Primary break-up: DNS of liquid jet to improve atomization modelling

T. Ménard, P. A. Beau, S. Tanguy, F. X. Demoulin & A. Berlemont
CNRS-UMR6614-CORIA, Rouen University, France

Abstract

Two different approaches for numerical simulations of primary break-up of liquid jet are described. In the ELSA model (Eulerian Lagrangian Spray Atomization) the liquid and the gas are considered as two species of a same mixture, but without necessarily the same velocity. The drift velocity and the liquid mass dispersion are exactly related to the turbulent liquid mass flux. To describe the topology of the spray the liquid/gas interface density per unit of volume is used instead of the droplet diameter that has no meaning in the dense part of the spray. To establish definitely the model for the turbulent liquid mass flux and for the liquid/gas interface density equation, DNS simulations are carried out to obtain information in the dense zone of the spray where nearly no experimental data are available. Interface tracking is ensured by the Level Set Method and the Ghost Fluid Method (GFM) is used to capture accurately sharp discontinuities for pressure, density and viscosity. Coupling between the Level Set and VOF method is used for mass conservation. Fluid motion is predicted with a projection method for incompressible flows.

Keywords: Level Set, Ghost Fluid Method, VOF, DNS, atomization modelling, liquid jet.

1 Introduction

Extensive studies have been devoted to the transport of spray of droplets, but the atomization process remains a challenging topic of research. It clearly appears that specific approaches must be developed when it is necessary to describe interface behavior. In recent years a number of studies have been proposed for the modelling and numerical simulation of moving interfaces. Two approaches are described in this paper. Vallet et al [1] proposed a new approach that permits to compute all the atomization process and that included the primary break-up zone: the ELSA
model [1, 2]. The model is based on a single-phase Eulerian model, and describes the whole process from inside the injector to the final dilute spray region. The classical transport equations of the mean mixture variable are considered. Unclosed correlation terms appear in the set of equations. A $k - \epsilon$ model is used to model the turbulence. The liquid turbulent diffusion discussed in previous papers [3], will be treated using a classical gradient law since the purpose of this paper is to study the transport equation for the mean liquid/gas interface density. We will focus our work on this original equation first introduced by Vallet et al [1]. This equation was postulated in comparison with the flame surface density equation. Despite initial successes of the method there is a lack of experimental data to establish definitely the model for the turbulent liquid mass flux and for the liquid/gas interface density equation. DNS simulations are carried out to obtain information in the dense zone of the spray where nearly no experimental data are available. We are here concern by the primary break-up of a jet: a lot of topological changes occur (interface pinching or merging, droplet coalescence or secondary break-up) and the Level Set Method thus appears well designed for our purpose. Osher and Sethian [9] proposed a Level Set method which describes the interface with the zero level curve of a continuous function defined by the signed distance to the interface. To describe the interface discontinuities, we use the ghost fluid method (GFM), which has been derived by Fedkiw et al [5] to capture jump condition on the interface. A projection method is used to solve incompressible Navier-Stokes equations that are coupled to a transport equation for the level set function. It is well known that numerical computations in the re-distancing algorithm of the method can generate mass loss in under-resolved regions. This is the main drawback of level set methods, but to improve mass conservation extension of the method can be developed, namely a coupling between VOF and Level Set (Sussman and Puckett [11]). Specific care has been devoted to improve simulation capabilities with MPI parallelization. The numerical methods have been applied to investigate physical processes, involved during the primary break-up of an atomizing jet. The chosen configuration is close as possible of Diesel injection.

2 Overview of the Eulerian Lagrangian Spray Atomization (ELSA)

2.1 The mean liquid/gas interface density transport equation

The ELSA model is an atomization model. It means that this modelling has to predict the characteristics of the liquid droplets or blobs in the dense part of the spray. Concerning the diameter, Vallet et al [1]. introduced a more general equation than an equation for the diameter: the mean liquid/gas interface density equation. This equation avoids us to assume the shape of the droplets and allows us to describe complex liquid topology like liquid ligaments. This variable $\bar{\Sigma}$ (in $m^{-1}$) corresponds to the quantity of liquid/gas interface per unity of volume. In this part, we
rather use the quantity of liquid/gas interface per unity of mass $\tilde{\Omega}$ (in $m^2.kg^{-1}$) to simplify the equations and most especially the treatment of the diffusive term.

