Application of the immersed boundary method to simulate flows inside and outside the nozzles

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Abstract

The objective of the present work consists in a strong coupling between internal and external flows simulations by keeping the same numerical tools. Three phases have to be accounted for (solid, liquid and gas) as well as two types of interface (liquid/gas and fluid/solid). The chosen numerical approach is based on the implementation of the discrete immersed boundary method (IBM) in the academic code Archer initially developed for the study of primary breakup processes. This paper briefly describes the implementation of the method and two 2D test cases are investigated: the equilibrium of a droplet on a solid surface and the simulation of an injection event. These test cases show the efficiency and the accuracy of the method.

Introduction

In the last years, the direct numerical simulations were carried out to reproduce the primary breakup of liquid jets [1-3]. Recent works [3-4] have shown that internal flow characteristics strongly influence the breakup processes. These results led us to conduct numerical simulations able to take into account both internal and external flows by ensuring a strong coupling. In the case of complex geometries, meshes are often unstructured and irregular. On this type of mesh, two phase flow simulations are less accurate. In addition, with moving walls, this technique needs to remesh at each time step; this increases drastically the computational time. A possible approach consists in using a method where the solid frontiers are immersed in a structured Cartesian mesh. The main advantage of such a method is that the solid displacement is only based on the tracking of the interface position. Another advantage is the flexibility which allows the use of high order numerical schemes and fast solvers. The work presented here consists in the implementation of such a method. The objective here is to show that it can allow the simulation of both internal and external flows simultaneously.

The method which was found the best adapted to our situation is the Immersed Boundary Method (IBM) based on a direct forcing. This paper will first present the method briefly where the difficulty to account for the three phases (solid, gas and liquid) is highlighted. The approach is first validated in the situation of a drop lying on either horizontal or inclined walls. Second, the simulation of an injection event in a 2D configuration is carried out. In the investigated situation, the flow regime is weakly turbulent and the frequency analysis clearly shows the correlation which exists between the frequency of the velocity fluctuations at the nozzle exit and the perturbations that are present on the discharged liquid system.

Numerical Method

Governing equations of two phase flows in the absence of walls

The DNS of two phase flows remains an important topic of research. The main challenge is to capture the interface behavior in the nozzle vicinity with a good accuracy. To describe the dynamics of liquid/gas interfaces, the academic numerical code Archer was developed and validated in the case of liquid jet primary breakup [1]. In the code, the most suitable methods were coupled that is to say the level set method for the interface tracking, the Ghost Fluid Method (Fedkiw et al [5]) captures accurately sharp discontinuities and the VOF method ensures mass conservation as proposed by Sussman and Puckett [6]. To solve incompressible Navier Stokes equations, a projection method is used. A uniform staggered grid is used for convective terms; spatial discretization is carried out with a WENO scheme. The Poisson equation is solved by a multigrid algorithm to precondition a conjugate gradient method. Finally, a specific care was carried out to improve simulation capabilities with MPI parallelization.

Implementation of an immersed boundary method

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The immersed boundary method is based on the direct forcing which was originally proposed by Mohd Yusof [7]. It consists in the application of a velocity and a pressure field inside the solid. The approach is then based on the modification of the Navier Stokes equation to be solved as showed in Equation (1).

$$\rho\left(\frac{\partial u}{\partial t} + u.\nabla u\right) + \nabla p = \mu\Delta u + \mathrm{f} \quad (1)$$

where f is a corrective force. This force is chosen to construct the fictive flow inside the solid in such a way that the physical boundary conditions at the fluid/wall interface are respected.

In the present work, the level set method is employed to represent the solid/fluid boundary. The use of such a mathematical function allows to easily separate mesh points that belong to the fluid domain from those which are in the solid. The characteristics of the level set function are helpful to retrieve the geometrical information such as the distance from the interface and components of the vector normal to the interface. The mesh points that belong to the solid are the ghost points. The determination of the flow characteristics inside the solid is based on the flow characteristics in the fluid and close to the walls (neighboring points) by ensuring that physical conditions are respected on the fluid-solid boundary.

