determined in the near region around a spherical object, approximatively two diameters around the droplet. The presence of others objects will disrupt the flow motion and the definition of the Weber number based on the target droplet can not be accurate due to inaccuracy on the slip velocity A solution could be the implementation of a local Weber number based on the shear velocity, see Pelerkar et al. [12]

In the literature, the only parameter to transform back from PTM to ICM is a distance parameter and this is how the transformation occurs, see figure 2 and figure 3. The particle has to be in the vicinity of any interface to validate this hypothesis.

Next, collision between particles are considered in this communication only between IBM. Tomar et al. [9] and then Zuzio et al. [3] integrated solid collision algorithm between particles. Here, the impact Weber number, We_{impact}, and the impact distance parameter, b, are considered in order to define the collision regime, rebound or coalescence as seen in the thesis of Rabe, figure 8. [13]

$$We_{impact} = \frac{\rho_{droplet} |V_{rel}^2| d_*}{\sigma} \tag{2}$$

Where d_* is the smallest diameter between the two colliding droplets and V_{rel} the relative velocity between these droplets.

$$b = \frac{2\delta}{d_1 + d_2} \tag{3}$$

Where $d_{1,2}$ represents the diameters of the particles and δ represents the distance between the projected relative belocity of collision from the center of the droplet 1 and the center of the droplet 2. When $\delta = 0$, the collision is frontal.

A coalescence lead to important modification of the geometry of the particle and on the surrounding motion. The strategy of this communication is then to treat such interaction between IBM particles with a reverse transformation into ICM in order to let the deformation occurs.

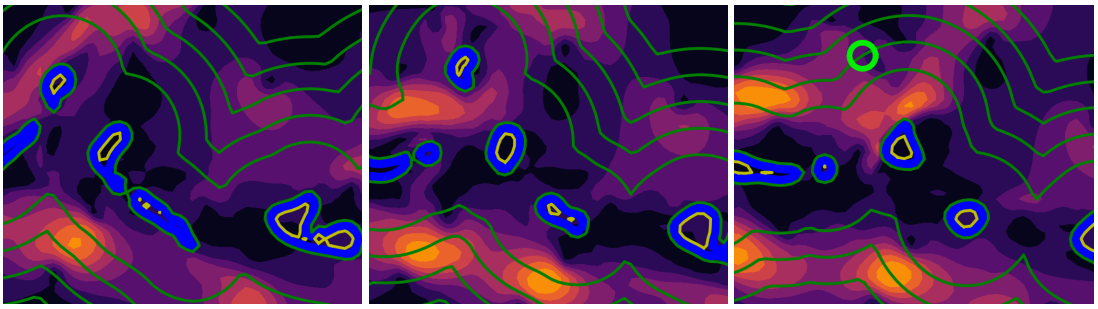

FIGURE 2 – Focus on Droplet transformation into Particle when isolated from other structures in an atomized jet, ICM in blue, PTM in light green, Iso Level-Set in shadow green.

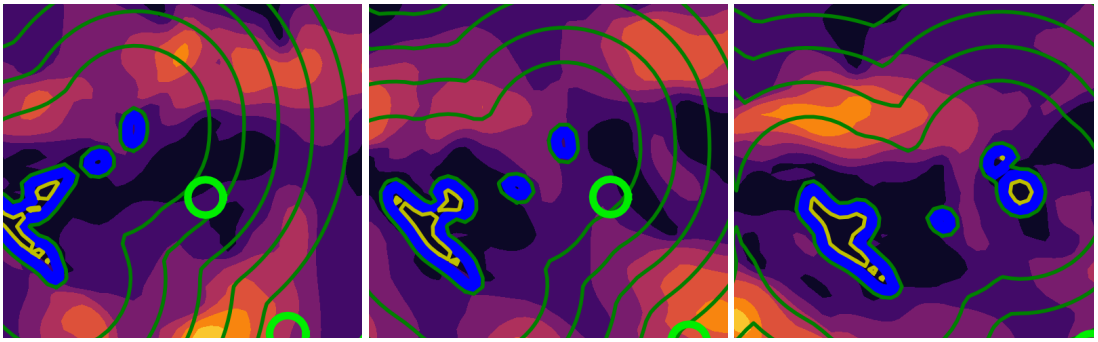

FIGURE 3 – Focus on Droplet-Particle coalescence in an atomized jet, ICM in blue, PTM in light green, Iso Level-Set in shadow green.