The transport equation for the mean liquid/gas interface density has the following general form:

$$
\frac{\partial \rho \tilde{\Omega}}{\partial t} + \frac{\partial \rho \tilde{\Omega} \tilde{U}_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_t \frac{\partial \tilde{\Omega}}{\partial x_j} \right) + \tilde{\rho} \left( \dot{\tilde{\Omega}}_{\text{mixture}} + \dot{\tilde{\Omega}}_{\text{stress}} + \dot{\tilde{\Omega}}_{\text{breakup}} + \dot{\tilde{\Omega}}_{\text{coalescence}} \right) 
$$

with $\tilde{U}$ the mean mixture velocity, $D_t$ the turbulent diffusivity and $\tilde{\rho}$ the mixture density.

2.2 Initialization $\dot{\tilde{\Omega}}_{\text{mixture}}$

This first term corresponds to a production of liquid/gas interface due to the mixing of liquid and gas phases. In fact, if the liquid and the gas phases are mixed together, there is obviously production of liquid/as interface.

$$
\dot{\tilde{\Omega}}_{\text{mixture}} = 2D_t \frac{6\tilde{\rho}}{\rho_1 \rho_2 L_t} \frac{\partial \tilde{X}_2 \partial \tilde{X}_2}{x_i} \quad \text{if} \quad \tilde{X}_2(1 - \tilde{X}_2) \leq 0.001 \tag{1}
$$

$$
\dot{\tilde{\Omega}}_{\text{mixture}} = 2D_t \frac{\tilde{\Omega}}{\tilde{X}_2(1 - \tilde{X}_2)} \frac{\partial \tilde{X}_2 \partial \tilde{X}_2}{x_i} \quad \text{otherwise} \tag{2}
$$

where $L_t$ is the turbulent length scale and $\tilde{X}_2$ is the liquid mass fraction, $\rho_1$ and $\rho_2$ stands respectively for the gas and liquid densities. By introducing this term, we assume that the first scale of the liquid blob produced is the turbulent length scale.

2.3 Production due to the turbulent stress $\dot{\tilde{\Omega}}_{\text{stress}}$

The second term represents the production of the interface due to the turbulent stretching. This term expresses that the liquid/gas interface is wrinkled by the turbulent flow. The simplest model is:

$$
\dot{\tilde{\Omega}}_{\text{stress}} = \frac{\tilde{\Omega}}{\tau_t} \quad \text{with} \quad \tau_t \quad \text{the turbulent time scale.}
$$

2.4 Production due to the break-up $\dot{\tilde{\Omega}}_{\text{breakup}}$

The third term deals with the effect of the droplet break-up due to collisions. This phenomenon seems to be the most important one in the dense spray region. The break-up phenomenon is not only controlled by the turbulence but mainly by the collisions occurring in the dense part of the spray.

$$
\dot{\tilde{\Omega}}_{\text{breakup}} = \frac{\tilde{\Omega}}{\tau_{\text{col}}} \quad \text{with} \quad \tau_{\text{coll}} = \frac{L_{\text{coll}}}{S_{\text{eff}} \Delta v} \quad \text{the collision time scale.}
$$

The characteristic collision length scale is $L_{\text{coll}}$, the characteristic collision velocity is $\Delta v$ and the effective section of the colliding droplets is $S_{\text{eff}}$. 

www.witpress.com, ISSN 1743-3533 (on-line)
2.5 Destruction due to the coalescence $\dot{\Omega}_{\text{coalescence}}$

The fourth term stands for the coalescence effects. This is a destruction term of the liquid/gas interface. The liquid/gas interface density equation must reach an asymptotic state, i.e. the destruction term must balance the production terms. It means that the Sauter mean diameter tends to a steady value. Vallet et al [1] propose a critical diameter given by:

$$D_{\text{crit}} = \frac{\sigma^{3/5}}{k} \left( \frac{\bar{\rho} \bar{X}_2}{\rho_2^{11/15}} \right)^{2/15} \quad \text{and} \quad \Omega_{\text{crit}} = \frac{6 \bar{X}_2}{\rho_2 D_{\text{crit}}}$$  \hspace{1cm} (3)

