# LES of atomization: From the resolved liquid surface to the subgrid scale spray

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**Abstract**

The first objective of this work is to use a Level set DNS database dedicated to the atomization of a turbulent liquid jet to characterise the small structure contribution (SGS terms) on the transport equations. Additionally SGS models are compared to their exact counter parts. Data are extracted from a DNS of a liquid jet performed by Berlemont [1]. In this framework, the evaluation of existing subgrid model shows that the scale similarity model reproduces correctly the SGS fluctuations.
In a second part, a LES model for atomization is detailed. Application of this method to the atomization of a Diesel jet is presented. LES results are then compared to a DNS data base which has been obtained on the same configuration [2, 1].

## Introduction

Liquid injection takes an important part in many physical processes. For instance, in internal combustion engines (ICE) new direct injection strategies are used to control the flow inside the combustion chamber. It follows that injector manufacturers propose more and more performing injection systems. Parameters and geometries become numerous then to characterize. In order to evaluate and use these new generation of injectors, accurate numerical tools are expected. Up to know the RANS (Reynolds Averaged Navier-Stokes) approach has been widely used, both in Eulerian and Lagrangian frameworks. Several works [2, 3] have been developed in our team to represent, in a realistic manner, the dense part of the spray in order to capture the details of the flow at the exit of the injector. One of the advantages is the possibility to use directly a simulation of the flow inside the injector to initiate the computation of the final spray. However, in one hand computations of injection process are often non stationary RANS while in the other hand LES simulations in single phase flows are known to be more accurate than RANS. Then naturally LES of atomization seems to be a necessarily step forward.
Characteristics of LES are there ability to treat realistic situations beyond those than can be computed directly with DNS (Direct Numerical Simulation). Inversely when the available mesh is fine enough, it is expected that LES tends to DNS results. Atomization or more generally liquid-gas flows are characterized by a special treatment of the interface where jumps of variable such as density can occur. And this is also where the surface tension forces take place. In addition of the special care on the transport equations when dealing with LES formalism, a special attention is necessarily to represent the interface. Two limit cases may happen:

- The liquid surface can be well captured with the available mesh size (or filter size) and the LES formulation must recover the DNS methods used to track the interface (Level Set, VOF…)
- The liquid surface wrinkles are below the mesh size and the two-phase LES formulation must recover the LES used for spray flows where finally droplets are considered very small by comparison to the mesh size.

Previous LES simulations of atomization are only able to represent the first limit [4]. In this work we present a possible LES method for two phase flows that can reach dynamically and continuously these two limits. It is shown that the unresolved SGS (Sub Gris Scale) term that appears in the phase function equation plays an important role. Even if it is very small by comparison to the resolved contribution [5].

## Filtered transport equations

In order to obtain the LES transport equations a convolution operation must be applied on the classical Navier-Stokes equations. By applying the filtering operation on the transport equations of the two-phase flow, the LES transport equations are obtained :

- Continuity : $\frac{\partial \overline{U}_i}{\partial x_i} = 0$ (1)
- Phase function : $\frac{\partial \overline{\phi}}{\partial t} + \frac{\partial \overline{U}_j \overline{\phi}}{\partial x_j} + \frac{\partial \tau_{interf\_j}}{\partial x_j} = 0$ (2)
- Momentum : $\frac{\partial \overline{\rho}\,\overline{U}_i + \tau_{temp\_i}}{\partial t} + \frac{\partial \overline{\rho}\,\overline{U}_i \overline{U}_j + \tau_{conv\_ij}}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} +$

$$\frac{\partial}{\partial x_j}\left(\overline{\mu}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_j}\right) + \tau_{diff\_ij}\right) - \tau_{superf\_i} \quad (3)$$

With the following unclosed SGS terms:

$$\tau_{interf\_i} = \overline{U_i \phi} - \overline{U}_i \overline{\phi} \quad (4)$$

$$\tau_{conv\_ij} = \overline{\rho U_i U_j} - \overline{\rho}\,\overline{U}_i \overline{U}_j \quad (5)$$

$$\tau_{temp\_i} = \overline{\rho U_i} - \overline{\rho}\,\overline{U}_i \quad (6)$$

$$\tau_{diff\_ij} = \overline{\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)} - \overline{\mu}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) \quad (7)$$

