

Simulation of liquid/gas interface break-up with a coupled Level Set/VOF/Ghost Fluid method

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Abstract: Recent progress in numerical simulations allows reproducing the primary breakup of liquid systems in gaseous media. Our approach is based on the coupling of Level Set, Ghost Fluid and VOF methods. Results concern bubble trapping during liquid jet atomization, ligament break-up, and liquid/gas interface break-up with a high density ratio and a large velocity difference between the two phases.

Keywords Level Set method, Ghost Fluid, Two phase flow, atomization.

1 Introduction

Numerical simulations are a very powerful tool to investigate a wide field of physical processes, thanks to constant developments and high efficiency of computer resources. A major interest of simulations lies in their ability to produce extensive 3D data where complex phenomena are involved, with a large amount of information that can help in physical understanding. DNS of two phase flows remain a main topic of research. In the particular case of atomization simulations, classical Eulerian or Lagrangian methods have been extensively developed to describe the spray behavior in the dilute regime very far from the initial break-up. To go further on in numerical simulations, the main challenge is to be able to catch the interface behavior before the dilute regime with enough accuracy to get a description of the primary break-up. We thus developed a numerical code (ARCHER) for interface tracking in order to describe the dynamic of liquid/gas interface. Notice that this numerical approach has the drawback to be limited to quite small domains to keep reasonable computing times, even if massively parallel computers can help in managing billion grid points. Nevertheless the primary break up takes place in a quite small area often limited to few injector diameters in the downstream direction.

The most common approaches to track liquid/gas interfaces are volume of fluid (VOF) method (Hirt and Nichols [1] Gueyffier et al [2], Scardovelli and Zaleski [3]), front tracking method (Unverdi and Tryggvason [4]) and level set methods (Sethian [5]) among others. Regarding advantages and disadvantages of these different methods, the choice may depend on the problem under study. A good strategy is to benefit from the advantage of each approach. In liquid atomization, a lot of topological changes occur (interface pinching or merging, droplet coalescence or secondary break-up) and the numerical method should describe the interface motion precisely. Moreover artificial smoothing of the interface can produce some unreliable results when comparing with a method that handles jump conditions at the interface, and obviously mass conservation must be satisfied. We thus decide to couple several methods where interface tracking is performed by a Level Set method, the Ghost Fluid Method is used for jump conditions on discontinuous variables, and a coupling between the Level Set and VOF methods ensures mass conservation. Incompressible Navier-Stokes equations are solved following a projection method and they are coupled to a transport

equation for the level set function. Poisson equation is solved with second order central scheme, and a multigrid algorithm for preconditioning a conjugate gradient method is used. Specific care has been carried out to improve simulation capabilities with MPI parallelization.

2 Numerical approach

2.1 Level Set

The basis of the Level Set methods has been proposed by Osher and Sethian [6]; the interface is described with the zero level curve of a continuous function ϕ which is defined by the algebraic distance between any point of the domain and the interface. The interface is thus described by $\phi=0$. A convection equation determines the evolution of the interface in a given velocity field \mathbf{V} (Sethian [5]):

$$\frac{\partial \phi}{\partial t} + \mathbf{V} \cdot \nabla \phi = 0 \quad (1)$$

Some problems may arise when solving that equation, such wide spreading and stretching of the level sets, and ϕ will no longer satisfies the property $|\nabla \phi| = 1$ of a distance function. A re-distancing algorithm (Sussman et al [7]) is then applied to keep ϕ as the algebraic distance to the interface.

To avoid singularities in the distance function field, a 5th order WENO scheme is used for convective terms and temporal derivatives are computed with a third order Runge Kutta scheme.

One advantage of the level set method is to easily provide geometrical informations of the interface, such as normal vector \mathbf{n} or curvature κ :

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|} \quad \kappa(\phi) = \nabla \cdot \mathbf{n} \quad (2)$$

2.2 LevelSet/VOF

It is well known that numerical computation of Eq. (1) and re-distancing algorithm can generate mass loss in under-resolved regions, or when a strong stretching occurs near the interface. This is a problem of level set methods, but the mass conservation extension of the method can be improved, namely a coupling between VOF and Level Set. The numerical method that we set up in our code is quite similar to the CLSVOF of Sussman and Puckett [8], details are extensively described in Ménard et al [9]. The main differences with the CLSVOF consist in keeping the initial re-distancing algorithm in our approach, and we modified the reconstruction technique to define the interface in a cell from the Level Set position.

2.3 Ghost Fluid Method

The interface is defined by two different phases and discontinuities must be taken into account for density ρ , viscosity μ and pressure p . Specific treatment is thus needed to describe the jump conditions numerically.

The pressure jump related to surface tension σ and to the interface curvature reads:

$$[p] = \sigma \kappa(\phi) + 2[\mu] (\nabla u \cdot \mathbf{n}, \nabla v \cdot \mathbf{n}, \nabla w \cdot \mathbf{n}) \cdot \mathbf{n} \quad (3)$$

where $[.]$ represents a jump for the considered variable.