The implementation of the Immersed Boundary Method in Archer was first investigated with single phase flows and validated on academic situations such as confined channel flows and unstable flows past a cylinder. It was verified that the position of the immersed body inside the computational domain does not modify the accuracy of the numerical solution. This first approach led us to investigate the much complex situation of two phase flows interacting with a solid surface. The major difficulties to be tackled are presented briefly here.

When a two phase flow interacts with a solid surface, a contact line which separates the liquid, the gas and the solid exists. This discontinuity is called the *triple line* and is reduced to a triple point in a 2D configuration. In this latter situation, the angle that makes the liquid/gas interface with the wall is called the contact angle and is an important characteristic to consider. From a macroscopic description, this angle is found to be either constant (θ_s) when the fluid is at rest or dependent of the triple point velocity otherwise (Sikalo et al [8]). In the present paper, all the test cases assume a constant contact angle although this hypothesis is not critical as far as numerical implementation is concerned.

The major difficulty in the implementation of the immersed boundary method in the Archer code concerns the determination of the flow characteristics on each ghost points that is to say the level set value, the velocity and the pressure. In the present investigation, two level set functions have to be considered. First the level set which is called the *solid level* set represents the solid walls; second the level set that needs to be physically reconstructed at each time step is the liquid/gas interface and is called the *fluid level set*. The determination of the flow characteristics on each ghost points is summarized below:

1. The imposition of the contact angle leads to the determination of the fluid level set value on the ghost points in the immediate vicinity of the walls only; the values on the other ghost points are deduced from the classical constant extension (Aslam [9]) while the redistance algorithm ensures the distance function properties.
2. On the fluid-solid boundary, a no slip condition is imposed for the velocity. To determine the velocity components on the ghost points, an algebraic method is proposed. In a 2D configuration, the velocity of the ghost point is deduced from a linear interpolation. This interpolation takes into account the velocity components of the two closest points in the fluid (neighboring points) and the velocity on the walls.
3. In a similar way, the pressure in the solid phase is deduced from a linear interpolation with the knowledge of the pressure in the fluid and by imposing a zero normal gradient pressure on the wall. The most difficult configuration concern situations where the two neighboring fluid points belong to two different fluids (liquid and gas). We assume that the derivative jump of the pressure by density ratio is zero across the liquid/gas interface. The jump conditions at the interface between the liquid and the gas phase has to be accounted for in the discretization of the Poisson equation also. The problem to solve is illustrated on Figure 1 whereas equation (2) shows the discretized Poisson equation.

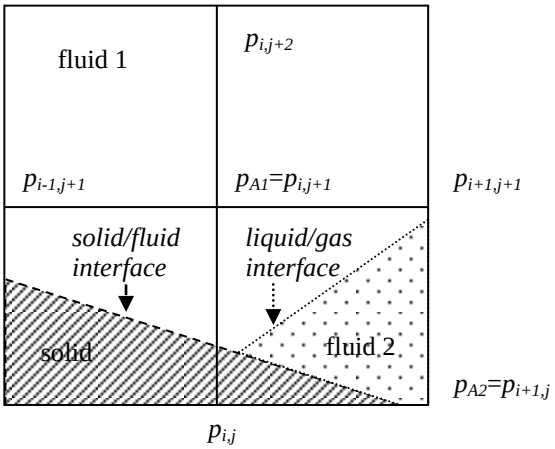

Figure 1 Illustration of the local discretization to solve the Poisson equation.

$$\frac{\Delta p_{i,j+1}}{\rho} = \frac{\frac{1}{\rho_1}(p_{i+1,j+1}+p_{i-1,j+1}+p_{i,j+2}-3p_{i,j+1})}{\Delta^2} + \frac{\frac{1}{\rho^*}\alpha_G(p_{A_2}-\alpha_\Gamma-p_{A_1})}{\Delta^2} \quad (2)$$

where Δ is the cell size, ρ^* is an effective density depending on the distance between the nodes and the liquid/gas interface, α_G is a geometrical parameter related to the local curvature of the interface and α_Γ accounts for the pressure jump between fluids 1 and 2 according to the Laplace's law.