The characteristic time scale of the coalescence is the collision time scale because coalescence occurs only if there is collision. We obtained for the coalescence destruction term:

$$\dot{\Omega}_{\text{coalescence}} = - \frac{1}{\tau_{\text{coll}}} \frac{\dot{\Omega}_2^2}{\Omega_{\text{crit}}}$$ \hspace{1cm} (4)

3 Overview of DNS simulation

3.1 The Level Set method

Level Set methods are based on the transport of a continuous function $\phi$ which describes the interface between two mediums (Sussman et al [12] and Sethian [10]). That function is defined by the algebraic signed distance ($|\nabla \phi| = 1$) between any point of the domain and the interface. The interface is thus described by the 0 level of the level set function. Solving a convection equation determines the evolution of the interface in a given velocity field $U$ [10]:

$$\frac{\partial \phi}{\partial t} + U \cdot \nabla (\phi) = 0$$ \hspace{1cm} (5)

Particular attention must be paid to this transport equation. Some problems may arise when the level set method is developed, namely a high velocity gradient can produce large spreading and stretching of level set, such as $\phi$ will no longer remains a distance function. A re-distancing algorithm [12] is then applied to keep $\phi$ as the algebraic distance to the interface. The algorithm is based on the iterative resolution of the following equation:

$$\frac{\partial d}{\partial \tau} = \text{sign}(\phi)(1 - |\nabla d|) \quad \text{where} \quad d(x, t, \tau)_{\tau=0} = \phi(x, t)$$ \hspace{1cm} (6)

where $\tau$ is a fictitious time. We solve equation (6) until steady state is reached, thus close to the exact steady state solution namely either $\text{sign}(\phi) = 0$, meaning that we are on the droplet interface, or ($|\nabla d| = 1$) which mathematically defines a distance function. In our simulations two or three iterations per physical time step of re-distancing algorithm are sufficient to ensure that $d$ is a signed distance. The main advantage of the above algorithm is to provide us with the required
property for $\phi$ without changing its zero level set. Equations (5) and (6) are hyperbolic types. Specific care must be devoted to the discretization method, as discontinuities are often observed in the results. To avoid singularities in the distance function field, we thus use a 5th order WENO scheme for convective terms Jiang and Shu [6]. Temporal derivatives are at least computed with a second order Runge Kutta scheme.

One advantage of the level set method is its ability to represent topological changes both in 2D or 3D geometry quite naturally. Moreover, geometrical information on the interface, such as normal vector $n$ or curvature $\kappa$, are easily obtained through:

$$n = \frac{\nabla \phi}{|\nabla \phi|} \quad \kappa(\phi) = \nabla \cdot n \tag{7}$$

As previously mentioned, mass loss can occur in under-resolved regions when eqns. (5, 6) are solved. Two main extensions of the method can be developed, namely the particle level set (Enright et al. [4]) or a coupling between VOF method and Level Set method (Sussman and Puckett [11], Van Der pijl et al. [14]). Our choice is to develop Level Set Method with GFM and coupling with VOF approach.

### 3.2 Coupling VOF and Level Set method

We recall here the main ideas of the CLSVOF method extensively discussed by Sussman and Puckett [11]. To couple the VOF method and the Level Set method, we first define the volume fraction $F$, in a grid cell $\Omega$ of the domain, at time $t$, as a function of $\phi$ (assuming 2D formalism for simplicity):

$$F(\Omega, t) = \frac{1}{|\Omega|} \int_{\Omega} H(\phi(x, y, t)) \, dx \, dy \tag{8}$$

where $H$ is the Heaviside function:

$$H(\phi) = \begin{cases} 1 & \text{if } \phi > 0 \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