To overcome smoothing of the Continuum Surface Force method, the Ghost Fluid Method (GFM) has been developed by Fedkiw et al [10]. The formalism respects jump discontinuities across the interface and avoids an interface thickness. Discretization of discontinuous variables is more accurate and spurious currents in the velocity field are much lower than with CSF methods. As defined above, the interface is characterized through the distance function, and jump conditions are extrapolated on some nodes on each side of the interface, the discontinued functions are extended continuously and then

derivatives are estimated. More details can be found in Liu et al [11] and Tanguy et al [12] on implementing the Ghost Fluid Method to solve the Poisson equation with discontinuous coefficients and to obtain solution with jump conditions.

2.4 Navier Stokes equations

The Level Set/VOF/Ghost Fluid approach is coupled with a projection method for the direct numerical simulation of incompressible Navier-Stokes equations expressed as follows:

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} + \frac{\nabla p}{\rho(\phi)} = \frac{\nabla(2\mu(\phi)\mathbf{D})}{\rho(\phi)} \quad \mathbf{D} = \frac{1}{2}(\nabla \mathbf{V} + \nabla \mathbf{V}^T) \quad \nabla \cdot \mathbf{V} = 0 \quad (4)$$

Spatial derivatives are estimated with a 2nd order central scheme, but convective terms are approximated by 5th order WENO scheme discretization in order to ensure a robust behavior of the solution. Temporal derivatives are approximated with an Adams Bashforth algorithm or 3rd order Runge Kutta scheme. Poisson equation discretization, with a second order central scheme, leads to a linear system; the system matrix is symmetric and positive definite. Different methods can be derived to solve that system. According to different authors the MultiGrid method for preconditioning Conjugate Gradient methods (MGCG) combines Incomplete Choleski Conjugate Gradient (ICCG) robustness with the multigrid fast convergence rate. The MGCG method greatly decreased computational time compared to the ICCG algorithm.

2.5 Validation and parallelization

Extensive discussions on the methods and numerical validations are reported in Ménard et al [9, 13]. Among these validations, Zalesak's [14] disk problem (2D), circle in a vortex (2D), droplet collisions (2D and 3D), sphere in a three dimensional velocity field (LeVeque [15]) and Rayleigh instability of liquid jets are well designed to estimate the chosen methods are numerical schemes.

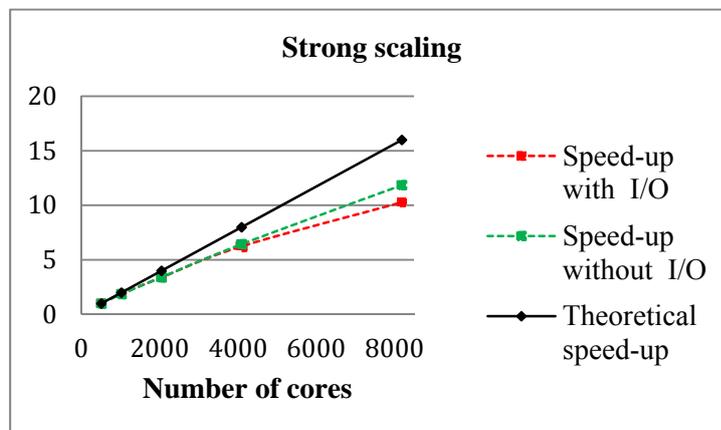


Figure 1: Strong scaling of the code

Specific care has been also devoted to improving simulation capabilities with MPI parallelization and using specific allocatable variables, the memory storage is also optimized. The code ARCHER shows quite good speed-up when increasing the number of cores as shown in Figure 1 by the strong scaling results on the Blue Gene/P computer at IDRIS (calculations have been carried out with 268 million points on the jet atomization test case). Improvement of the speed-up efficiency is still under development.

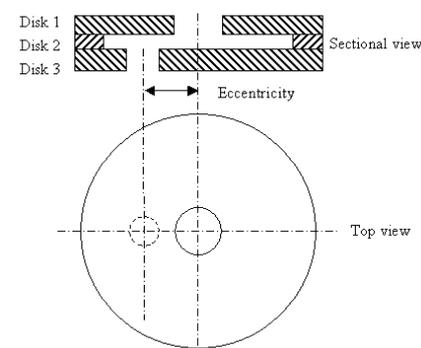
One of the first detailed simulations of jet primary break up under realistic conditions (Diesel automotive injector) have been published by Ménard et al [9] and several papers have then reported on similar cases such Herrmann [16], Desjardins et al [17], and a highly refined (6 billion points) study by Shinjo & Umemura [18]. However experimental investigations are quite difficult in the initial break-up of sprays, and very few experimental data are available to compare simulations and measurements in the first step of the atomization. The spray is very dense, the liquid volume fraction is close to one, and the liquid/gas interface is very complex. As a consequence it is very difficult to get experimental results in order to characterize this zone. We thus choose in the following results two different configurations that allow discussions between simulations and experimental results.