Results and Discussion

Case 1: Equilibrium of a drop on a solid surface

The present test case is devoted to simulate the shape of a droplet at equilibrium in the absence of gravitational effects. This study was investigated by Dupont and Legendre [10] with a different numerical approach. The drop which is initially semicircular (the radius is R_0) is released on a wall and the initial contact angle with the wall is 90° (Figure 2). Then, as the constant angle (θ_S) is assumed to be constant and possibly different from 90°, the contact line moves and the drop shape changes with time by respecting the contact angle value. This test case takes the advantage to provide an analytic expression of the droplet geometry when the equilibrium is reached. As a matter of fact, its final form is given by the radius R, the length L and the thickness e (Figure 3). When the contact angle θ_S is known, based on geometrical consideration and mass conservation, it can be showed that:

$$R = R_0\sqrt{\frac{\pi}{2(\theta_s - sin\theta_s cos\theta_s)}}, L = 2Rsin\theta_s, e = R(1-cos\theta_s) \quad (3)$$

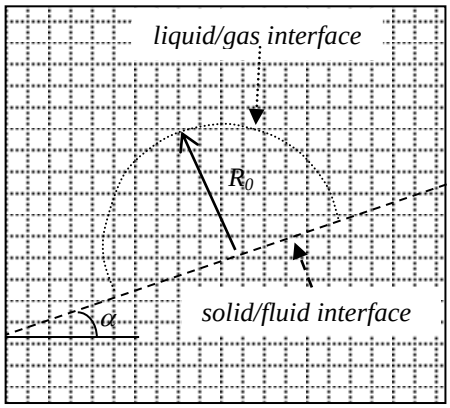

Figure 2 Initial conditions of the 3 phases in the regular Cartesian mesh.

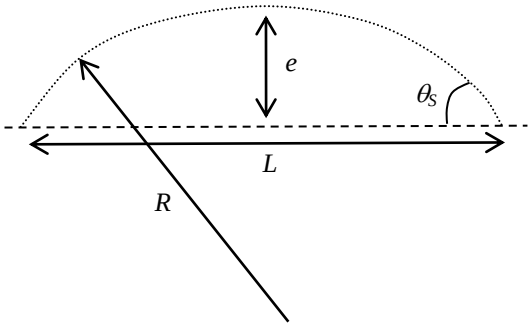

Figure 3 Droplet characteristics at the equilibrium.

The physical domain is 0.004 m x 0.004 m and the physical parameters are:

R_0 = 6.349x10^{-4} m, ρ_1 = 1.204 kgm^{-3}, ρ_2 = 1x10^3 kgm^{-3}, μ_1 = 1.78x10^{-5} kgm^{-1}s^{-1}, μ_2 = 1x10^{-3} kgm^{-1}s^{-1}, σ_{12} = 7.09x10^{-2} Nm^{-1}.

Indices 1 and 2 refer to the gas and the liquid respectively whereas σ_{12} is the surface tension coefficient.

In the present investigation, static angle was varied from 30° to 120°, two inclination angles α were considered (0° and 18°) in order to evaluate the influence of the wall position inside the computational domain. Finally two different meshes were used (MESH1: 64x64 and MESH2: 128x128). In the case of the coarsest mesh (MESH1), 10 cells describe the initial radius R_0.

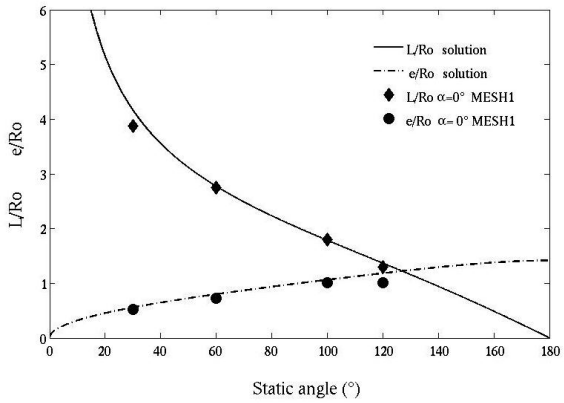

Figure 4 Influence of the static angle on the drop shape (horizontal wall).

