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Multi-scale spray atomization model

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Abstract

The purpose of the present article is to present a dynamic multi-scale approach for turbulent liquid jet atomization in dense flow (primary atomization), together with the possibility to recover Interface Capturing Method (ICM) / Direct Numerical Simulation (DNS) features for well resolved liquid-gas interface. A full ICM-DNS approach should give the best comparison with experimental data, but it is not industrially affordable for the time being, therefore models are mandatory. A numerical representation based on full ICM-DNS, for the initial destabilization of the complex turbulent liquid jet, going up to the spray formation, for which well established numerical models can be used, is appealing but has not yet been applied. Indeed such an approach requires the ICM-DNS to be applied up to the formation of each individual droplet. Hence, in many situation models have to be applied to the dense, unresolved and turbulent liquid-gas flow. To achieve this goal, the most important unresolved phenomena to address are, the sub-grid turbulent liquid flux and surface density, in which models based on the so-called Euler-Lagrange Spray Atomization (ELSA) concept, were developed and have been successfully applied to an Engine Combustion Network (ECN) database, in both RANS/LES (Reynolds-Averaged Navier-Stoke/Large Eddy Simulation) context. An innovative coupling between ICM and a complete ELSA approach was tested based on Interface Resolved Quality (IRQ) sensors to determine locally and dynamically whether or not the interface can be well captured. The ultimate aim is to conduct numerical simulations of fuel injection in an industrial scale, for which comprehensive database has been set up. The test case has been chosen for two reasons: (i) previous numerical studies showed, on the same test case, that RANS turbulence model requires a strong modification to get appropriate results, hence prompted the use of LES models. And (ii), liquid Reynolds and gas Weber numbers are relatively low, compared with ECN test cases, hence more flow regions are expected to be resolved. Results showed that using a fully resolved interface model in the whole domain, provides results in good agreement with the experiment in the primary atomization region only. Indeed, it effectively captured the surface instabilities and liquid structure detachments. In the far field, however, this model becomes rapidly unadapted downward in the dispersed spray region, and the ICM-ELSA model was able instead to treat low volume fractions of atomized liquid, where velocity fluctuations become important.

Keywords

Resolved/unresolved interfaces, Primary atomization, Air-blast atomizer.

Introduction

Multiphase flow can be classified in discrete and separated flow, however, when it comes to atomizing turbulent liquid jets, a combination of both is rather preferable. Indeed, just at the exit of the injector nozzle, the amount of liquid is very high, and this phase cannot be decomposed as sets of discrete droplets. Moreover, bubbles could be present in the liquid flow due to penetration of the surrounding gas during the breakup process, and previous cavitation inside the nozzle injector. Consequently, the carrier phase would be the liquid and the discrete phase, the gas bubbles. On the contrary, further downstream, a spray is generated, in which the carrier phase is the gas and the discrete phase corresponds to liquid droplets. Between these two limits, a two-phase flow exists with unclear discrete and carrier phases [1]. The key point of the proposed ELSA model, is the analogy between atomization, liquid dispersion and turbulent mixing of a jet, with large density difference with the ambient medium [2]. By using single-fluid approach, the choice of both carrier and discrete phases, is avoided [1]. Therefore, the two-phase flow is studied as a single-phase turbulent flow composed of two species with highly variable density. Noteworthy, the notion of two-phase flow still applies, in the sense that there are two velocities: one for the liquid and one for the gas that can be recovered thanks to the QME (Quasi–Multiphase Eulerian model) extension of ELSA approach [3]. In this section, applying the Reynolds averaging technique for incompressible isothermal fluids, governing equations for continuity, momentum and liquid volume fraction are presented, respectively:

$$\left\{ \begin{array}{l} \nabla \cdot \bar{\mathbf{U}} = 0 \quad , \\ \frac{\partial \bar{\rho} \bar{\mathbf{U}}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{U}} \otimes \bar{\mathbf{U}}) = -\nabla \bar{p} + \nabla \cdot [\bar{\rho} \bar{\nu} (\nabla \bar{\mathbf{U}} + \nabla \bar{\mathbf{U}}^t)] + \rho \bar{\mathbf{f}}_b - \nabla \cdot \mathbf{R}_U + \tau_\rho \quad , \\ \frac{\partial \bar{\alpha}_l}{\partial t} + \nabla \cdot (\bar{\mathbf{U}} \bar{\alpha}_l) = -\nabla \cdot \mathbf{R}_{\alpha_l} \quad . \end{array} \right. \quad (1)$$

The averaged (or filtered in LES framework) mixture velocity \bar{U} , and the liquid volume fraction $\bar{\alpha}_l$, follow the classical transport equations in which \bar{p} is the normal stress in two-phase medium at equilibrium, ν is the kinematic mixture viscosity, $\bar{\rho}$ is the mixture density, and finally \bar{f}_b , is the body forces per unit of mass. Whenever it is not possible to solve these equations directly at all scales, some filtering or averaging process is applied, thus necessarily introducing the so-called Reynolds stress tensor R_U , and the turbulent liquid flux R_{α_l} (colored in red) in eq. (1). It is important to notice, that one of the first feature that is lost, is the accurate position of the interface. Previously, the liquid volume fraction field, or any other phase indicator, was sufficient to determine the position of the interface. For instance, any iso-surface of the liquid volume fraction, within the range [0,1], is identical if the liquid volume fraction profile is a step profile across the interface. Nevertheless, averaging or filtering will smooth the liquid volume fraction profile, and let undetermined the actual position of the interface. Any other VOF method faces the same problem but in different ways e.g., by forcing a sharp transition between liquid and gas at the interface e.g., Level Set [4], Ghost-Fluid [5]. This compressive feature, is in contradiction with the averaging/filtering procedure in which, a smooth transition is considered, with the consequence to lose the interface position. Notice that, numerous successful works in the literature ignore these problems, and use averaged/filtered approaches whilst keeping a sharp transition between phases i.e., turbulence models such as RANS or LES, are used and combined with ICM. Normally, it is expected that such effects are negligible, if all scales of the flow are solved.