3 Simulations

The first case concerns a coupling between internal flow and primary breakup simulations in the case of a compound nozzle with a complex geometry. We focus on some remarkable behaviors of the liquid phase, such as bubble trapping inside the liquid jet and jet forming when they burst at the interface. The second case concerns a configuration that remains quite difficult to simulate, that is liquid/gas interface break-up with a high density ratio (about 1000) and large velocity difference between the two phases.

3.1 Triple disk compound injector

Compound nozzles are designed in order to enhance atomization under high turbulence level of the liquid flow. They consist of the superposition of two or three disks with eccentric orifices that impose drastic deflections to the internal flow. We consider here the case with three disks (Figure 2). The liquid enters the nozzle through disk 1, passes through the cavity disk (disk 2) and issues from the nozzle through the discharge disk (disk 3). The passage in each disk is circular. These compound nozzles are very efficient for liquid atomization for low-pressure gasoline injection. Besides the turbulence level, the liquid flow at the exit section exhibits a double vortex secondary flow.



Disk	Thickness (μm)	Diameter (μm)	Eccentricity (μm)
1	177	300	0
2	75	2254	0
3	75	180	200

Figure 2: Nozzle geometry



Figure 3: Liquid jet experimental view from a compound nozzle (Triballier et al [19])

The consequence of this flow structure on the jet was confirmed by both numerical calculations and experimental observations (Triballier et al. [19]) As observed in the figure 3 the secondary flow is flattening the liquid jet as soon as it leaves the nozzle discharge.

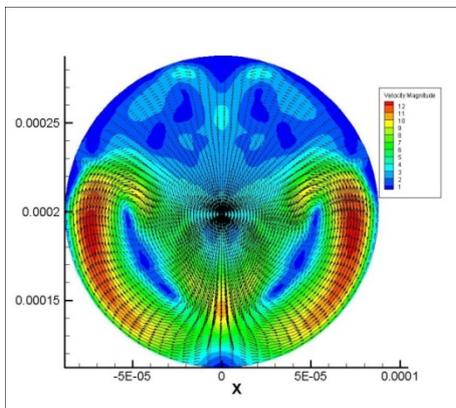
Due to the large computational times, the present study focuses on one single case. In order to compare experiment results and numerical simulation, the studied case is part of Dumouchel et al [20] work. The Reynolds number is equal to 2974 and corresponds to an injection pressure that equals 0.4 MPa. This pressure was chosen to investigate a situation where turbulence acts on the breakup process and promotes the droplet production.

3.1.1 Overview of the results

One important problem in the simulations of liquid jet atomization is to know the inlet boundary conditions, on the exit of the injector. As no experimental data are available, preliminary numerical

simulations have been carried out for the internal flow using the CFD package Fluent 6.2. These predicted data are used as input conditions for the DNS of atomization.

Several simulations have been run during the development of this study. The first one was without any turbulence in the liquid on the exit. We observed that the initial round jet is converted into a liquid sheet with thick edges on both sides as experimental visualizations, but the interface remains very smooth without any waves or wrinkles. In a second simulation, we then introduced the turbulence of the liquid on the jet exit. Starting from the prediction of the turbulence energy and its dissipation (RNG model), a random correlated scheme has been used to generate fluctuating velocities. We clearly observed that the turbulence induces much more perturbations on the liquid interface, both on the edges and on the liquid sheet; the liquid surface topology becomes much wrinkled and the whole flow appears very turbulent and chaotic. But the break-up of the liquid sheet arises at a time shorter and closer to the injector nozzle when turbulence is included, when it is compared to experiments. Moreover the jet angle is in both cases much greater than in experiments (46° instead of 24°). However it is quite well known that predictions with (K- ϵ) model are not the most suitable for swirling flows at moderate Reynolds numbers. We thus decide to start new simulations with inlet profiles taken from LES simulations of the internal flow in the triple disk injector (Cousin et al. [21]). A first case with roughly 8 million grid nodes to describe the break-up of the jet was initially performed in order to confirm that starting with LES predictions improves the simulation results. Then a refined simulation presented below was performed.



The size of the domain is (2d, 8d, 8d) i.e. 0.00036 m, 0.00144 m, 0.00144 m and the uniform cartesian grid is 1024x256x1024 nodes (256 million), which leads to $1.44 \mu\text{m}$ for the mesh size (a half geometry was considered only regarding the nozzle geometric properties). The number of cells at the nozzle outlet is 6136 close to the one used for LES simulations. A typical instantaneous velocity field that is taken as inlet conditions is shown on figure 4. The time step between two stored data (from LES simulations) is 10^{-8} s and 20,000 input profiles are used to initiate the instantaneous liquid velocities in the DNS interface tracking. Running time is typically 20 hours wall time on 1024 cores for 2000 time

steps.

