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SUBGRID MODELLING OF LIQUID ATOMIZATION

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ABSTRACT

The recent advances of large eddy simulation (LES) and interface tracking methods, such as volume of fluid (VOF) or level set, are promising for the development of a numerical tool for atomisation if they are associated. However, if LES is largely developed and utilised nowadays with monophasic or dispersed flows, its extension to atomisation is still recent ands leads to many difficulties. The LES formalism induces subgrid scale (SGS) terms which appear on the transport equations. For liquid Gas flow specific SGS terms appear due to the physical property jump between liquid and gas phase at the interface. So the 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], which combines two interface tracking methods: Level-Set to reconstruct easily the interface and VOF to conserve liquid mass. Thanks to the fine grid mesh, a filter width characteristic size, realistic for LES, is applied carry out *a priori* estimations of the SGS contributions to the momentum and VOF/Level-Set fields. In this framework, the evaluation of existing subgrid model shows that the scale similarity model reproduces correctly the SGS fluctuations.

INTRODUCTION

Background

Injection of liquid fuel in the combustion chamber of automobile engines is a fundamental process that plays a major role from spray formation to mixture combustion.

It is necessary to control the atomisation process to develop efficient engines in good agreement with actual pollution and economical constraints.

Many experimental and numerical studies have been dedicated to the analysis of spray formation and droplets tracking. However, the understanding and the prediction of the primary atomisation process is still an open field.

There is a lack of knowledge concerning liquid jet topology and its interactions with the surrounding turbulent field leading to the spray formation. Complex interactions between both liquid and gas phases, the presence of an interface and the difficulties to carry out measurements close to the injector explain the difficulty to obtain detailed experimental results of this complex configuration.

A possible way is to use numerical simulations that are detailed enough to capture the interface properties and behaviour.

In this framework, direct numerical simulations (DNS) may be useful. Indeed, DNS resolves all the scales of the flow. When one-phase flows are considered, if accurate numerical methods are used, DNS is considered to be exact although it is limited to small turbulent Reynolds numbers because of its expensive computational cost. In the case of two-phase flows, some numerical models may be added to the DNS solver to take into account the presence of an interface.

However, a skyrocketing numerical cost forbids the complete simulation of any automobile injector although encouraging progresses were made recently [1].

Large Eddy Simulation (LES) seems to be a promising way between industrial codes (mainly RANS) and academic codes (rather DNS). Indeed, LES solves only the largest scales of the flow and thus, it take into account the major unstationnary effects. Considering that the behaviour of the smallest scales is relatively independent, only the low frequency part (largest scales) of the turbulent field is simulated, the higher frequency (small scales) contribution being modelled through subgrid scales (SGS) models.

The objective of this work is to use *a priori* test to estimate and to quantify the subgrid contributions to use to envision a complete LES of primary atomisation of a diesel liquid jet.

State of Art

During the last decade LES underwent a strong development, in particular with the Smagorinsky works [2] and the improvement made by Germano et al. [3][14] and Lilly [4] with the introduction of the dynamic models. However, even if LES is largely developed in monophasic cases, its extension to two phase flows is not so simple or validated In particular in the case of primary atomisation. Its implementation requires the use of SGS terms because only the largest scales of turbulence are indeed simulated. These terms have to be modelled to completely solve the flow. Several difficulties appear, because of the implicit filtering due to the LES formalism: new SGS terms appear in regards with the two-phase aspect.

Most LES works related to atomisation process are done in dispersed phases, where only one phase is actually solved. Many other works are related to the study of the free surfaces computation in particular for the study of breaking waves process, [5][6][7] or of bubbling process [8]. Toutant *et al.* [9][10] propose an estimation and a closure of the SGS terms for droplets tracking. Thank to the fact that their LES grid is fine, this one describe all the interface inclusions (e.g. the

smaller). Most simulation does not take into account the surface tension effects regarding to the simulation scales. Concerning primary atomisation, Gosman *et al* [11] conducted in 2004 a LES by using a VOF method. They used the continuum surface force method of Brackbill [12] to calculate the surface tension forces from VOF function. However, the SGS surface tension forces are neglected in this simulation. The authors think that this fact can be justified because of the high Weber number of the turbulent jet and thanks to the relative fine mesh, which minimises the subgrid contribution.