Discretization of eqn. (8) requires to define the interface in a cell $\Omega_{(i,j)}$. We thus introduce a reconstructed level set function ($\phi^R$), that is defined by a line in 2D (a plane in 3D):

$$\phi^R_{i,j} = a_{i,j}(x - x_i) + b_{i,j}(y - y_j) + c_{i,j} \tag{10}$$

The coefficients $c_{i,j}$ represent the normal distance form the interface to the points $(x_i, y_j)$. The coefficient of eqn. (13) are determined by the minimization of the error (for a nine point stencil):

$$E_{i,j} = \sum_{i' = i-1}^{i+1} \sum_{j' = j-1}^{j+1} w_{i',j'} \delta_{\epsilon}(\phi_{i',j'})(\phi_{i',j'} - a_{i,j}(x_{i'} - x_i) - b_{i,j}(y_{j'} - y_j) - c_{i,j})^2 \tag{11}$$
\( \delta_\epsilon (\phi_{i',j'}) \) is a smoothed Dirac distribution with thickness \( \epsilon \) \( (\epsilon = \sqrt{2} dx) \) and \( w_{\alpha,\beta} \) are weighting factors which are maximal on the cell central point \((i, j)\). One advantage of the approach is that we can choose the number of points in the stencil. For example, when two interfaces are in the nine point stencil but only one interface is in the considered cell, the approximation can be unrealistic. A six point or four point stencil is then used in eqn. (11).

Equation (8) then reads:

\[
F_{i,j} = \frac{1}{\Delta x \Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} H(a_{i,j}(x-x_i)+b_{i,j}(y-y_j)+c_{i,j}) \, dx \, dy \quad (12)
\]

In order to calculate the above integral a change of coordinate system is first applied such as the origin of the new coordinate system is on the lower left hand corner of the cell and the normal to interface points towards the origin. In other terms we will always have liquid in the lower left hand corner and the new coefficient \( c'_{i,j} \) is the distance from the new origin to interface. A new equation is obtained for interface:

\[
a'_{i,j}(x-x_{i-1/2}) + b'_{i,j}(y-y_{j-1/2}) + c'_{i,j} = 0 \quad (13)
\]

and eqn. (12) is now the sum of two parts (figure 1): the area I is calculated with geometrical rules and the area II is estimated by \( \frac{1}{dx \, dy} \int (y(x)) \, dx \) which now represents the liquid volume under the line. In 3D geometries the same steps are applied with a little bit more calculus.

![Figure 1: Illustration to determinate the Volume Fraction in a cell.](image)

Note that the above coupling between VOF and Level Set method is applied in two cases. When we want to verify mass conservation in the level set transport and
re-distancing algorithm, we assume that the volume fraction $F_{i,j}^n$ is known and the following constraint at time $n$, is applied:

$$\frac{1}{\Delta x \Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} H(a_{i,j}(x-x_i) + b_{i,j}(y-y_j) + c_{i,j}) \, dx \, dy = F_{i,j}^n \quad (14)$$

We use an iterative Newton method with a given precision to get the final value of $c'_{i,j}$ and then $c_{i,j}$. Finally we write:

$$\phi^n(i,j) = c_{i,j} \quad (15)$$

But the transport of the liquid volume fraction is also solved with the above coupling. In order to get the value $F_{i,j}^{n+1}$, eqn. (12) is used but the integral limits are modified, namely the velocity is used to determine the volume of liquid passing from one cell to a neighbourd cell. Detailed information can be found in Sussman and Puckett [11].

3.3 Projection method for Navier-Stokes

Incompressible Navier-Stokes equations can be written as:

$$\frac{\partial U}{\partial t} + U \cdot \nabla(U) = -\nabla(p) + \frac{\nabla(2\mu(\phi)D)}{\rho(\phi)} + g \quad (16)$$

$$\nabla \cdot U = 0 \quad (17)$$

$p$ is the pressure, $\rho$ and $\mu$ are the fluid density and viscosity respectively. Spatial derivatives are estimated with 2$^{nd}$ order central scheme, but convective terms are approximated by 5$^{th}$ order WENO scheme discretization in order to get a robust behavior of the solution. Temporal derivatives are approximated by Adams Bashforth formulation. Linear system deduced from Poisson equation is solved with a multigrid algorithm for preconditioning conjugate gradient method (Tanguy [13]).