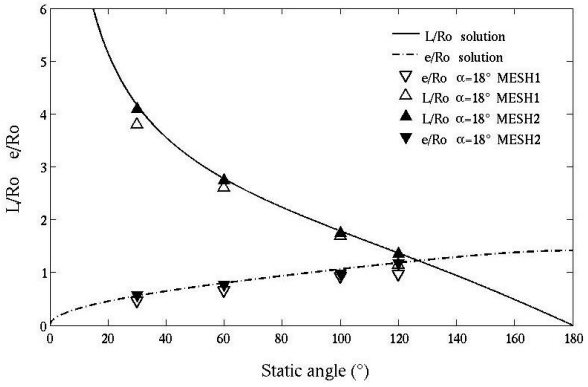

Figure 5 Influence of the static angle on the drop shape and effects of the mesh size (inclined wall).

Figure 4 shows the results given by the simulations in the situation of the coarsest mesh where the solid surface is horizontal and located at the half distance between two horizontal gridlines. First, it can be observed that numerical results are in a good agreement with the analytical solution despite the mesh coarseness. For small and large values of static angles, a lack of accuracy is observed. This discrepancy can be strongly reduced by refining the computational mesh as it can be observed in Figure 5. On this latter figure, the angle that makes the solid surface with the gridlines is also different from zero (18°); therefore the wall is not aligned with the gridlines anymore. Results are accurate and allow validating the efficiency of the method to investigate two phase flows. The complete simulation of the temporal oscillations of the droplet needs the knowledge of the dynamic contact angle dependency with the triple line velocity. This can be achieved by using empirical relationships from the literature (Sikalo et al [8]) where this angle is expressed as a function of a capillary number through an analytical power law.

Case 2: An injection test case

The second test case investigates the capability of the approach to simulate a whole injection event where inflow and outflow are computed with the same numerical solver. The geometrical configuration is 2D, the nozzle is 0.5 mm thick and 5.7 mm long. Water is injected in air at rest and the physical properties of these two fluids are the same as those used in the previous test case. The simulation is carried out with a regular Cartesian mesh with 2048 cells along the longitudinal direction and 1024 cells in the transverse direction. As far as boundary conditions are concerned, a flat velocity profile with no fluctuations is imposed at the nozzle inlet with a velocity set to 8 ms^{-1}. The resulting Reynolds number based on the thickness of the nozzle orifice is then 4,000 representative of a weakly turbulent flow. The time step of the simulation is about 3.36x10^{-8} s. At the start of the simulation, the fluid domain is filled of air at rest. Figure 6 shows the temporal evolution of the liquid phase. At the start of injection, water fills the nozzle; the leading edge of the liquid/gas interface presents a curvature due to the imposition of a constant contact angle set to 120°. The choice of a constant contact angle is not critical, as a matter of fact, regarding the contact line velocity, we are in conditions where capillary numbers are important indicating that the dynamic contact angle weakly depends on the triple line velocity. When the liquid emerges from the orifice, some disturbances along the liquid/gas interface due to the existence of fluctuating velocities at the nozzle exit are observed. These velocity fluctuations have an intermittent character; five turbulent spots were observed during the whole simulation. These spots have enough momentum to locally disturb the liquid/gas interface. However, these perturbations do not present a natural unstable character. The application of the linear theory on a flat liquid sheet reveals that the wavenumbers of the disturbances generated by the turbulent spots are too large and the surface tension forces are strong enough to avoid a growth of these disturbances.