Objectives

It appears that the recent advances in LES and interface tracking methods could lead to a very effective and rapid tool if both methods were coupled. The main objective of this work is to use Level-Set/VOF DNS data of the atomisation of a turbulent liquid jet in order to characterise the SGS contribution of the small structures to the total amount.
Data are issued from a DNS performed by Berlemont *et al* [1] that combines two interface tracking methods: namely Level-Set, which allows precise interface reconstruction and VOF, to guarantee mass conservation.
Finally this DNS uses the Ghost Fluid method initiates by Fedkiw *et al* [13] to consider jumps across the liquid/gas interface.
Considering that the mesh size of the DNS is fine enough to describe all the significant scales of the flow, it becomes possible to extract the exact SGS contribution with *a priori* tests (for momentum and phase function balance equations) and then compare this real DNS contributions with models.
In this study we propose an evaluation of the classical "scale similarity" subgrid models used in LES.
Applying the filtering operation to these equations allows us to point out the SGS terms. Eventually, "scale similarity" SGS models are evaluated for interfacial, temporal and convective terms in the case of primary atomization.

NOMENCLATURE

Symbols	*Units*	*Signification*
P	Nm^{-2}	Pressure
U_i	ms^{-1}	Velocity (i^{th} direction)
L_{ij}		Leonard tensor
Φ		Phase function
ρ	$k_g m^{-3}$	Density
ν	$m^2 s^{-1}$	Kinematic viscosity
μ	$k_g m s^{-1}$	Dynamic viscosity
σ	Nm^{-1}	Surface tension coefficient
κ	m^{-1}	Local surface curvatare
δ		Dirac delta function
$\overline{\Delta}$	m	Filter length
Operator		
$\nabla\cdot$		Gradient
$\bar{\cdot}$		Filtering operation (implicit level)

NUMERICAL CONSIDERATIONS

DNS and injection configuration

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 is schematized in figure 4 where the dimensions and configuration of the domain are given. Figure 1 and 2 present a visualisation of the jet (iso-ϕ=0.5 on fig. 1). *A priori* tests are carried out in the study zone presented in figure 4 where the turbulence is well developed.
The table 1 shows physical parameters of the simulation.

parameter	**symbol**	**value**
gaz density	$\rho_g(kg.m^{-3})$	25
liquid density	$\rho_g(kg.m^{-3})$	696
gaz viscosity	$\mu_g(kg.m^{-1}s^{-1})$	$1.\text{x}10^{-5}$
liquid viscosity	$\mu_l(kg.m^{-1}s^{-1})$	$1.18\text{x}10^{-3}$
surface tension	$\sigma(N.m^{-1})$	0.06
jet diameter	$D(\mu m)$	100
debitant velocity	$U_d(m.s^{-1})$	79
liquid Renolds	Re_l	4659
liquid Weber	We_l	7239
turbulence intensity	$\overline{u'u'}/U^2$	0.05
characteristic turbulence scale	$L_t(m)$	$0.1D$

Table 1 : DNS configuration, physical properties.

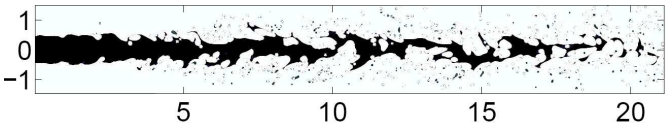

Figure 1 : Planar cut of theVOF field along injection direction.

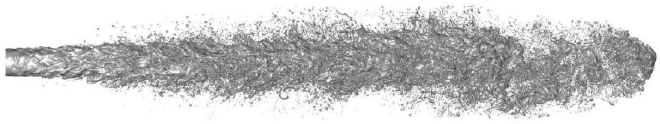

Figure 2 : Instantaneous image of the DNS of the liquid jet.

