NUMERICAL SIMULATION OF THE AIR-BLASTED LIQUID SHEET : DEVELOPMENT OF A DNS SOLVER BASED ON THE LEVEL-SET METHOD

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Abstract

Our goal is to build a CFD tool able to simulate the phenomenon of atomization, and particularly the air-blasted planar liquid sheet. After many years of research in this area both from experimental and theoretical approaches, scientific community is still very perplexed to explain basic physical mechanisms driving a liquid sheet atomization. We present here the development of a DNS solver for a two-phase incompressible flow with interface capturing feature for non miscible fluids. This interface is captured by a Level-Set method, which has become very popular during the last ten years. However, unlike classical approaches, stress tensor jump conditions through interface are explicitly taken into account without introducing any smoothing. Different simulations of interfacial instabilities are presented, we will show the potentiality of the Level-Set method coupled with an explicit expression of jump conditions. Our first numerical simulations of a spatially developing liquid sheet surrounded by co-flowing air streams at moderate velocities is presented.

Governing Equations

As we are mainly interested by the simulation of liquid sheet desintegration by coflowing air streams at moderate velocities, we will use the incompressible Navier-Stokes equations :

$$\begin{aligned} \nabla.\mathbf{u} &= 0 \\ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} &= -\frac{1}{\rho}(\nabla p + \nabla(2\mu\mathbf{D})) \end{aligned} \tag{1}$$

Here $\mathbf{u} = (u, v, w)$ is the velocity, ρ the density, p the pressure and $\mathbf{D}$ is the viscous stress tensor. We consider two immiscible viscous fluids, an interface clearly separate the two fluids through we can write the dynamic boundary conditions :

$$\begin{aligned} [p] - \mathbf{n}\cdot[\mu\mathbf{D}]\cdot\mathbf{n} &= \sigma\kappa \\ \mathbf{t}\cdot[\mu\mathbf{D}]\cdot\mathbf{n} &= 0 \end{aligned} \tag{2}$$

Here σ is the surface tension coefficient, κ the curvature, $\mathbf{n}$ and $\mathbf{t}$ are respectively the normal and the tangent at the interface. Basically, these relation imply a jump for the pressure at the interface and the appearance of a surface force called surface tension, which do need an appropriate numerical treatment.

Numerical Methods

Navier-Stokes Solver

Before dealing with the special numerical treatment of the interface separation of two immiscible viscous fluids, we need to build an efficient and accurate Navier-Stokes solver as we use a one fluid approach to deal with this problem. We use a classical projection method to enforce incompressibility constraint. Finite volume spatial discretization is based on staggered MAC cartesian grid for the velocity components, all others quantities are cell-centered. The convection terms in the momentum equations are approximated in a non-conservative way with 5^{th} order accurate WENO schemes [1]. This particular choice has been motivated by the robustness and low numerical dissipation of such schemes. Time integration is performed with a 2^{nd} Adams-Bashforth scheme. This kind of time integration ensures a good temporal accuracy and only one pressure Poisson equation to solve each time step.

Level-Set Method and Redistance Equation

One need to define a mathematical function to locate in space and in time the interface. We chose to use the Level-Set function to capture this interface. For a point of the computational domain, $\phi(x, y, z, t)$ is defined by the signed normal (minimal) distance to the interface. This definition implies numerous interesting properties :

- the sign of ϕ determine the position of each fluid
- interface is described by the zero level of ϕ
- ϕ is a smooth function, $||\nabla\phi|| = 1$

The time evolution of the Level-Set follows the advection equation :

$$\phi_t + (\mathbf{u}.\nabla)\phi = 0 \tag{3}$$

As for the momentum conservation equations, this equation is solved using a 5^{th} order non-conservative WENO scheme for spatial discretization and time integration is performed by a 3^{th} order TVD Runge-Kutta scheme [1].

While advection Eq.(3) will move each level at the correct velocity, and particulary the interface contour $\phi = 0$, Level-Set function will no longer be a distance function ($||\nabla\phi|| \neq 1$). In consequence, we obtain a lack of information around the position of the interface. Since we use the distance property of the Level-Set for curvature interface calculation, the result will be damaged. Indeed, the Level-Set function must be regularly reinitialized to keep signed distance property. This is achieved by finding the steady state solution of the following Hamilton-Jacobi equation :

$$\begin{aligned} \Phi_t &= S(\Phi_0)(1 - ||\nabla\Phi||) \\ \Phi(x, y, z, 0) &= \Phi_0 = \phi(x, y, z, t) \end{aligned} \tag{4}$$

Where S is the sign function. For numerical purposes it is useful to smooth this function. Eq.(4) has the property that ϕ remains unchanged at the interface, the zero of Φ_0 and Φ will be the same and Φ will converge away to the interface to $||\nabla\Phi|| = 1$. Eq.(4) is solved by a Godunov type scheme with a 5^{th} order WENO scheme [2].