Regarding the Reynolds stress, single-phase flow model is initially tested. Following Boussinesq's proposal, the turbulent momentum transport is assumed to be proportional to mean gradients of velocity [6]. By analogy, turbulent transport of a scalar is taken to be proportional to the gradient of the mean value of the transported quantity. Thus, the turbulent liquid flux is seen mainly as a dispersion term for the liquid due to the random turbulent motion. Finally, the Reynolds stress tensor and the turbulent liquid flux are presented, respectively:

$$\left\{ \begin{array}{l} R_U = (\overline{U \otimes U} - \bar{U} \otimes \bar{U}) \quad , \\ \quad \approx -\frac{\nu_t}{Sc_t} (\nabla \bar{U} + \nabla \bar{U}^t) \quad . \\ R_{\alpha_l} = (\overline{U \alpha_l} - \bar{U} \bar{\alpha}_l) \quad , \\ \quad = \bar{\alpha}_l (\bar{U}|_l - \bar{U}) \quad , \\ \quad \approx -\frac{\nu_t}{Sc_t} \nabla \bar{\alpha}_l \quad . \end{array} \right. \quad (2)$$

where ν_t , is the turbulent viscosity (or sub-grid stress in LES framework) and Sc_t , is the turbulent Schmidt number. In eq. (2), R_{α_l} is the *turbulent liquid flux*, that represents the transport of the liquid volume fraction induced by velocity fluctuations, and is related to the unresolved part of the velocity that is known to produce additional dispersion. This formulation is only valid in the absence of mean slip velocity between phases. Additionally, it has been proven [1, 3] that even with this single flow approach, it is possible to recover the different mean liquid and gas velocities $\bar{U}|_l$, and $\bar{U}|_g$, respectively, by means of a drift flux model. Additionally, density correlations represented by τ_ρ in eq. (1), appears on this Reynolds formalism. Their effect is still subject of research, e.g. density fluctuations in combustion processes are not necessarily applicable when the density ratio tends to infinity, which is also the present study case. On the other hand, by using the Favre averaging (i.e., the mass formulation) in two-phase flow simulation, there is not an explicit approximation, in modeling liquid-gas turbulent fluctuation stresses, as compared with the Reynolds formalism. However, further development in the Favre formalism for two-phase flow, revealed implicitly an equivalent density correlation issue, especially for high density ratios $\left(\frac{\rho_l}{\rho_g}\right)$. Therefore, since this article will treat the conservation equation using a Reynolds formalism (LES/RANS), based on volumetric variables, the density correlations will be considered as part of the global Reynolds/Residual stress model.

The purpose of the present article is to present a dynamic multi-scale approach suitable to perform LES for liquid jet atomization, together with the possibility to recover ICM/DNS features for well resolved interface flow. To achieve this goal, the most important unresolved phenomena to address are, the sub-grid turbulent liquid flux, eq. 2, and liquid gas interface density, namely Σ , which represents the liquid/gas surface interface per unit of volume [2, 7].

Numerical method

The goal is to propose a less computationally demanding model than DNS (e.g., RANS / LES), dynamically adaptable to turbulent interface fluctuations i.e., interface resolution dependent. To that end, a pondering parameter C_α is proposed, to evaluate when it is necessary to consider either an Interface Capturing Method (ICM) for resolved interface, or subgrid modeling (ELSA) for unresolved interface. Indeed, an expected feature of LES model theoretically, is to retrieve DNS i.e., by using proper mesh resolution tending to Kolmogorov length scales for single-phase flow, then the residual stress tensor eq. (2) would vanish from the filtered equations. On the contrary, in liquid-gas flow, it means that unresolved interface modeling such as ELSA, has to be modified for high mesh resolution, in order to recover resolved interface features, by using approaches such as: ICM. Therefore, for highly resolved flow, LES should switch from ELSA to ICM. In the following part, considering the known shortcomings of unresolved interfaces approaches, in the dense spray region, and in order to develop a model suitable also in the dilute spray

region, a coupling technique between ELSA and an interface capturing method ICM is proposed and detailed, as displayed in figure 1, highlighted in red.