$$\tau_{superf\_i} = \overline{\sigma \kappa n_i \partial} \quad (8)$$

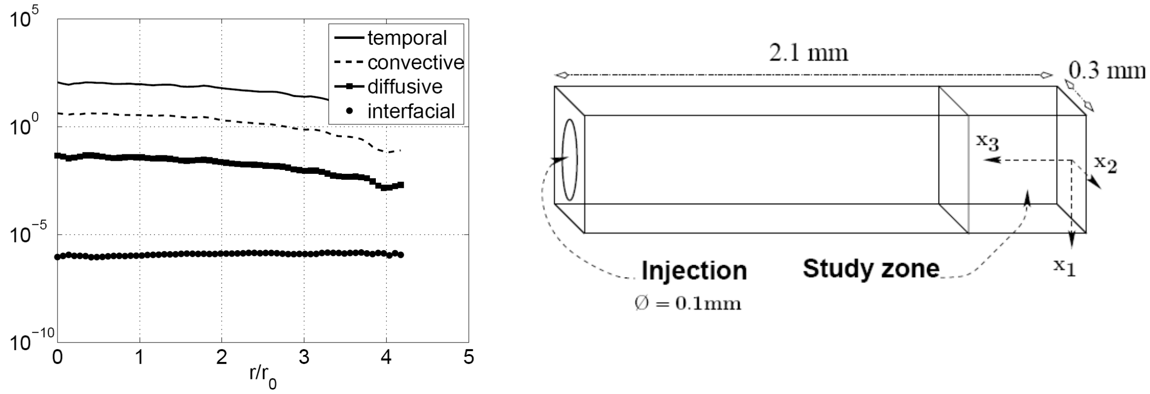
**SGS terms sorting and *a priori* tests**

To carry out our *a priori* tests, we used the results of a DNS of liquid jet primary atomisation conducted by Berlemont *et al* [1]. This simulation solves directly the equations of mass momentum and one transport equation for the phase function (Level-set and VOF). Discontinuities are taken into account with the ghost fluid method. The total grid is 256x256x2048, the computational domain can be se on figure 1(b). Considering the cylindrical geometry of the problem, it is possible to average each term (5), (6), (7) and (8) at radius r in order to sort the SGS terms.

On figures 1(a) the relative dimensionless SGS budget contribution to the streamwise momentum equation against $r/r_0$, with $r_0$ the jet injection radius, since the two other direction gives almost the same result, one can notices that:

$$\frac{\partial \tau_{temp\_i}}{\partial t} > \frac{\partial \tau_{conv\_ij}}{\partial x_j} >> \frac{\partial \tau_{diff\_ij}}{\partial x_j} >> \tau_{superf\_i}$$

According to this result, the diffusion term $\tau_{diff\_ij}$ and superficial term $\tau_{super\_i}$ are neglected in this type of configuration. As a result only the temporal term $\tau_{temp\_i}$ and convective term $\tau_{conv\_ij}$ SGS modelling are addressed here.




(a) (b)

**Figure 1 :** Dimensionless Streamwise momentum, semi-log scale (a), computational domain (b).

**Modeling**

As we saw in the preceding sections, when filtering the transport equations, unclosed subgrid terms appear. These terms have to be modelled to reproduce the subgrid phenomena. The subgrid modelling panorama is nowadays well extended. The first model was suggested by Smagorinsky [6]. Major improvement made recently by Germano [7] and modified by Lilly [8] gives good results when compared with experimentations or DNS in monophasic flows. The tests we have conducted with the Smagorinsky/Lilly model have not lead to a good approximation. In this paper the scale similarity model is tested in the particular case of primary atomization.

**Scale similarity model**

The model proposes to use only the Leonard [9] term $Lij$ in order to models the SGS terms. The SGS terms models are for the phase function and the velocity:

$$\tau^{model}_{interf\_i} = \overline{\overline{U}_i\overline{\phi}} - \overline{\overline{U}}_i\overline{\overline{\phi}} \quad (9)$$

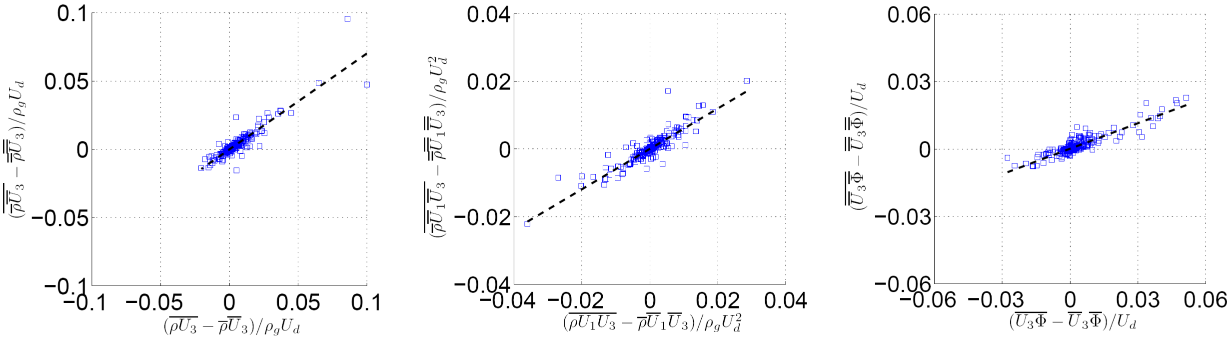
$$\tau^{model}_{conv\_ij} = \overline{\overline{\rho}\,\overline{U}_i\overline{U}_j} - \overline{\overline{\rho}}\,\overline{\overline{U}}_i\overline{\overline{U}}_j \quad (10)$$