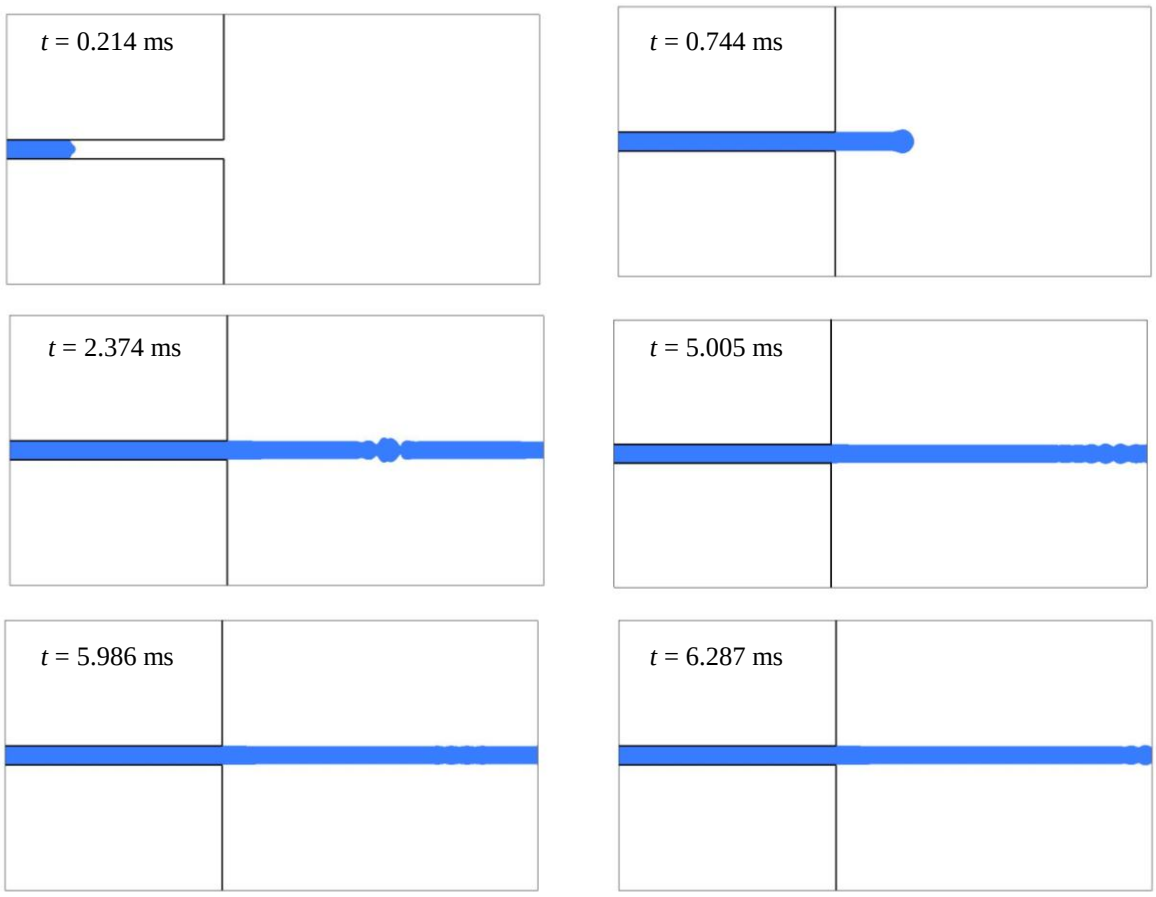

Figure 6 Temporal evolution of the flow inside and outside the nozzle.

The mean and standard deviation of the two components of velocity at the nozzle exit are given in Figures 7 and 8; they are normalized by the inlet velocity. *u* denotes the longitudinal velocity whereas *v* denotes the transverse velocity. The symmetry of the mean velocity profiles is well reproduced as well as the level of fluctuations which stays small. The highest levels of fluctuations are obviously obtained in the vicinity of the walls. The temporal fluctuations of the velocity are responsible of the disturbances on the liquid sheet observed downstream the nozzle tip. The temporal velocity fluctuations at the nozzle tip were analyzed and represented under the form of the power spectral density in Figure 9. This figure shows the power spectral densities of three characteristics; the two firsts are the longitudinal and transversal fluctuating velocity and the last one is a relative liquid/gas interface length which informs us on how the interface is perturbed. We can clearly observe that the characteristic time scales of the flow emerging from the nozzle are strongly linked to the time scales related to the interface deformation process.