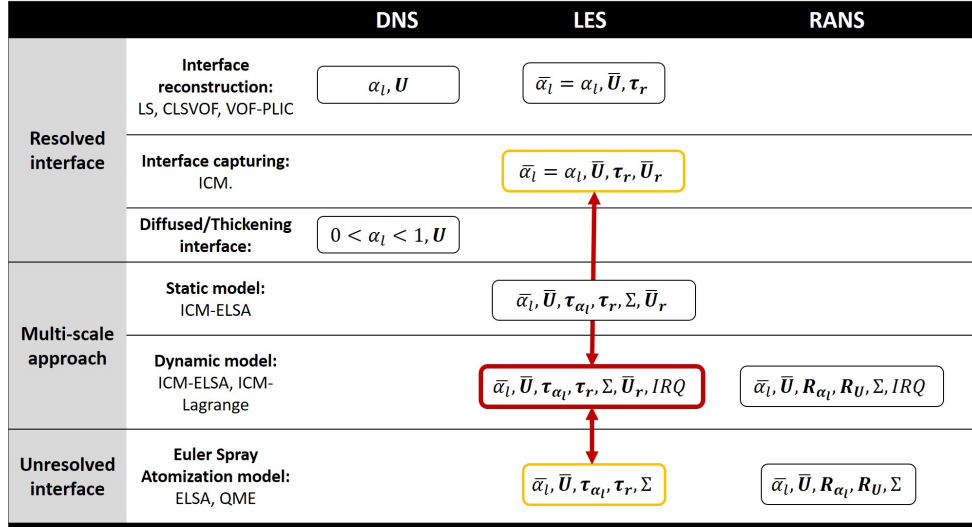


Figure 1. Physical-modeling representation of atomization process in turbulent liquid-gas flow. Transition from resolved interface to unresolved interface approach, namely *ICM – ELSA*, using LES framework (highlighted in red).

There are some issues that have to be clarified. Firstly, f_σ , is the additional force in the momentum equation due to the surface tension depending on the local curvature of the interface, and defined as $f_\sigma = \sigma \kappa \delta(x - x_s) n$. To compute this force, and to apply the jump of any variable, the most accurate ICM-DNS code applies interface reconstruction, along with dedicated high order numerical schemes. There are many successful examples in the literature of these fully resolved approaches, combining ICM method with DNS using mesh resolution high enough to compute all the flow scales, based on the curvature, VOF-PLIC (piecewise-linear interface construction), VOF/level-set coupling for unstructured and non-uniform meshes, octree meshes, among others [8] (Top-left/center in figure 1). For instance, the ARCHER code [9], is based on coupled *VOF-Level set* method for interface reconstruction, together with a *ghost-fluid* approach, to represent accurately the discontinuity of variables such as density, pressure and viscosity at the interface. This reconstruction process generally depends on the mesh geometry, hence are difficult to reproduce for body-fitted methods based on unstructured mesh, which are generally used to address complex geometries. Notice that several proposals exist, for example in the open source software: OpenFOAM® to improve this point, in particular the isoAdvector approach [10], and the so-called *interFoam* [11].

For full-scale resolution, ICM method aims at keeping a sharp interface, thus a discontinuous profile across the phases exits in particular during the convection process. This property is either directly included in the numerical scheme (VOF, Level-Set, ghost-fluid, among others) or obtained by additional correction designed to prevent numerical diffusion that could smear the profile. The *interFoam* solver of OpenFOAM® is based on this last technique, where Weller [12] proposed to use an additional flux of liquid directed toward the interface proportional to the local velocity magnitude (U_r) and located only where a mixture of liquid and gas exists (i.e. $\alpha_l \in [0, 1]$), in such a way that the local flow steepens the gradient of the volume fraction and thus the interface resolution is improved [13]. This method is often referred as the VOF method, even if there is no real reconstruction of the interface. On the other hand, following the modeling approach in this article, LES filtering framework is used. As for instance, diffusive methods are designed to smear the interface over several mesh cells, to recover a continuous behavior of any variable. It is important to emphasize that the drift/slip behavior of the residual (unresolved) liquid flux, is not compatible with the ICM method, since the former assumes the profile to be discontinuous, thus both approaches can not coexist at the same place. For unresolved interface approach, the general two-phase flow spray atomization model, originally develop by Vallet and Borghi [2] is used. In this model, the boundary separating pure liquid and pure gas, is considered as a mixing zone. Mass and volume formulation of the conservative variables (Liquid Volume Fraction, LVF $\bar{\alpha}_l$, and interface surface density Σ), have been already validated against available experimental and DNS data, under LES and RANS formalism, by using to that end, the so-called ELSA model [1, 7, 14, 15, 16] (Bottom-right/center in figure 1). Hence, starting from the system reported in eq. (1), the liquid volume fraction equation is modified, considering C_α , which is a pondering parameter between the ELSA and the ICM approach:

$$\frac{\partial \bar{\alpha}_l}{\partial t} + \nabla \cdot (\bar{U} \bar{\alpha}_l) + \underbrace{C_\alpha \nabla \cdot [U_r \bar{\alpha}_l (1 - \bar{\alpha}_l)]}_{ICM} = (1 - C_\alpha) \underbrace{\nabla \cdot (R_{\alpha_l})}_{ELSA} \quad . \quad (3)$$

The advantages of the proposed model, is to determine a resolution of the interface with ICM in a limited region, whereas it would be disabled when R_{α_l} prevails (i.e. when the interface fluctuations become significant, for instance

in LES framework). The switching strategy is introduced through C_α . Two different criteria were proposed to determine its value, based on the interface resolution and the curvature of the interface. C_α was set to zero (0), when the interface is poorly-resolved (dilute region) and set to one (1) otherwise (dense region). The interested reader is referred to [17], in which Interface Resolution Quality (IRQ) criteria are developed. On the one hand, as mentioned before, DNS should be capable of resolving all two-phase flow scales, theoretically. Nowadays, however, it is unfeasible industrially speaking. On the other hand, the proposed dynamical model i.e., eq. 3, is thus able to take advantage of a full-interface resolution, to recover a DNS formulation with ICM, and to switch to a diffusive (residual or sub-grid) LES approach, only when necessary. Note that ICM is not compatible with diffusive models, hence C_α is dynamically adjusted to (1) one or (0) zero, depending on the interface resolution within the cell(s). Furthermore, when the spray is formed and diluted, it is more accurate to use a regular method dedicated to solved the Williams-Boltzmann Equation (WBE) [18], and therefore a Lagrangian formulation should be initiated.