$$\tau^{model}_{temp\_i} = \overline{\overline{\rho}\,\overline{U}_i} - \overline{\overline{\rho}}\,\overline{\overline{U}}_i \quad (11)$$

**A priori tests**

The models presented in the theoretical part is being tested here by using the a priori test of the liquid jet DNS. The goal of this part is to estimate if the presented SGS model is sufficient and convenient in the case of LES liquid atomisation. So, to carry out the tests, the filtering operation is applied to extract the exact value of the SGS terms. They are compared with the computed models terms i.e. equations (9), (10) and (11). Tests are carried out far from the inlet of the liquid jet as shown on figure 1(b). The results are presented as scatter plots allowing to compare SGS contribution from against the models.

Figures 2(c) confirm the potentiality of the model to represent the $\tau_{interf\_i}$ of the phase function equation. The figures 2(a) show the correlation between $\tau^{exact}_{temp\_3}$ and $\tau^{model}_{temp\_3}$ for $\overline{\Delta} = 5\delta_x$. The models are well suited to represents these SGS terms, since the scatter point are distributed around line plotted in these graphs. Concerning the $\tau^{model}_{conv\_13}$ term this is almost the same result, figure 2(b). The model well reproduces the real SGS terms.




(a) (b) (c)

**Figure 2 :** Comparison between exact terms vs. modeled terms for $\tau_{temp\_3}$ (a), $\tau_{conv\_13}$ (b) and $\tau_{interf\_3}$ (c).

**LES model for atomization**

The aim of the model is resumed on the figure 3. The idea is to use method dedicated to interface tracking when the interface is well resolved i.e. when the interface length scales are captured by the mesh size (near the injector nozzle on figure 3). In the dilute phase (on the right, figure 3), where appear droplets which diameters are under the mesh size, the model slip gently to a continuous vision. Indeed, the interface tracking methods like VOF does not provide information on the subgrid spray since these schemes are made to be non-diffusive. So we propose to solve the equation (2) for $\overline{\Phi}$ with the associated SGS terms.

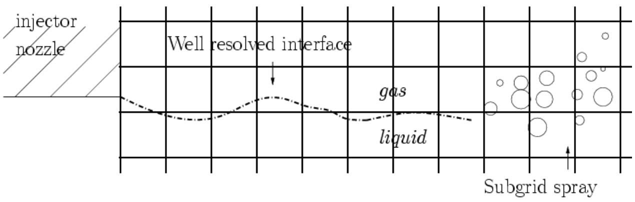



**Figure 3 :** Scheme of a liquid injection process on the calculation mesh.

The liquid volume fraction $\overline{\Phi}$ is not sufficient to well describe the subgrid spray. Indeed this variable doesn't give any information about the size of the liquid parcels. In order to circumvent this problem, the model uses the interface density, which allows obtaining more information on the spray. The interface density is defined to be the quantity of interface within a calculation cell, such as:

$$\Sigma = S_{\text{int}} / V_{cell}$$

With $S_{\text{int}}$ the interface surface in a cell and $V_{cell}$ the volume of this one. The idea is to use a regular form (postulated) of the surface density transport equation proposed initially by Valet *et al* [10]. This equation can be written:

$$\frac{\partial \overline{\Sigma}}{\partial t} + \frac{\partial \overline{U}_j \overline{\Sigma}}{\partial x_j} = -\frac{\partial \overline{U_j \Sigma} - \overline{U}_j \overline{\Sigma}}{\partial x_j} + \dot{\Sigma} + S_{\Sigma \min} \quad (12)$$

Where $\dot{\Sigma}$ is a source term of creation or destruction of interface, due to breakup and coalescence process for examples. One can obtain from the Reitz [11] model modified by Iyer and Abraham [12] and Lebas *et al* [2, 3], the difference between the surface velocity and the mixture velocity is represented thanks to a diffusive process.