Figure 4: Instantaneous velocity field

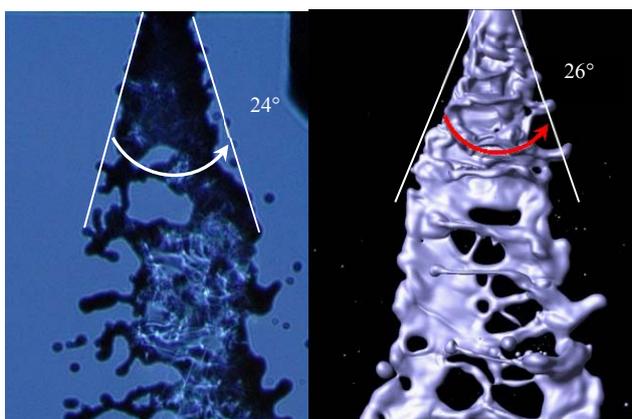


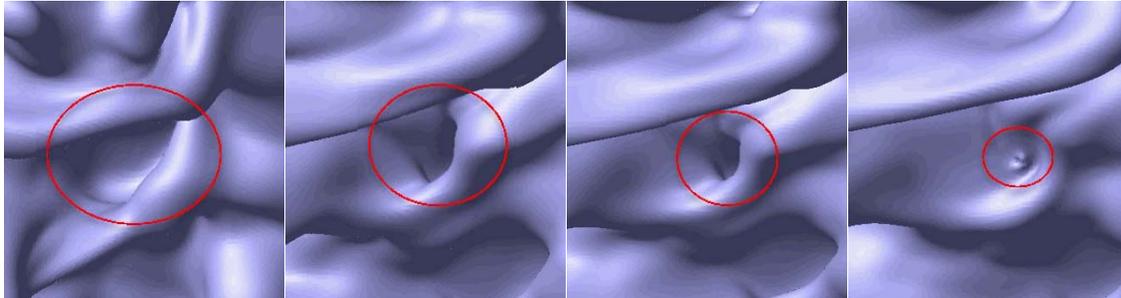
Figure 5: Jet breakup
left: visualization, right: simulation

length of 0.74 d for the experiments whereas this length equals 0.64 d for refined simulation.

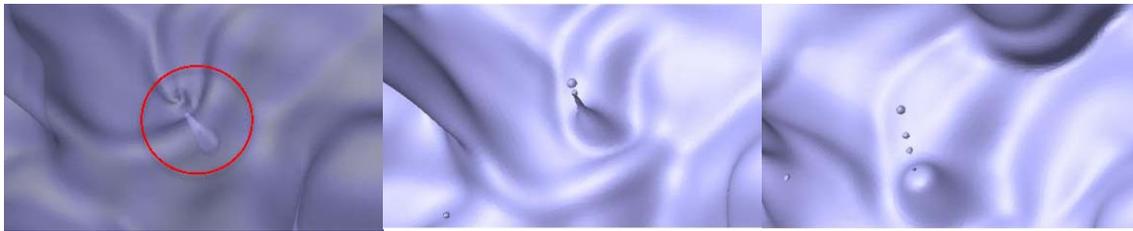
Figure 5 presents the comparison between both visualized and simulated jets during steady flow operations. One can first observed that the jet morphology is well described by the simulation. We then applied the same image analysis on both experimental and numerical images. The calculated jet angle (26°) is fairly close to the measured one (24°) (mean value on ten consecutive images). This result shows that the LES simulations provide much better initial conditions for the jet simulation compared to what was previously obtained. We also applied Fast Fourier Transforms on the angle signal as a function of the distance. We extracted the dominant mode of the perturbations. We found a characteristic

3.1.2 Trapped Bubble and burst

We took a closer look on the refined simulations and a remarkable behavior on the interface was observed. Experimental or numerical studies on bubble bursting on liquid surfaces have shown in the past that a ligament is often formed and breaks into droplets. Although the interface is stretched with a swirling motion, that particular behavior has been isolated in our results. The figures 6 present the gas trapping and figures 7 show the bubble bursting, jet forming and droplets.



Figures 6 a,b,c,d: Bubble trapping



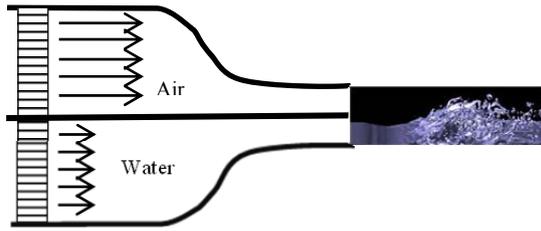
Figures 7 a,b,c: Bubble bursting and jet forming with droplets

The bubble trapping is clearly observed on the figures 6-a to 6-d. The gas stays in a hollow of the interface (Figure 6-a and 6-b) and due to the swirling motion of the liquid and stretching of the interface, the hole closes (Figure 6-c and 6-d). The Figure 7-a is at the same time than Figure 6-d, but we use transparency in the picture. We can see that some gas is trapped and a bubble stays under the interface with a teardrop shape, its smallest side being located just under the liquid surface. The bubble then bursts out and the liquid jet forming is observed with a first droplet on Figure 7-b and final break-up in the figure 7-c. Analyzing the images shows that the ratio between the drop diameter and the bubble diameter is between 0.07 and 0.15 which is in the range of ratios provided by Duchemin et al. [22] or Wu [23]. More details and discussion on the triple disk injector simulations have been recently published in Cousin et al [21].