Numerical test case

The previous section has described different available approaches to address the liquid-gas turbulent flow within dense zones. The ultimate aim, is to conduct numerical simulation of fuel injection in a industrial scale, for which one comprehensive data base has been set up by Stepowski et al. [19]. As a reminder, a full ICM-DNS approach should give the best comparison with experimental data, but it is not affordable for the time being, therefore models are mandatory. A numerical representation based on full ICM-DNS, for the initial destabilization of the complex turbulent liquid jet, going up to the spray formation, for which well established numerical model can be used, is appealing but has not yet been applied. Indeed such an approach requires the ICM-DNS to be applied up to the formation of each individual droplet. Hence, in many situation models have to be applied for the dense turbulent liquid-gas flow, among them the ELSA approach, which has been successfully applied for instance on an ECN database [20] by several teams [21, 22], both in RANS/LES context, leading to CPU cost compatible with industrial application. For the following test case, the interface can be: (1) treated as captured at the present mesh resolution, leading to an ICM approach or (2) treated as residual (or subgrid) interface, leading to a diffused interface approach, for which a turbulent liquid flux driven mainly by liquid dispersion is considered. The diffused interface approach combined with the dispersion model has already been successfully tested by Chesnel et al [14], in another framework by comparison with DNS results. Finally, in this article, a coupled approach is tested based on IRQ's sensors, to determine locally and dynamically whether or not the interface can be well captured. The following tests, correspond to a validation step, succeeding the previous development phase [21]. Results will be employed for further improvement of the dynamic switching approach of the model i.e., eq. 3.

The test case has been chosen for three reasons: (i) Experimental data are available, about the mean liquid volume fraction in the primary atomization region; (ii) previous numerical studies [15] showed, on the same test case, that RANS turbulence model requires a strong modification to get appropriate results, hence prompted the use of LES models. And finally (iii), liquid Reynolds and gas Weber numbers are relatively low, compared with previous ECN test case, hence more flow regions are expected to be resolved (i.e., with $C_\alpha = 1$). In the near nozzle field, the ICM will effectively capture the surface instabilities and liquid structure detachments. A fine resolution will thus be necessary in the near flow field. In the far field, however, the ELSA method might be able to treat low volume fractions of the liquid that has been atomized and dispersed. The configuration while being turbulent, a Large Eddy Simulation (LES) turbulent model will be employed, to model until certain extent, the small eddies of the flow.

The considered configuration, issued from Stepowski et al. [19], consists of injecting a low-speed liquid through a circular pipe, and a high-speed gas through an annular pipe, into a steady atmosphere. Experimentally, to obtain the near field of liquid volume fraction, α_l , the fluorescence emission of an additional specie, incorporated into the water, induced by a pulsed laser sheet was used [19]. The liquid used is pure water, and ambient gas is considered as dry air, leading to a density ratio of approximately 1000. The sketch of the injector geometry and mesh are presented in the figure 2 below. Geometrical characteristics of the experimental device, are as follows: $D_l = 1.8 \text{ mm}$, $D_g = 3.4 \text{ mm}$, $\Delta = 0.25 \text{ mm}$, $U_g = 115 \text{ m/s}$, $\rho_g = 1.2 \text{ kg/m}^3$, $U_l = 1.3 \text{ m/s}$, $\rho_l = 1000 \text{ kg/m}^3$. The non-dimensional Momentum flux ratio, J , plays an important role in destabilization of the liquid jet, and in the liquid core length, especially in this type of injector. Values of the known characteristic non-dimensional numbers, are reported in the following table:

Table 1. Simulated flow conditions.

$U_g \text{ (m/s)}$	$U_l \text{ (m/s)}$	We_g	Re_g	Re_l	J
115	1.3	500	8000	2600	10

Estimation for the minimal LES mesh resolution, $\Delta_x = 39 \text{ } \mu\text{m}$, based on the Taylor micro-scale and the turbulent length scale at gas nozzle exit, is the one recommended by Addad et al. [23]. Finally, the number of cells at liquid nozzle exit, 48, and the cell size both at liquid and gas nozzles, is $37.5 \text{ } \mu\text{m}$.