$$\frac{\partial \overline{U}_j - \overline{U_j \Sigma}}{\partial x_j} = \frac{\partial}{\partial x_j}(D_\Sigma \frac{\partial \Sigma}{\partial x_j})$$

$$\dot{\Sigma} = \frac{\overline{\Sigma}}{\tau_t}(1 - \frac{\overline{\Sigma}}{\Sigma_{crit}})$$

$\Sigma_{crit}$ is the surface density corresponding to a critical stable droplet diameter $D_{crit}$ and $\tau_t$ a classical breakup time. This critical stable state is obtained when the order of local Weber number is the unity. This last assumption leads to:

$$\Sigma_{crit} = \frac{\overline{\rho}\tilde{k}}{\sigma_{\lg}}$$

$S_{\Sigma \min}$ in the equation (12) is an initialization source term. Beau *et al* [3] proposed to use:

$$\frac{D_t}{l_\Sigma}\frac{\partial \overline{\Phi}}{\partial x_i}\frac{\partial \overline{\Phi}}{\partial x_i}$$

**Model results**

On figure 4, the $\overline{\Phi}$ scalar field with iso-line $\overline{\Phi} = 0.5$ is plotted. Near the injection it appears deformation of the interface which length scale bigger than $\overline{\Delta}$, here level-set-VOF [1] method is applied. Far from the injector nozzle $\overline{\Phi}$ is diffused in accordance with the model for $\tau_{\mathrm{int}\,erf\_i}$. In this zone subgrid spray appears, the droplets diameter is under the cells size. The liquid volume fraction allows to get the spray angle or moreover the penetration length to be recovered. The figure 5 shows the droplet size diameter D32 in the dilute zone directly calculated from the interface density. It is possible to see the initial deformation of the interface leading to the formation of droplets near this one. As the liquid core penetrates the resolved liquid vanished into smaller droplets (into subgrid spray). With the use of interface density we can access to the D32 diameter in the dilute phase. It is also possible to get the droplet size distribution from this field.

**Conclusion**

An overview if the filtered the two-phase equations exhibit the SGS terms for the phase function transport equation and momentum equation. Specific SGS terms related to multiphasic flows have been discussed. Closure based on classical models used in monophasic LES have been tested. The “scale similarity” SGS models have been tested thanks to an *a priori* procedure by using instantaneous fields resulting from a liquid jet primary atomisation DNS. The real contributions extracted from the DNS have been compared to the models for temporal, convective and interfacial SGS term. The results showed that the similarity scale model reproduces correctly the SGS terms for the temporal term, convective term and phase function term.

In a second part we have developed an LES formulation suitable for atomization. This model is based on two visions, discontinuous when the interface scales are resolved at the mesh size and continuous vision when the spray scales fall under the filter resolution. We have demonstrated the feasibility of our method by implementing this method on a LES solver. This model allows us to obtain several information about the geometry of the problem since the LES solve the largest scales of the flows with the use of interface density transport equation. It is also possible to obtain the droplets diameter, size distribution and repartition of the liquid in the domain.

For the perspectives the first step is to quantitatively validate our method compared with the DNS database for liquid atomisation. Further work would concern the evaporation and the combustion of the spray.

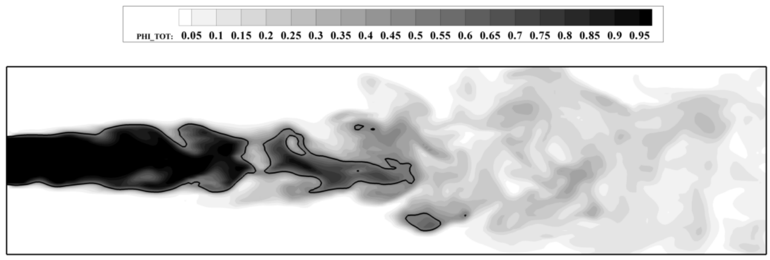



**Figure 4 :** $\overline{\Phi}$ , scalar field in the injection direction, iso-line $\overline{\Phi} = 0.5$

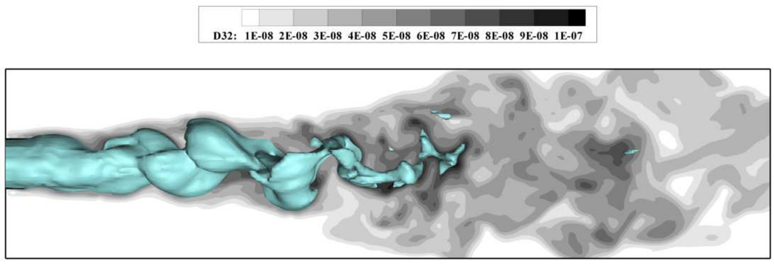



**Figure 5 : D32 droplet diameter obtained from interface density.**

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