3.2 Plane liquid/gas shear layer: first results

The second case concerns a configuration that remains quite difficult to simulate: the liquid/gas interface break-up with a high density ratio (air/water) and a large velocity difference between the two phases (10 to 100m/s). A literature survey shows that the simulation of primary atomization by high speed air and high density ratio often fails due to numerical instability issues. The main reason seems to be some difficulties for an accurate description of the momentum transfers between both phases. Recent new developments by several authors allow overcoming these troubles. In our case the coupling between the level set method and the VOF method has been proved very efficient.

The experimental set-up that is simulated has been extensively studied by Matas et al [24] and Ben Rayana [25]



Several preliminary simulations have been carried out on coarse grids, for different geometries or velocities. In order to compare the simulations and experiments, a well-documented case has been chosen. The ratio $M = \rho_g U_g^2 / \rho_l U_l^2$ is equal to 16, $U_g = 30$ m/s and $U_l = 0.26$ m/s. In order to keep

reasonable computing times, the width of the channel is equal to 24 mm instead of 80 mm in the experiments. Main characteristics of the domain geometry for the simulations are given in the figure 8 and inlet conditions are given in the figure 9. Note that crude profiles are taken to respect the boundary layers on the middle flat plate.

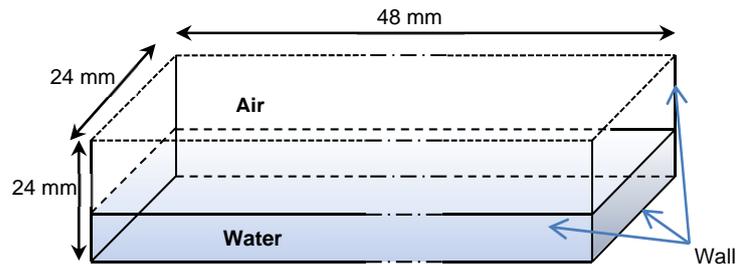


Figure 8: Computational domain

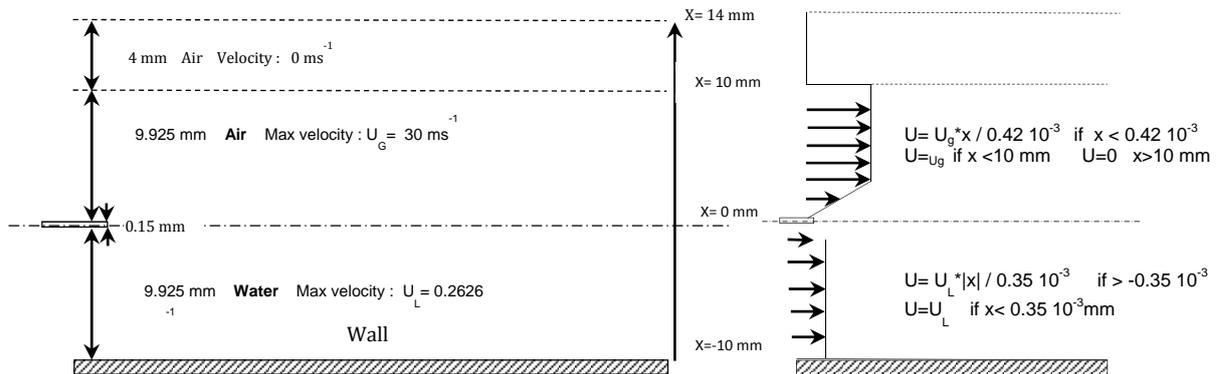


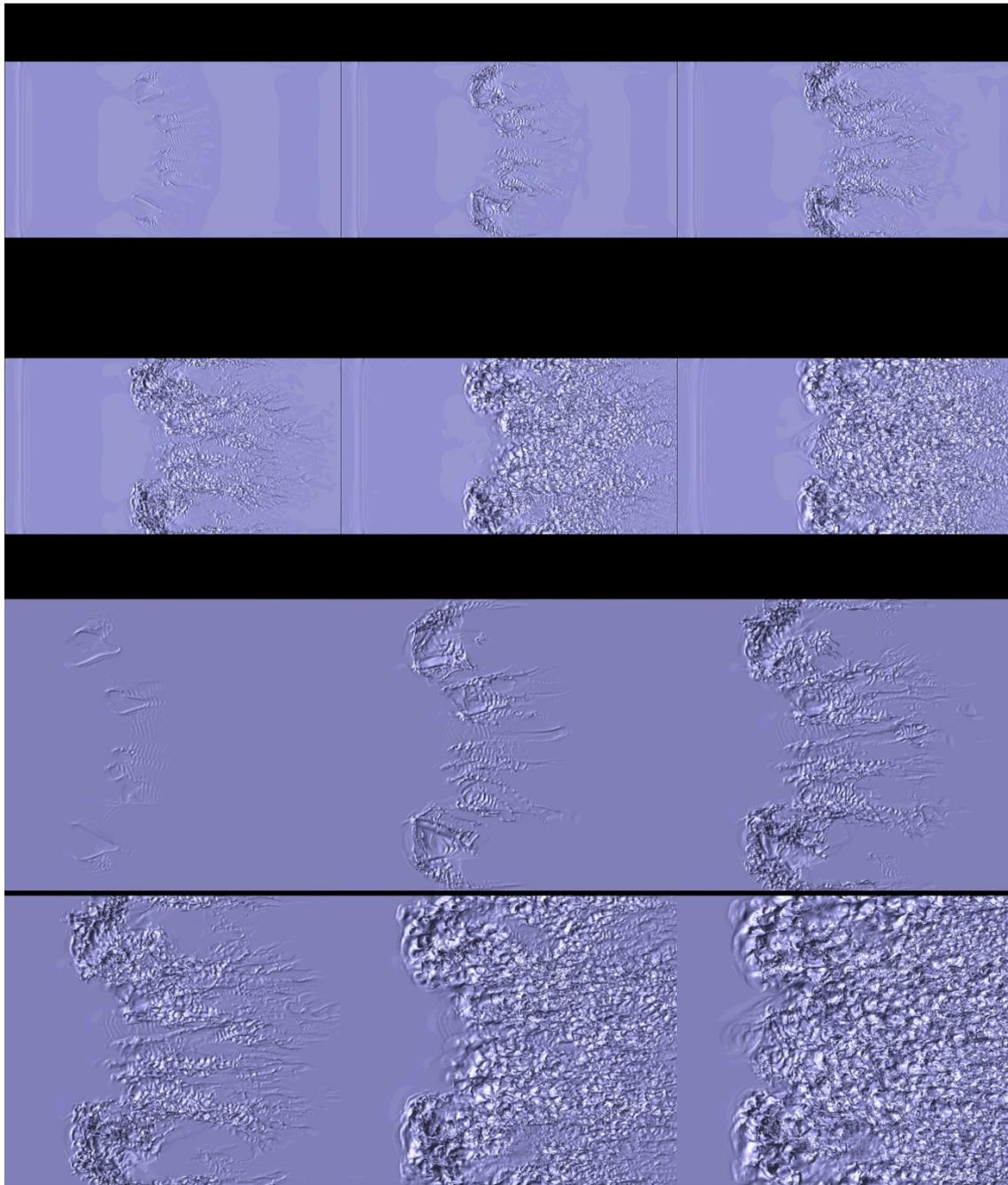
Figure 9: Inlet conditions

The grid is 512x512x1024 nodes and the mesh size equals 48 μ m. Calculations have been run on 2048 cores, and the running time is roughly 20 hours wall time for 3500 time steps ($\sim 10^{-6}$ s). The results have been stopped after 70,000 time steps.