Results and discussion

The experimental data available consists of mean liquid volume fraction fields, obtained with 2500 independent samples [19]. In the numerical simulations, mean fields are obtained by averaging within a certain period of time. Consequently, to eliminate the initial transient part, time averaging process was started after 3 liquid advection times,

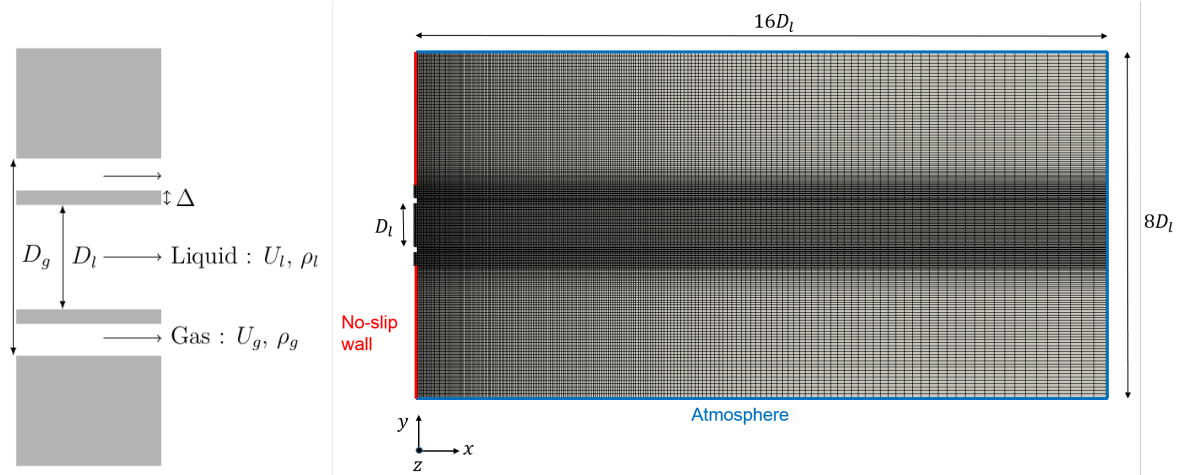


Figure 2. Schematic image of air-blast injector used by Stepowski et al. [19] (left). Dimensions and boundary conditions of the computational domain (right).

tU_l/D_l , that corresponds to 150 gas advection times, tU_g/D_g . Convergence of each simulation, is monitored with evolution of field averaged and variance volume fraction values. Convergence is obtained after 72 liquid advection times, tU_l/D_l , for both mean and variance values. Small fluctuations and variations are still observable at the end of simulations.

Figure 3 exhibits the Liquid Volume Fraction (LVF) averaged (top half of each image) and instantaneous (bottom half of each image) of ELSA [24], ICM, and ICM-ELSA. Mean LVF values of experiments are also displayed (bottom-right of the figure). Dark blue colors (1) represent the liquid and light yellow colors (0), the gas. All four (4) pictures are scaled with the same size. Firstly, the mean LVF values on top-left of the figure for ELSA exposes the diffused interface (LVF values nearly brown), as soon as the liquid is injected into the atmosphere. For ICM (on top-right), the liquid-gas interface is resolved next to nozzle exit, however, after a few diameters axially, some numerical diffusion starts to emerge, due to poor mesh refinement downstream of the flow, as expected. Specifically in the instantaneous field, it is observed that after $3D_l$, approximately, isolated liquid structures, are not correctly captured by the ICM. The iso-contour $\alpha_l = 0.5$ (black continuous line), is a relevant marker of resolved structures. This iso-contour, is absent due to the lack of mesh refinement, that is a source of numerical diffusion. Indeed, ICM is developed on the ideology of capturing the interface and keeping it sharp, which is a physically correct approach, but is limited to cases with high mesh resolution. Therefore, if the mesh is not fine enough, the model produces diffused interface, which is basically numerical diffusion. This is clearly visible on top-right of the figure 3 (instantaneous results), in which there are $0 < \alpha < 1$ values.