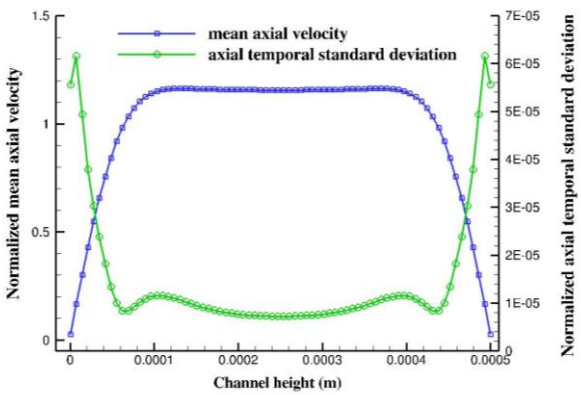

Figure 7 Mean and standard deviation of the axial velocity component.

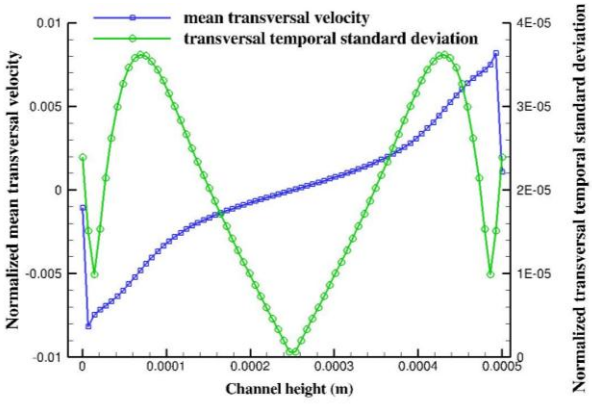

Figure 8 Mean and standard deviation of the transversal velocity component.

For the investigated case, the simulation reports dominant frequencies at 20, 40 and 60 kHz. These frequencies correspond to the period of the turbulent spots release, the duration of a turbulent spot and the period of the fluctuations during a single spot respectively. In addition, a signal analysis was also performed on the interface position at an instant of the simulation where perturbations are observed along the liquid/gas interface. The power spectral density (Figure 10) reveals also the presence of three main modes directly related to those observed on Figure 9. The values of the observed perturbation wavelength are too small to allow a natural growth as proved by the application of the linear theory.

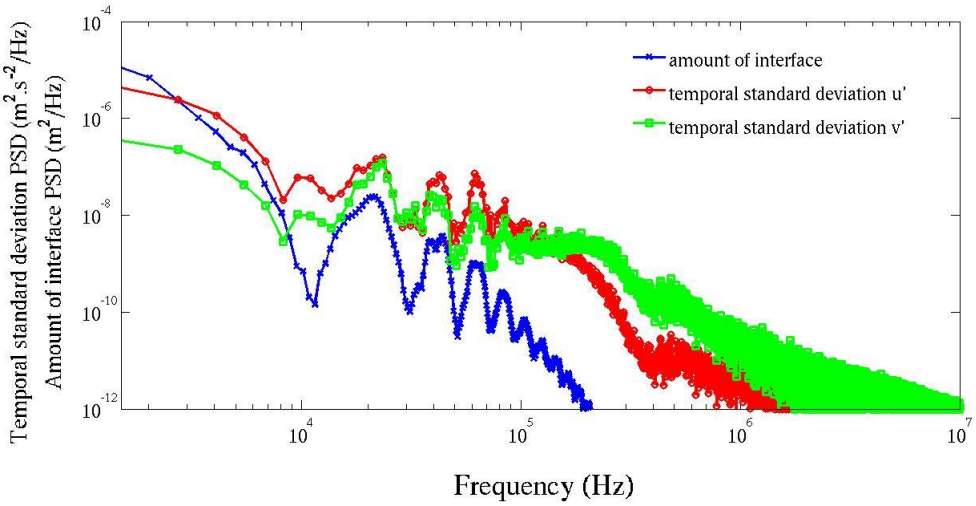

Figure 9 Power spectral densities of the fluctuating velocity and interface length