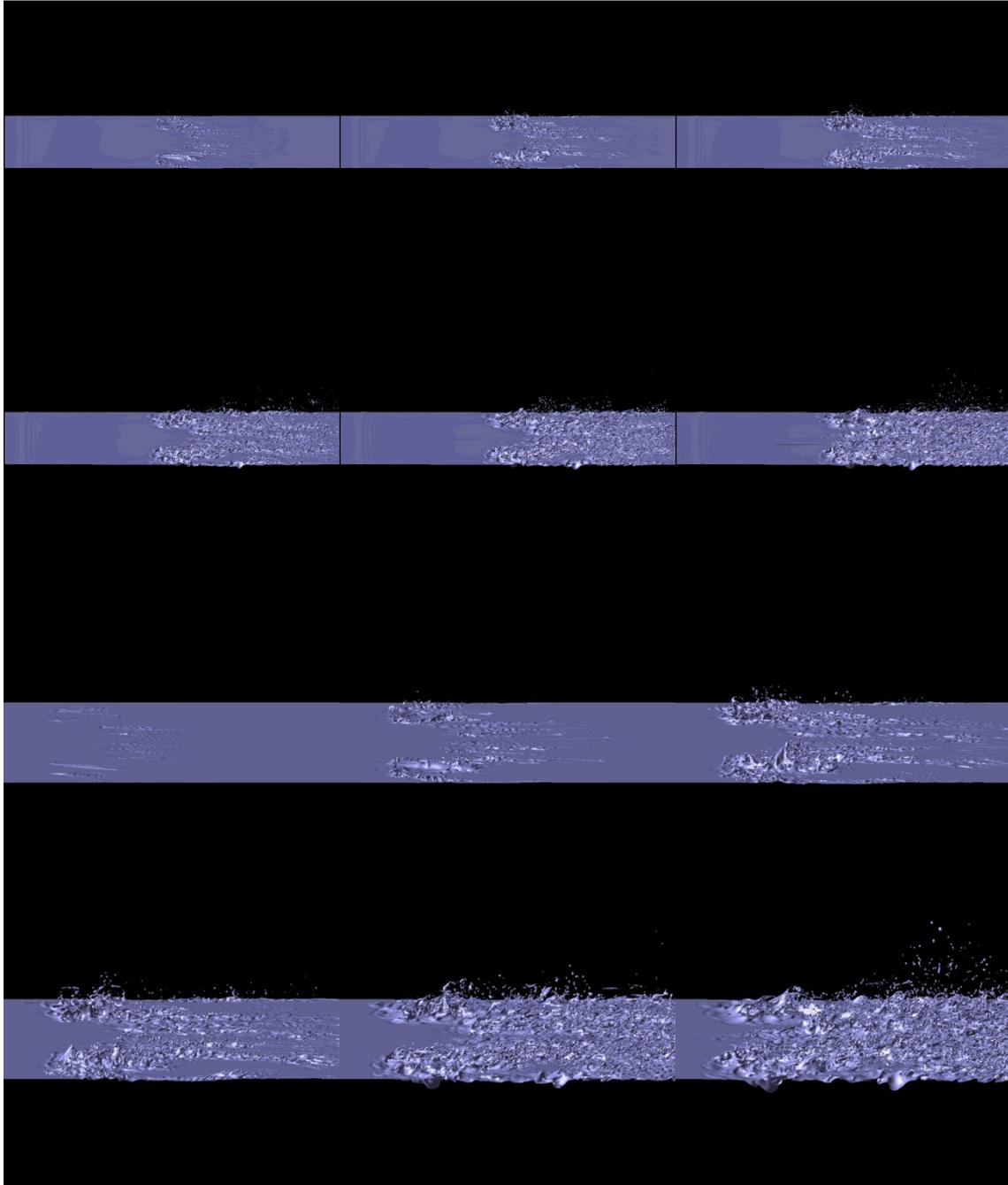
Developments on the instabilities on the interface and atomization of the liquid sheet are presented on figures 10 (top views) and figures 11 (side views). These first simulations confirm that the code is able to handle large density ratio with high shear induced by the gas flow. We clearly observed at the beginning some small wrinkling and waves that are amplified and cover more and more the liquid interface. Note that both axial and transversal instabilities are generated. As time increases, perturbations on the interface grow, crests are developing and liquid parcels and droplets are formed. On the last images of the sequence, the interface is totally disturbed at the end of the domain.

However some questions arise on these simulations and comparisons with experiments remain quite difficult at this stage of development. The mesh size (48 μ m) is still too large and our

simulations are clearly under-resolved. We can also observe that initial perturbations are coming from the walls. As we decreased the width of the domain for numerical reasons, it seems that either we have to enlarge it, either we have to go forward in these simulations to obtain the same behavior on the entire width of the domain. When referring to Ben Rayana [25] and Hong [27] studies, the destabilization of the liquid sheet happens closer to the edge of the plate in the experiments. Recalling the importance of the inlet conditions in the triple disk injector, we have run a simplified configuration to confirm that behavior on the liquid shear layer.

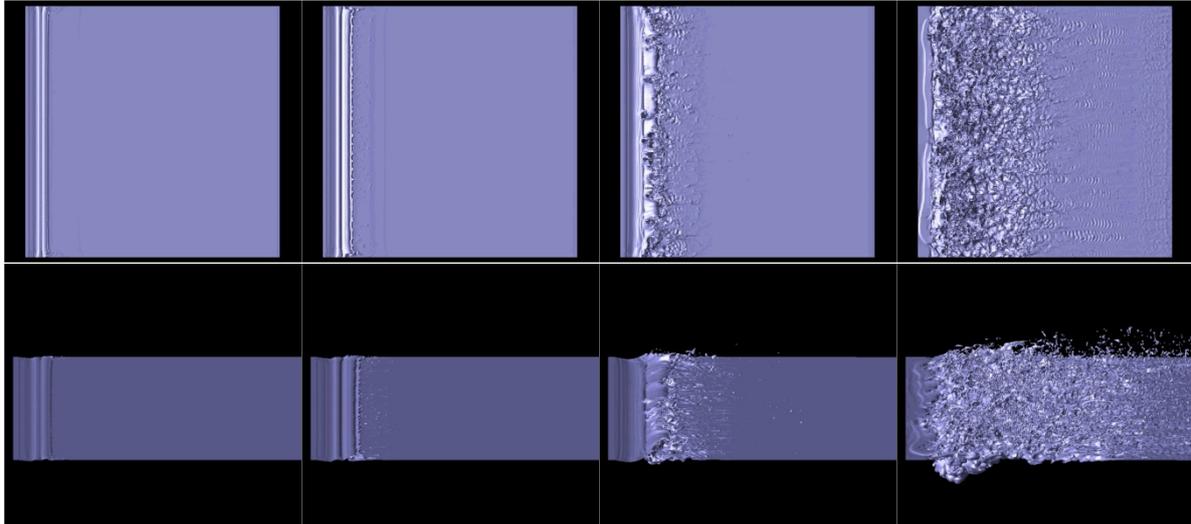


Figures 10: Top view of the liquid interface: Entire domain (6 on the top), zoom (6 on the bottom)