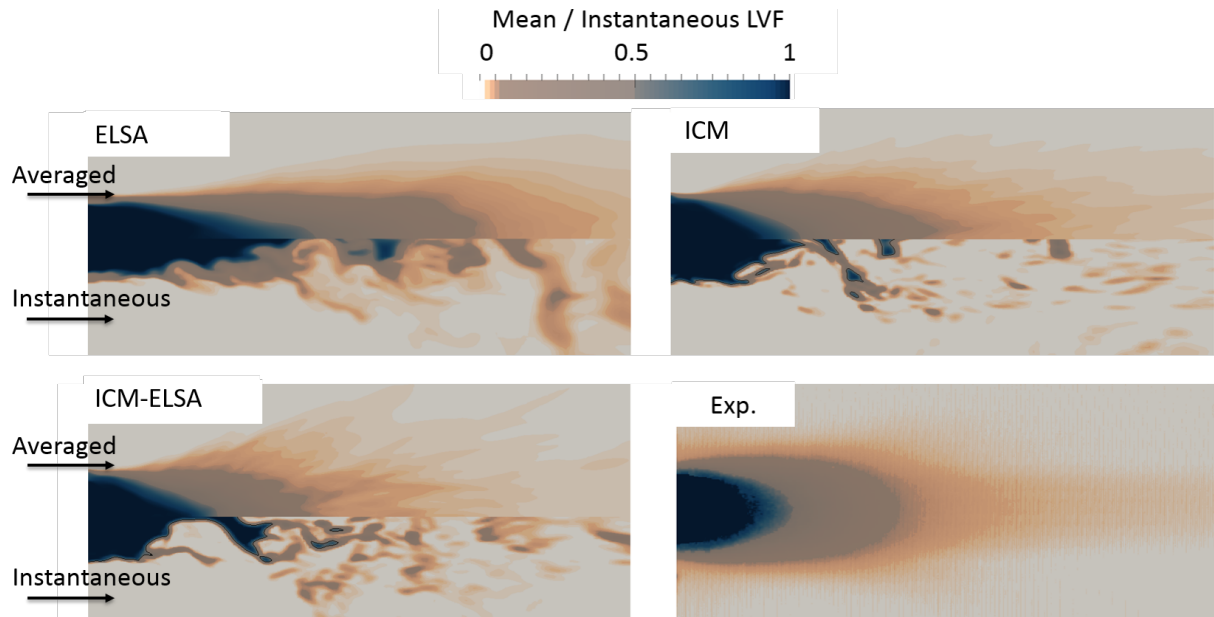


Figure 3. Mean (top half of each image) and instantaneous (bottom half of each image) values of Liquid Volume Fraction (LVF) fields of ELSA [24], ICM, ICM-ELSA. Mean LVF of experiments (bottom-right of the figure).

Further increasing of the mesh resolution (thus reducing the numerical diffusivity) would bring another type of numerical error i.e., an additional surface tension, which is a numerical force that prevents droplets breakup at smaller scales than the cell size, as similarly found in previous validation test case [21]. This type of numerical behavior has to be prevented and replaced by a physical approach. Consequently, ICM-ELSA should give an intermediate result between ICM, near nozzle exit, and ELSA, in the last part of the domain, which is in fact, the expected behavior of the model. Finally, by using ICM-ELSA, the numerical diffusion is replaced by the residual turbulent liquid flux, which is a more physical and preferable subgrid approach. Regarding the averaged LVF values, ELSA is over-predicting the liquid penetration compared with experiments, supposedly due to the inadequate interface modeling resolution approach, next to the nozzle exit. Likewise, ICM-ELSA performs better compared with experiments. Nonetheless, experimental liquid core shape, is here more spherical, due to repeating flapping in radial directions. This shape is not observed with numerical simulations, in which it tends to a conic shape. Insufficient convergence in time may be an explanation. One can expect to catch this shape with a longer period of simulated time. Another explanation may be the influence of the small inner walls before the nozzle exit, with eddies production overestimation injected in the gas flow. Henceforth, it is to be mentioned that ICM results will be omitted for comparison purpose due to the numerical diffusion exhibited in the fig. 3 below, especially from $x/D \geq 1.9$.

Quantitative results are presented in figure 4 by the time-averaged axial profiles of Liquid Volume Fraction (LVF) and compared with line-measured experimental data. In this case, ELSA model is exposed to be unadapted for the air-blast atomizer test case, especially for the primary and secondary atomization zone. Even though a sufficient mesh refinements was employed for all cases (Taylor micro-scale), ELSA axial profiles are far from experimental ones. Indeed, the turbulence in this test case, takes time to destabilize and to provoke detachment of liquid structures. This is mainly the liquid-gas shear layer that promote the liquid dispersion. An additional plausible explication, is that the employed *LES* model, is a single-phase turbulent model, hence is unadapted to modelize small scales of liquid-gas interface. A two-phase *LES* model combined with ELSA model, might be better to correctly predict the liquid core length. This air-blast atomizer test case, is in fact, quite distinct from the ECN test case previously explained [20], in which there is a clear resolution of the liquid-gas interface at the exit of the injector. Therefore, an ICM suitability is then prompted only in the near flow field region, in which the liquid-gas interface can be much better captured than the ECN test case, and then switched it off, when the residual stresses due to mesh resolution, arise. The latter state is exactly what the ICM-ELSA was designed for.

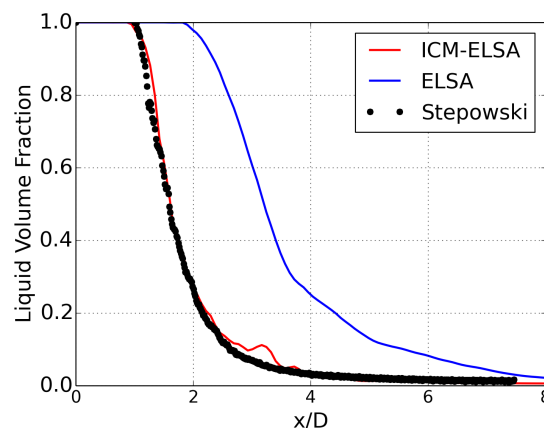


Figure 4. Mean axial values of Liquid Volume Fraction (LVF).

Figure 5 displays the time-averaged radial profiles of LVF for ICM-ELSA, and experiments. Firstly, as expected, ICM-ELSA agrees well with experiments at an axial position $X/D = 1$ (figure on the left). Within this near flow field, is where *ICM* can resolve the small velocity fluctuations i.e., residual stresses would be negligible or very small. However, at $X/D = 1.9$ (figure on the right), regarding ICM-ELSA, in which a physical modeling approach is deployed, in the far field region, the differences with experiments are mainly due to a lack of convergence. Finally, it has been shown by means of a coaxial injector simulation, that the proposed ICM-ELSA model, is capable of both improving results. It has been shown that using a resolved interface model, namely ICM or a fully unresolved model such as ELSA, in the whole domain, provides fairly good agreement with the experiment in the primary atomization region only (up to $X/D \approx 1$). However, in the far field, this model is unadapted upward in the dispersed spray region, as shown in figure 4. It is therefore pertinent in this region to keep a moderate mesh refinement and to switch to a residual or subgrid model, where velocity fluctuations become important.