3.4 Ghost Fluid Method

To handle interface discontinuities we use a Ghost Fluid Method which has been derived by Fedkiw et al [5] to capture jump condition on the interface. For example, the pressure jump related to surface tension $\sigma$ and to the interface curvature reads:

$$[p] = \sigma \kappa(\phi) + 2[\mu](\nabla u \cdot n, \nabla v \cdot n, \nabla w \cdot n) \cdot n \quad (18)$$

The Ghost Fluid Method 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 thus much lower than with other approach such Continuous Surface Force method. We have used this procedure to discretize all discontinuous variables, namely density, viscosity, pressure and viscous tensors. Details can be found in Fedkiw [5], Tanguy [13], Kang et al [7].
3.5 Simulation

All the simulations presented here are thus carried out with the Level Set Method, with Ghost Fluid Method for interface discontinuities and coupling with VOF Method for mass conservation. Numerical codes have been developed for 2D, 2Daxi and 3D geometries, and MPI parallelization is used.

4 Turbulent liquid jet

We present a comparison between these two approaches. We perform a simulation in 3D with the DNS method in the primary atomization zone of a turbulent jet where conditions are given in Tab. (1). The uniform mesh size is $128 \times 128 \times 896$ and dimensions of the domain are $(0.0003, 0.0003, 0.0021)$ in the $(x, y, z)$ directions.

Generation of turbulent inflow boundary conditions is still a challenging task for studying turbulent spatially developing flow like jet with DNS or LES. Here we use a method, devised by Klein et al [8], which consists in generating random velocities with a prescribed length scale. In our computation that scale is equal to the turbulent integral scale $L_t$ of the cylindrical channel flow ($L_t = 0.1D$). Turbulence intensity is 0.05 of inlet mean velocity.

Table 1: Characteristics of the spray.

<table>
<thead>
<tr>
<th>Diameter (D)</th>
<th>velocity</th>
<th>turbulent intensity</th>
<th>turbulent length scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 $\mu$m</td>
<td>100m.$s^{-1}$</td>
<td>$\frac{u'}{\bar{U}} = 0.05$</td>
<td>0.1D</td>
</tr>
</tbody>
</table>

For the RANS simulation, the model is implemented in CFD code STARCD V 3.15 through user-subroutines. Since only mean values are computed, a 2D non-uniform mesh is sufficient for the modelling part. The total number of cells is $100 \times 55$ and the dimension of the domain are $(0.046, 0.097)$ in the $(x,y)$ direction. There are 10 cells along the diameter of the injector hole. The aspect ratio of the cells near the orifice is close to one in order to achieve good numerical accuracy.

5 Results

Typical result for both methods are represented on figure 2. Figure 2.a shows an instantaneous 3D result using the level set method. From the injector nozzle, the
turbulence initiates some perturbations of the liquid surface, that are enhanced by the mean shear between the liquid jet and the surrounding air. The interface becomes very wrinkled and some break-up are initiated. The induced liquid parcels show a wide range of shapes. The surface is not organized and no clear process of break-up seems dominant. On the figure 2.b and 2.c a cut through the middle of the jet is used to show the mean value of the liquid volume fraction. Figure 2.b is obtained by averaging the level set results and figure 2.c is the result of the ELSA model. The global behavior is well captured by the model even if the length of the liquid core is overestimated. These results imply that the representation of the initial liquid break-up and dispersion by a turbulent flux is an appropriate model in such atomization process, even if it has to be improved.

Figure 2: Comparison between DNS and ELSA results. (a) instantaneous DNS result at $t = 40\mu s$; (b) center cut, mean liquid volume fraction (DNS); (c) center cut, mean liquid volume fraction (ELSA model). (b), (c) Black area correspond to liquid core ($\phi_{VOL} > 0.99$), line: external contour of the spray ($\phi_{VOL} = 0.01$).
Extensive numerical simulations are still carried out to compare other means quantities. Space limitation, however, does not allow us to discuss all of the results in this paper.

References