Ghost Fluid Method

As we have already said, one need an adequate numerical treatment of the dynamic boundary equation at the interface between two immiscible viscous fluids. We chose the Ghost Fluid Method for which one can obtain a discontinuous numerical solution for the pressure whereas classical approaches to model surface tension incorporate a smooth source term in momentum conservation equations, implying a smoothed pressure solution over few cells around the interface location. With the Ghost Fluid Method, surface tension is treated in an implicit way, allowing better approximation of the physic of the problem.

The idea of the Ghost Fluid Method is quite simple and very efficient. If we use classical numerical approaches to discretize a differential equation where the solution is discontinuous through an interface, local discrete derivatives near interface can't be evaluated. If one considers a node near the interface, one must use a node locate on the other side of the interface to calculate the derivative, blue nodes on Fig.(1). To overcome this drawback, a ghost node is artificially created by continuous prolongation of the node where the derivative has to be calculated. The jump at the interface, explicitly taken into account via Eq.(2), is shifted on this ghost node, red nodes on Fig.(1). This new node can be used to calculate the local discrete derivative. In consequence, a "ghost fluid" is created, which is the continuous prolongation of one fluid on the other side of the interface. We can use an analogous reasoning if we consider a derivative jump through the interface. The complete mathematical details can be found in [3]. We can develop the boundary conditions Eq.(2) and obtain numerous jump conditions in each spatial direction for pressure as for velocities and pressure derivatives.

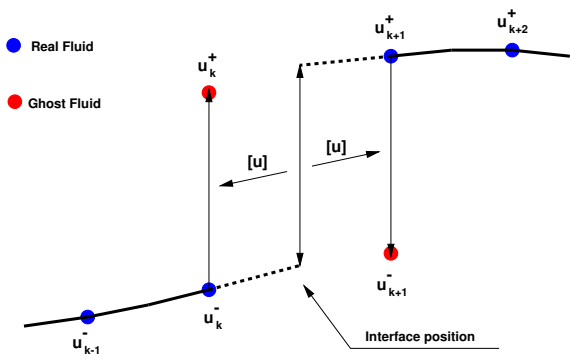

FIGURE 1: Ghost Fluid Method

Summary

First, we calculate ϕ^{n+1} along the Eq.(3) with high order schemes. This choice have been done in order to ensure incompressibility constraint, $\nabla.\mathbf{u}^{n+1} = 0$, in the sense that we use the interface position to discretize viscous terms and the pressure Poisson equation in the projection method :

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u}^n.\nabla)\mathbf{u}^n = \frac{1}{\rho}(\nabla(2\mu\mathbf{D})) \quad (5)$$

$$\nabla.\left(\frac{\nabla p}{\rho}\right) = \frac{\nabla.\mathbf{u}^*}{\Delta t} \quad (6)$$

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} + \frac{\nabla p}{\rho} = 0 \quad (7)$$

- Eq.(5) an intermediate velocity $\mathbf{u}^*$ is determined. Convective terms are evaluated in a non-conservative way with a 5^{th} order WENO scheme. Viscous terms are evaluated using a classical finite volume method with a specific treatment at the interface using the Ghost Fluid Method.
- Eq.(6) this classical Poisson equation is discretized using the Ghost Fluid Method. The MGCG method of Tatebe [4] is used to solve our system of equations, in other words, to invert the resulting matrix. This method, based on a conjugate gradient algorithm preconditioned by a multigrid method, is very fast and robust despite the ill-conditioned problem resulting from the Ghost Fluid Method.
- Eq.(7) the Ghost Fluid Method is again used to evaluate the pressure gradient

Assuming an explicit scheme to advance in time our system, time step have to be restrict. It is done in the same way of Fedkiw and al. [5].

Interfacial Instabilities Simulations

Numerous academic test cases have been calculated in order to check stability and accuracy of the developed DNS code, like static air bubble, showing us the accuracy of the Ghost Fluid Method [6]. Oscillating liquid drop or damped surface wave are another test problems where surface tension is dominant, and results are very close with the analytic solution.