Conclusions

The present work concerns two approaches to simulate liquid injection system, in flow regimes characterized by high Reynolds and Weber numbers. The focus is on the description of the dense liquid-gas flows, in which the spray

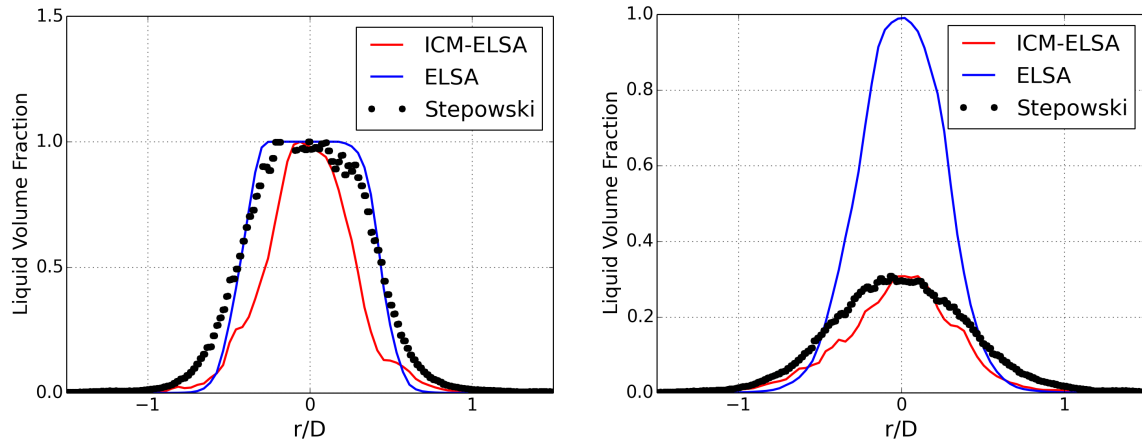


Figure 5. Mean radial values of Liquid Volume Fraction (LVF) at axial position $X/D = 1$ (left), and $X/D = 1.9$ (right), respectively.

is not yet formed. Even though, the area covered by this kind of turbulent liquid-gas flow is often less than a few diameters away from injector nozzle, it is mandatory to address it, to link the inside injector flow to the final spray. It is recognized, that DNS coupled with accurate ICM approaches, are very valuable and accurate tools to describe this flow, as soon as the mesh resolution is sufficient. This requires that the subgrid turbulent liquid flux could be neglected. It is also important to recognize that in many practical applications, such level of mesh refinement is not affordable and physical models, able to represent the subgrid liquid dispersion, are expected. Since the work of Vallet and Borghi [2], the so-called ELSA model, have been designed for this purpose. On the other hand, the proposed dynamical model i.e., eq. 3, is thus able to take advantage of a full-interface resolution, to recover a DNS formulation with ICM, and to switch to a diffusive (residual or sub-grid) LES approach, only when necessary. A particular numerical test was assessed, namely Air-blast atomizer test case. Hence, the above solver ICM-ELSA was applied to predict the primary breakup of a single cylindrical liquid jet. The test case has been chosen for three main reasons: (i) Experimental data are available, about the mean liquid volume fraction in the primary atomization region; (ii) previous numerical studies [15] showed, on the same test case, that RANS turbulence model were unsuitable, which required a strong modification in the turbulence model to get appropriate results, hence prompted the use of LES models. And finally (iii), liquid Reynolds and gas Weber numbers are less, compared with the previous ECN Spray-A test case, hence more flow regions are expected to be resolved. It has been found, in the near nozzle field, the ICM effectively captured the surface instabilities and liquid structure detachments. A fine resolution was necessary in the near flow field. Nevertheless, in the far field, the ELSA was able to treat low volume fractions of the liquid that has been atomized and dispersed. This particular test case showed the importance or resolved interface approaches such as (ICM), when dealing with moderate liquid Reynolds and gas Weber numbers. On the contrary, the ECN Spray-A test case, displayed highly turbulence flow inside the nozzle that atomized rapidly the liquid. Therefore, the unresolved interface approach such ELSA was more suitable for this case. More importantly, the proposed multi-scale solver ICM-ELSA was able to dynamically adapt to those interface-subgrid instabilities.

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Nomenclature

U	Mixture velocity [m/s]
p	Mixture pressure [Pa]
α_l	Liquid volume fraction (LVF)
R_U	Reynolds stress tensor
R_{α_l}	Turbulent liquid flux
Sc_t	Turbulent Schmidt number
\bar{U}_l, \bar{U}_g	Mean liquid, gas velocities [m/s]
Σ	Interface Surface density [1/s]
ρ_l	Liquid density [m^3/s]
ρ_g	Gas density [m^3/s]
τ_r	Subgrid Stress tensor
Re	Reynolds number
We	Weber number
IRQ	Interface Resolution Quality
ICM	Interface Capturing Method
DNS	Direct Numerical Simulation

<i>ELSA</i>	Euler-Lagrange Spray Atomization
<i>QME</i>	Quasi–Multiphase Eulerian model
<i>RANS</i>	Reynolds-Averaged Navier-Stoke
<i>LES</i>	Large Eddy Simulation
<i>LVF</i>	Liquid Volume Fraction
<i>J</i>	Momentum flux ratio