Back on 2 and figure 3, it is possible to see that in both way, the distance function is rewritten when the droplet or particle is transformed. This is part of a process of numerical and physical rewritting of the transformed area as schemed on figure 4 where one can see the rewritting of the *Level-Set*.

First on figure 4, for case a. and case b, a target area is selected around the droplet where modification will occurs. For figure 4 a., on figure 2, the *VOF* inside of the droplet, which is set to 1 when the cell contains liquid is set to 0, to vanish the presence of the droplet. Then, the velocity field inside of the droplet and outside of the droplet in a defined area is rewritten with respect to the work of Ling et al., [2] in order to conserve the momentum. On figure 3, the distance function is rewritten in the vicinity of the transformed droplet, iterations are needed to redefine correctly the distance function and to obtain the expected slope. A lagrangian particle does not affect the distance function within the code as seen on figure 3 b and c.

For the opposite transformation, schemed on figure 4 b., the creation of the droplet is based on the droplet

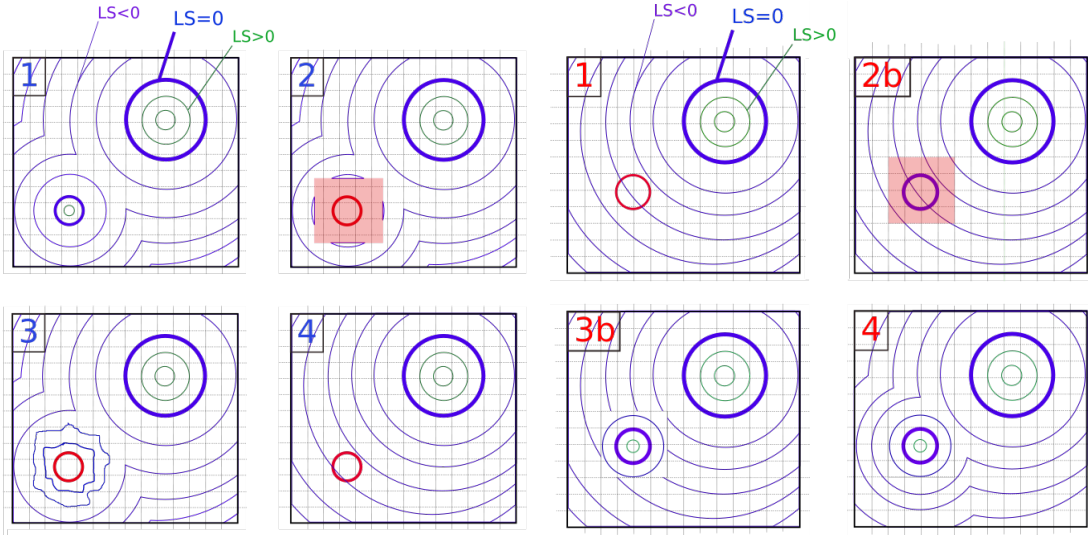

FIGURE 4 – a) On left with blue indices, droplet to particle transformation. b) On right with red indices, particle to droplet transformation.

of the radius by the initialization of a *Level-Set*. Then, with the algorithm of the *CLSVOF*, cells inside of the droplets are fullfill with the right amount of *VOF*. To respect the conservation of the momentum, velocity field is also rewritten in the vicinity of the transformed particle. Finally, with iteration on the distance function, one is able to pass from 3b to 4, and this can also be observed on figure 3.

Application

To apply our local and global transformation criteria on a real application, we used the results of Mukundan et al. [14] of a planar sheet airblast atomizer. Details on the configuration can be found in its communication. Here we analyze with our criteria a time step of this atomization process. The selected snapshot is given on figure 5. The purpose of this analyzis is to validate the implementation of the hybrid treatment of small droplets and to validate the matter of velocity, *VOF* and distance function reconstruction without any burst of velocity during the simulation. On figure 5, green represents the smallest droplets transformed into LPP with a radius smaller than $2\Delta x$ while red represents medium droplets of radius between $2\Delta x$ and $4\Delta x$. The spatial representation of those smallest droplets is surrounding the main liquid structures. The bigger are the droplets, the closer they are from the structure.