Rayleigh-Taylor Instability

A classical test problem for two-phase flow simulation is the Rayleigh-Taylor instability, where a heavy fluid is placed on the top of a light fluid with a small initial perturbation of the interface.

We present here results for a short time evolution, where an initial sinusoidal perturbation is growing, according to the inviscid linear theory, exponentially with time as e^{nt} with a growth rate given by :

$$n^2 = kg\left(\frac{\rho_g - \rho_l}{\rho_g + \rho_l} - \frac{k^2\sigma}{g(\rho_g + \rho_l)}\right) \quad (8)$$

Here k is the wave number of the perturbation, g the gravity, σ the surface tension coefficient, ρ_l the density of the light fluid and ρ_g the density of the heavy one. From Eq.(8), we can define a critical surface tension σ_c for which $n = 0$. On Fig.(2), we compare the theoretical growth rate in the linear regime, black line, and the computed ones, color points ($\rho_l = 3\ kg/m^3$, $\rho_g = 1\ kg/m^3$, $k = 1\ m^{-1}$ and $g = 10\ m/s^2$). We can observe a good agreement between calculations and theory even for coarse grids.

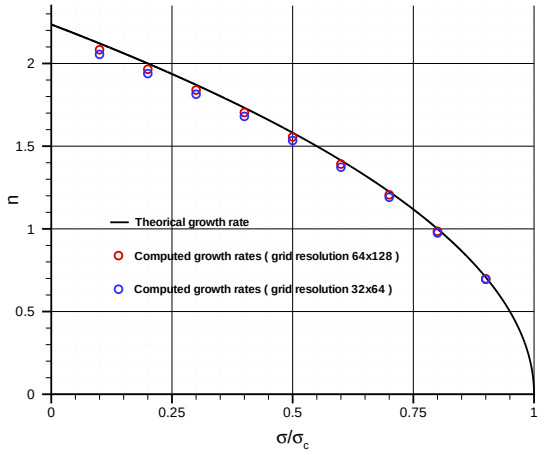

FIGURE 2: Rayleigh-Taylor Instability Simulation

Kelvin-Helmholtz Instability

The Kelvin-Helmholtz instability of an initially flat interface separating two fluids moving with different velocities is the closest well understood problem of the liquid sheet primary atomization. This problem show us how a perturbed sheared interface evolves in time into a row of vortices or how surface tension can develop fingers breaking into drops. Because of a lack of space, we just present here two simulations with same dimensional parameters of Tryggvason and al. [7].

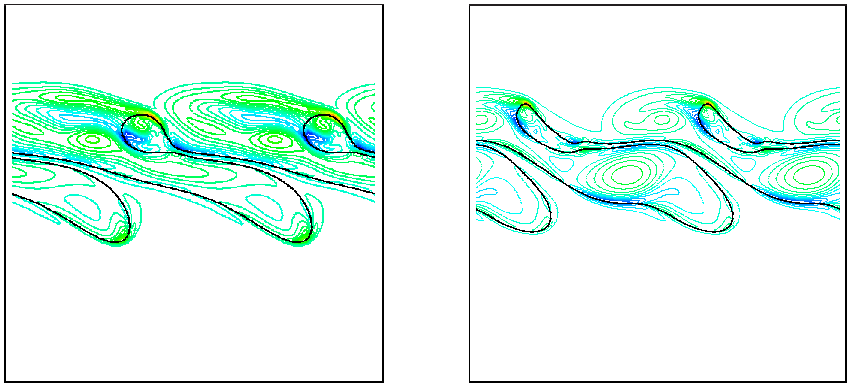

FIGURE 3: Numerical simulation of the Kelvin-Helmholtz instability (interface and vorticity contours) with a resolution of 256x256 grid points

Results are very close with ones found in [7] where a front tracking method is used to capture interface, interface shape and vortex position are approximatively the same.