Figures 11: Side view of the liquid interface: Entire domain (6 on the top), zoom (6 on the bottom)

The domain is reduced to 10 mm for water flow and 10 mm for air above (no plate thickness). The inlet velocity profiles are flat (no more boundary layers), both in the gas and the liquid (30m/s and 0.26m/s). The domain is 0.2mx0.4mx0.4 m and the grid is 256x512x512 (the mesh equals 78 μ m). An image sequence of the entire domain is given in figure 12 (top view and side view). We clearly notice that the break-up of the liquid sheet is much closer to the separation plate. One can also observe that behind the initial wave, the perturbation on the liquid interface between both cases is quite similar on the last images, although the wave front is much more less pronounced on the figure 10. When comparing the side views (figure 11 and figure 12), the initial entrainment of the liquid sheet and break-up are different. In this last case, a first transversal wave is generated that is then stretched and breaks into liquid blobs and droplets. In the first case, lot of small waves were generated, then amplified and disintegrated.



Figures 12: Interface break-up: top view and side view

Moreover we observe in this simplified configuration a well-known mechanism for droplet formation. As reported by Zaleski et al [26] in the Figure 13, we observe the deformation of a transversal wave to give birth to a liquid finger that breaks into droplets due to the relative velocity between both phases. Even if the mesh is too coarse to catch accurately that kind of ligament break-up, this behavior was not observed in the first simulations. It can be stated that once more the inlet conditions on the separation plate are essential to allow comparisons between experiments and simulations.

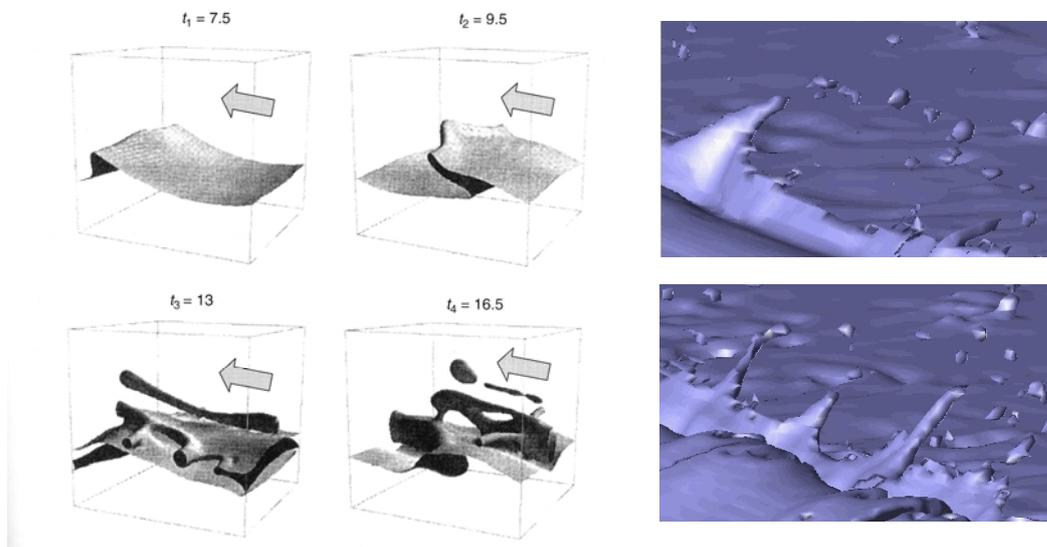


Figure 13: Ligament formation and break-up (Zaleski et al[26]) and simulations

3 Conclusion and future work

The main objective of our work is to develop direct numerical simulation tools for the primary break up of liquid interfaces. We develop a 3D code, where interface is represented by a Level Set, the Ghost Fluid Method is used for discontinuities, and the Level Set and VOF methods are coupled for

mass conservation. Specific care has been devoted to improve computing time with MPI parallelization.

The numerical methods have been applied to investigate physical processes that are involved in break-up a liquid jet generated by a triple disk injector and on a plane liquid/gas shear layer. We clearly observe the strong coupling between internal and external flows, and the sensitivity of break-up mechanisms to inlet conditions is one of the biggest difficulties to tackle when comparing experiments and simulations. However, our code ARCHER remains stable when large density ratio and high gas shear are considered.

To go further on we decide to implement an immersed boundary method in our code to be able to run simulations from inside the injector until atomization of the liquid. That method will be coupled with AMR, which is also under development. The final objective is to realize a virtual injector, with a complete simulation from inside the injector to the break-up of the liquid interface and spray forming.

Acknowledgment

This work is supported by ANR VAA and MODEMI research programs, and FEDER program. Computations have been carrying out in IDRIS and CRIHAN computational centers.

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