In such engineering application, the high shear at the interface of the droplet, typically with a Reynolds number based on gas velocity, $Reynolds_{gas} = \frac{\rho_{gas} v_{shear} Lc}{\mu_{gas}}$, with Lc representing channel half width of the injection domain, of $\text{Reynolds}_{gas} = 13\,333$, and a velocity difference at the injection of $\frac{v_{gas}}{v_{liq}} = 100$, enhance the difficulty of the reconstruction and this show us the limit of number of cells inside of the diameter of the PTM that we use to transform medium droplets into particles.

Conclusions

This communication shows an efficient Eulerian/Lagrangian DNS simulation of two phase flow atomization to handle multiscale issue. The present method shows the implementation of transformation criteria added to prior hypothesis of transformation shown in the literature. It has successfully been applied on an airblast atomizer, from the jet injection to the dispersed area.

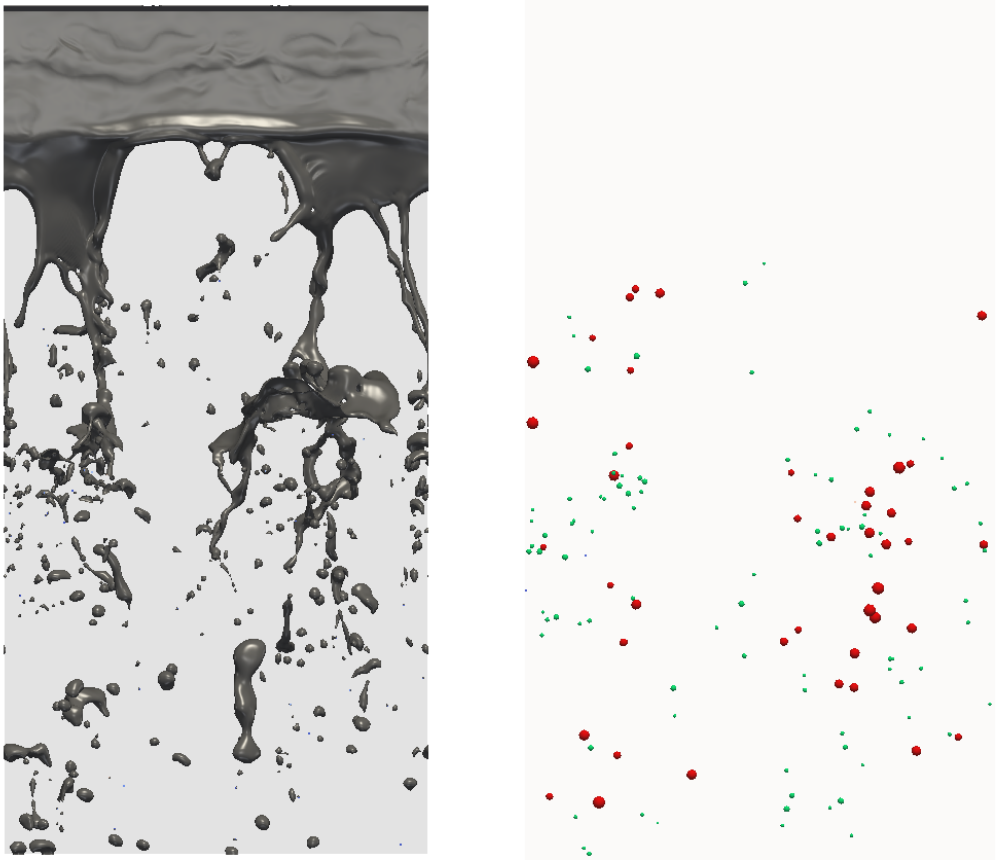

FIGURE 5 – Snapshot of Airblast atomizer, Right : CLSVOF Liquid structures, Left : Particles structure. Green : LPP $Radius < 1.5\Delta$, Red : IBM $Radius < 4.\Delta$

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