Air-Blasted Liquid Sheet Simulations

Two-dimensional Spatial Simulations

Simulation of the air-blasted liquid sheet is the main goal of this work. Liquid jet breakup and atomization by a high-speed gas stream is a complicated multi-parameter two-phase flow problem. Detailed studies of fundamental breakup mechanisms are needed in order to derive predictive models in combustion applications. Although most commercial configurations have an axysymmetric design, two-dimensional geometry is very popular because of its simplicity. A thin sheet of liquid is injected between two plates, respecting a Poiseuille flow, sheared by two air boundary streams from both side. There are several non-dimensional parameters which appear to be revelent, even if this question is still open :

$$R_{e_g} = \frac{\rho_g U_g \delta}{\mu_g} \quad , \quad R_{e_l} = \frac{\rho_l U_l a}{\mu_l} \quad , \quad W_e = \frac{\rho_g (U_g - U_l)^2 a}{\sigma} \quad , \quad M = \frac{\rho_g {U_g}^2}{\rho_l {U_l}^2} \tag{9}$$

U_g id the outer air velocity, δ the boundary thickness, U_l is the mean liquid velocity, $2a$ the liquid sheet thickness and σ the surface tension coefficient. We have performed several simulations with the same physical parameters, except outer air velocity.

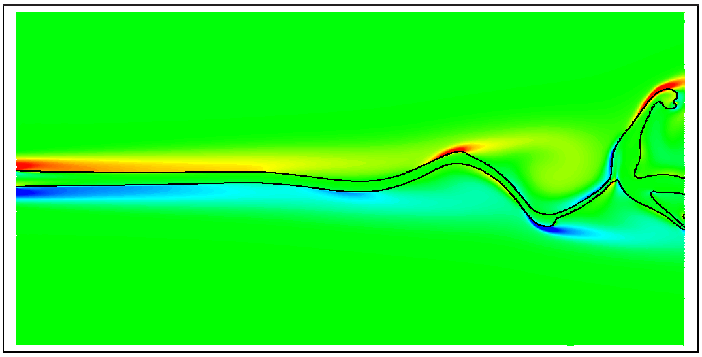

FIGURE 4: Numerical simulation of spatially developing air-blasted liquid sheet instabilities (interface and vorticity contours) $R_{e_g} = 103$, $R_{e_l} = 53$, $W_e = 16$, $M = 1.226$

For this first simulation Fig.(4), a moderate outer air velocity is considered ($U_g = 20\ m.s^{-1}$). Inflow perturbation is done by applying a random field independently on each side of the liquid sheet. The momentum flux ratio M is close to one in order to ensure a quick energy transfer from gas to liquid. For this air-blasted velocity, interface evolution is relatively simple resulting a poor atomization. However, physical mechanisms driving atomization are more evident in this case. An important vorticity sheet is localized on the maximum amplitude of the interface which produces downstream a vortex.

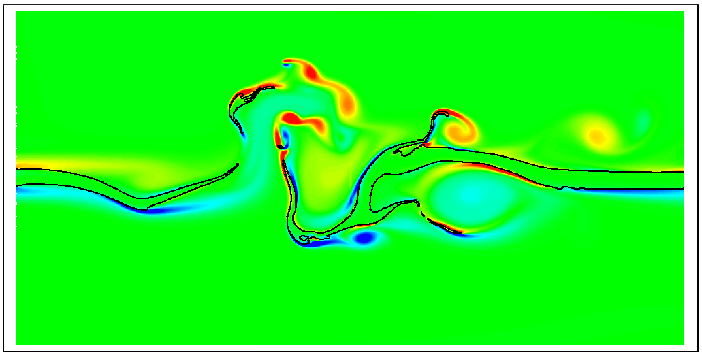

FIGURE 5: Numerical simulation of spatially developing air-blasted liquid sheet instabilities (interface and vorticity contours) $R_{e_g} = 207$, $R_{e_l} = 53$, $W_e = 73$, $M = 4.9$

This second simulation Fig.(5) has been done by doubling outer air velocity ($U_g = 40\ m.s^{-1}$). Interface evolution is much more complicated, numerous vortex are created downstream fingers. Liquid sheet is quickly broken into blobs which are accelerated by the air flow. However, this simulation suffers from mass loss, the biggest problem of the Level-Set method, coming from the fact that numerical redistancing Eq.(4) tends to move the zero level. In order to tackle this problem, we want to couple in the future our Level-Set method with an another interface tracking method, like front tracking or VOF, in order to ensure mass conservation.

Three-dimensional Temporal Simulations

Experimental investigation on an air-blasted liquid sheet clearly show us tridimensional instabilities despite the two-dimensional configuration. This phenomenon is as important as the air velocity is important. To take into account this effect, we have performed tridimensional simulation. Unfortunately, we don't have the possibility to perform spatial tridimensional simulation because the number of grid points needed is too important, we are presently limitated to temporal simulation. For the two simulations below, an initially flat liquid sheet is perturbed by longitudinal and spanwise modes.