References

- [1] R. Lebas, T. Menard, P. Beau, A. Berlemont, and F.X. Demoulin. Numerical simulation of primary break-up and atomization: Dns and modelling study. *International Journal of Multiphase Flow*, 35(3):247–260, 2009.
- [2] A. Vallet and R. Borghi. Modélisation eulerienne de l'atomisation d'un jet liquide. *Comptes Rendus de l'Académie des Sciences-Series IIB-Mechanics-Physics-Astronomy*, 327(10):1015–1020, 1999.
- [3] Antonio Andreini, Cosimo Bianchini, Stefano Puggelli, and FX Demoulin. Development of a turbulent liquid flux model for eulerian–eulerian multiphase flow simulations. *International Journal of Multiphase Flow*, 81:88–103, 2016.
- [4] Mark Sussman, Peter Smereka, and Stanley Osher. A level set approach for computing solutions to incompressible two-phase flow. *Journal of Computational physics*, 114(1):146–159, 1994.
- [5] Ronald P Fedkiw, Tariq Aslam, Barry Merriman, and Stanley Osher. A non-oscillatory eulerian approach to interfaces in multimaterial flows (the ghost fluid method). *Journal of computational physics*, 152(2):457–492, 1999.
- [6] Henk Kaarle Versteeg and Weeratunge Malalasekera. *An introduction to computational fluid dynamics: the finite volume method*. Pearson Education, 2007.
- [7] B Duret, J Reveillon, T Menard, and FX Demoulin. Improving primary atomization modeling through dns of two-phase flows. *International Journal of Multiphase Flow*, 55:130–137, 2013.
- [8] Fabian Denner, Duncan R van der Heul, Guido T Oud, Millena M Villar, Aristeu da Silveira Neto, and Berend GM van Wachem. Comparative study of mass-conserving interface capturing frameworks for two-phase flows with surface tension. *International Journal of Multiphase Flow*, 61:37–47, 2014.
- [9] Thibault Ménard, Sebastien Tanguy, and Alain Berlemont. Coupling level set/vof/ghost fluid methods: Validation and application to 3d simulation of the primary break-up of a liquid jet. *International Journal of Multiphase Flow*, 33(5):510–524, 2007.
- [10] Johan Roenby, Henrik Bredmose, and Hrvoje Jasak. A computational method for sharp interface advection. *Royal Society Open Science*, 3(11):160405, 2016.
- [11] Kent E Wardle and Henry G Weller. Hybrid multiphase cfd solver for coupled dispersed/segregated flows in liquid-liquid extraction. *International Journal of Chemical Engineering*, 2013, 2013.
- [12] HG Weller. A new approach to vof-based interface capturing methods for incompressible and compressible flow. *OpenCFD Ltd., Report TR/HGW/04*, 2008.
- [13] F Raees, DR Van der Heul, and Cornelis Vuik. Evaluation of the interface-capturing algorithm of OpenFOAM for the simulation of incompressible immiscible two-phase flow. Technical report, Delft University of Technology, Faculty of Electrical Engineering, Mathematics and Computer Science, Delft Institute of Applied Mathematics, 2011.
- [14] Chesnel. *Simulation aux Grandes Échelles de l'Atomisation, Application à l'Injection Automobile*. PhD thesis, University of Rouen, 2010.
- [15] Francois-Xavier Demoulin, Pierre-Arnaud Beau, Gregory Blokkeel, Arnaud Mura, and Roland Borghi. A new model for turbulent flows with large density fluctuations: Application to liquid atomization. *Atomization and Sprays*, 17(4), 2007.
- [16] Francois-Xavier Demoulin, Julien Reveillon, Bernard Duret, Zakaria Bouali, Philippe Desjonquieres, and Thibaut Menard. Toward using direct numerical simulation to improve primary break-up modeling. *Atomization and Sprays*, 23(11), 2013.
- [17] Nicolas Hecht. *Simulation aux grandes échelles des écoulements liquide-gaz : application à l'atomisation*. PhD thesis, University of Rouen, 2014.
- [18] F. A. Williams. Spray combustion and atomization. *Physics of Fluids*, 1(6):541–545, 1958.
- [19] D Stepowski and O Werquin. Measurement of the liquid volume fraction and its statistical distribution in the near development field of a spray. *Atomization and Sprays*, 14(3), 2004.
- [20] Engine Combustion Network. <https://ecn.sandia.gov/>. [cit. 2018-01-14].
- [21] J Anez, A Ahmed, N Hecht, B Duret, J Reveillon, and FX Demoulin. Eulerian–lagrangian spray atomization model coupled with interface capturing method for diesel injectors. *International Journal of Multiphase Flow*, 2018.
- [22] JM Desantes, JM García-Oliver, JM Pastor, A Pandal, E Baldwin, and DP Schmidt. Coupled/decoupled spray simulation comparison of the ecn spray a condition with the σ -y eulerian atomization model. *International Journal of Multiphase Flow*, 80:89–99, 2016.
- [23] Yacine Addad, Ulka Gaitonde, Dominique Laurence, and Stefano Rolfo. Optimal unstructured meshing for large eddy simulations. In *Quality and reliability of large-eddy simulations*, pages 93–103. Springer, 2008.
- [24] Felix Dabonneville. *Development of a multi-approach and multi-scale numerical method applied to atomization*. PhD thesis, Normandie Université, 2018.