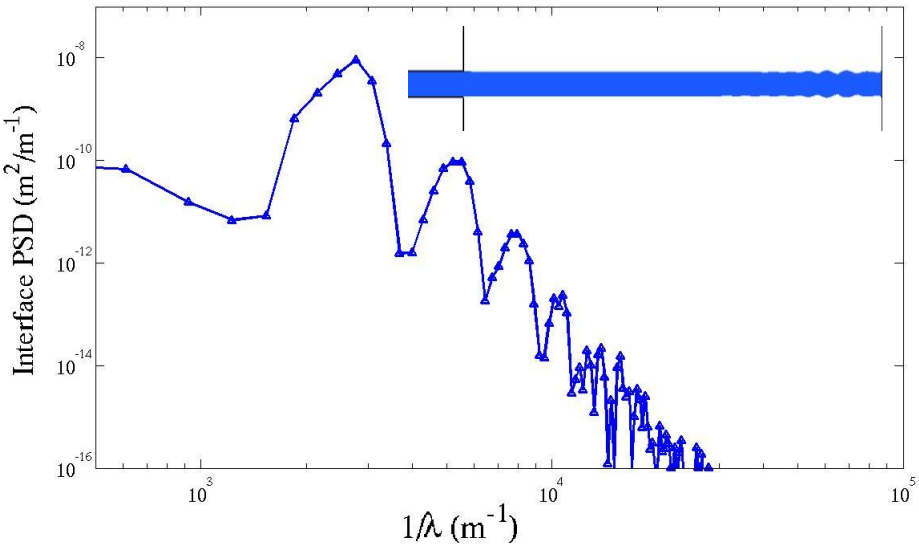

Figure 10 Power spectral density of the liquid/gas interface at 5 ms after the injection start (the studied liquid system is given on the top right of the figure).

Summary and Conclusions

The present work is devoted to the implementation of an immersed boundary method in the academic code Archer which was initially built to simulate the primary breakup of liquid jets without the presence of walls with complex shapes. The constraints related to the numerics in this field need the use of regular Cartesian meshes and led us to implement an immersed boundary method with a direct forcing. In the investigated situations, we are in the presence of three phases (solid, liquid and gas) and two level set functions are necessary to represent the fluid/solid and liquid/gas interfaces. The major difficulties concern the methodology to take into account the physical conditions at the interface crossing and are discussed in the paper.

In the present paper, two different test cases were investigated: the equilibrium of a droplet set on a solid wall and the discharge of a liquid sheet from a nozzle. The first test case showed the accuracy of the method and

the shapes of the droplets at the equilibrium were retrieved successfully regarding the analytical results. We showed that results are satisfactory even in situations where the fluid/wall interface is not aligned with the grid-lines. In addition, the accuracy of the numerical resolution was found better when the mesh is finer. The development of a mesh refinement is an efficient solution to improve the computations. Such an approach has to be automatic (AMR) in order to capture the liquid/gas interface whose shape evolves with time. Moreover this approach could be useful in the case of moving walls. For instance, the simulation of an injection event in automotive nozzles needs to describe the displacement of the needle which controls the amount of fuel to be discharged.

The second test case showed that the implementation of the immersed boundary technique in the code Archer is able to allow a strong coupling between internal and external flows. In particular we observed that the temporal characteristics of the velocity fluctuations are directly related to the disturbances on the discharged liquid sheet. These first results invite us to investigate other situations. In particular, it would be interesting to operate in conditions where the velocity fluctuations at the nozzle outlet generate disturbances that can grow naturally in the gaseous medium. To go in this direction, the application of the linear theory shows that with a Reynolds number set to 4,000, an increase of the gas density will lead to the growth of the perturbations created by the turbulence. Moreover actual investigations concern the effects of the nozzle shape. As a matter of fact, when convergent or divergent nozzles are used, mean and fluctuating velocities can change and affect the primary breakup process. This was already observed by Sander and Weigand [3] but in their investigation, the profiles they used were synthetic and the internal flow was not simulated contrary to the present investigation. The proposed approach is of paramount importance when the nozzle shape complexity is increased where no synthetic velocity profiles can be easily found.

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