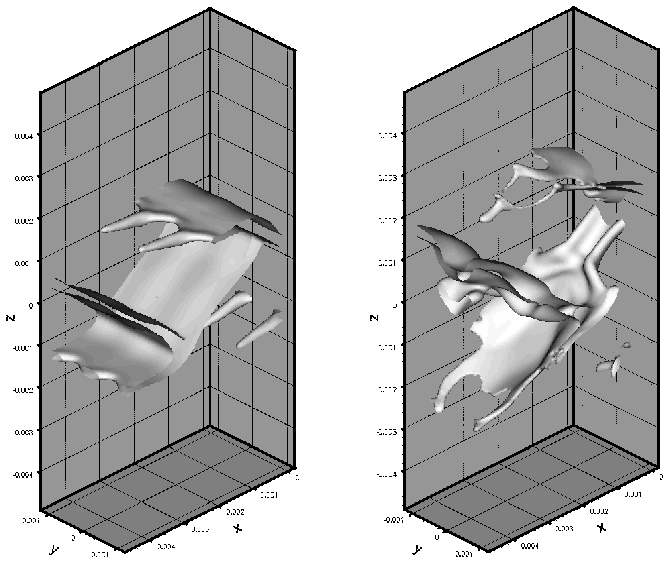

FIGURE 6: Numerical Simulation of Tridimensional Periodic Developing Air-Blasted Liquid Sheet Instabilities (left case and right case have respectively the same physical parameters than Fig.(4) and Fig.(5))

On the left case, we can see the formation of two fingers. On the right case, as the spatial simulation, interface evolution is much more intricated with a higher atomization level.

Conclusion

In this paper, we have developed a efficient DNS two-phase flow code and performed our first simulations of the air-blasted liquid sheet. We will continue our effort to develop this code, and particulary we will write an algorithm to ensure mass conservation, it will be probably a coupling with an another interface tracking method. We will continue to simulate the air-blasted liquid sheet with a parametric study of revelent parameters driving the liquid sheet atomization.

Nomenclature

Latin

$2a$	$[m]$	liquid sheet thickness
$\mathbf{D}$	$[s^{-1}]$	viscous stress tensor
g	$[m.s^{-2}]$	gravity
k	$[m^{-1}]$	wave number
M	-	momentum flux ratio
n	$[s^{-1}]$	growth rate
p	$[N.m^{-2}]$	pressure
R_e	-	Reynolds number
$\mathbf{u}$	$[m.s^{-1}]$	velocity vector
W_e	-	Weber number

Greek

δ	$[m]$	air boundary thickness
κ	$[m^{-1}]$	interface curvature
μ	$[N.s.m^{-2}]$	dynamic viscosity
ρ	$[kg.m^{-3}]$	density
σ	$[N.m^{-1}]$	surface tension coefficient
ϕ	$[m]$	Level-Set function

Subscript

l	liquid
g	gas

References

[1] C.W. Shu, ENO and WENO Schemes for hyperbolic conservation laws, *ICASE Report*, 1997

[2] G.S. Jiang and D. Peng, Weighted ENO Schemes for Hamilton–Jacobi Equations, *SIAM J. Sci. Comput.*, vol. 21, pp. 2126-2143, 1999

[3] R. Fedkiw, M. Kang and X.-D. Liu, A Boundary Condition Capturing Method for Poisson's Equation on Irregular Domains, *J. Comput. Phys.*, vol. 160, pp. 151-178, 2000.

[4] O. Tatebe, MGCG Method, A Robust and Highly Parallel Iterative Method, Ph.D. thesis, 1996

[5] R. Fedkiw, M. Kang and X.-D. Liu, A Boundary Condition Capturing Method for Multiphase Incompressible Flow, *J. Sci. Computing*, vol. 15, pp. 323-360, 2000

[6] F. Couderc and J.L. Estivalezes, Sharp Interface Capturing Methos based on Level-Set Method for Incompressible Flow with Surface Tension, ASME Annual Summer Meeting FEDSM2003-45151, Hawai, 2003

[7] W. Tauber, G. Tryggvason and S.O. Unverdi, The nonlinear behavior of a sheared immiscible fluid interface, *Physics of Fluids*, vol. 14, pp. 2871-2885, 2002