Equations

The approach used in the case of the DNS is known as monofluid, i.e. the two-phase flow is treated like a continuous flow field with variable density ρ and viscosity μ, which can be discontinuous through interface.
This approach allows using only one set of equations for all the flow. The interface is then considered as a discontinuity surface. The assumptions used for this simulation are:

- non compressible in each phase,
- ρ and μ constant in each phase,
- isothermal flow,

- no evaporation.

The continuity and momentum monofluid transport equation may be written.

Transport equations

- Continuity

$$\frac{\partial U_i}{\partial x_i} = 0 \quad , \tag{1}$$

- Phase function

$$\frac{\partial \phi}{\partial t} + U_j \frac{\partial \phi}{\partial x_j} = 0 \quad , \tag{2}$$

- Momentum

$$\begin{aligned} &\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \dots \\ &\frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_j}\right)\right) - \sigma \kappa n_i \delta \end{aligned} \tag{3}$$

Filtering operation

In order to conduct *a priori* testing it is necessary to apply a filtering operation on the various transport equations (1), (2) and (3), which are filtered according to a classical convolution operation.

Let G be the filter function and A, a fluctuating field, $\overline{A}$ is then defined by:

$$\overline{A} = \int_{\Omega} A(x') G(x - x', \overline{\Delta}) dx' \ . \tag{4}$$

The selected filter is a top hat filter. The filter size is symbolised by $\overline{\Delta}$. According to equation (4) this operation is reduced to a convolution of turbulent signal.

We used the same filter size along each direction: $\overline{\Delta_x} = \overline{\Delta_y} = \overline{\Delta_z}$

Filtered transport equations

By applying the filtering operation on the transport equations of the two-phase flow, the LES transport equations are obtained.

- Continuity

$$\frac{\partial \overline{U}_i}{\partial x_i} = 0 \quad , \tag{5}$$

- Phase function

$$\frac{\partial \overline{\phi}}{\partial t} + \frac{\partial \overline{U}_j \overline{\phi}}{\partial x_j} + \frac{\partial \tau_{\text{int}erf\_j}}{\partial x_j} = 0 \quad , \tag{6}$$

- Momentum

$$\begin{aligned} &\frac{\partial \overline{\rho}\overline{U}_i + \tau_{temp\_i}}{\partial t} + \frac{\partial \overline{\rho}\overline{U}_i \overline{U}_j + \tau_{conv\_ij}}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \dots \\ &\frac{\partial}{\partial x_j}\left(\overline{\mu}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_j}\right) + \tau_{diff\_ij}\right) - \sigma \overline{\kappa} \overline{n}_i \overline{\delta} - \tau_{\text{sup}erf\_i} \end{aligned} \tag{7}$$

With the following unclosed SGS terms:

$$\tau_{\text{int}erf\_i} = \overline{U_i \phi} - \overline{U}_i \overline{\phi} \quad , \tag{8}$$

$$\tau_{conv\_ij} = \overline{\rho U_i U_j} - \overline{\rho}\overline{U}_i \overline{U}_j \quad , \tag{9}$$

$$\tau_{temp\_i} = \overline{\rho U_i} - \overline{\rho}\overline{U}_i \quad , \tag{10}$$

$$\tau_{diff\_ij} = \overline{\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)} - \overline{\mu}\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) \quad , \tag{11}$$

$$\tau_{\text{sup}erf\_i} = \overline{\sigma \kappa n_i \partial} - \sigma \overline{\kappa} \overline{n}_i \overline{\partial} \ . \tag{12}$$

SGS terms sorting

Considering the cylindrical geometry of the problem, it is possible to average each term (11), (12), (13) and (14) at radius r in order to sort the SGS terms.

On figures 3 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 :

$$\frac{\partial \tau_{temp\_i}}{\partial t} > \frac{\partial \tau_{conv\_ij}}{\partial x_j} >> \frac{\partial \tau_{diff\_ij}}{\partial x_j} >> \tau_{\text{sup}erf\_i}$$

According to this result, the diffusion term τ_{diff_ij} and superficial term $\tau_{\text{sup}er\_i}$ are neglected in this type of configuration. As a result only the temporal term τ_{temp_i} and convective term τ_{conv_ij} need SGS modelling.

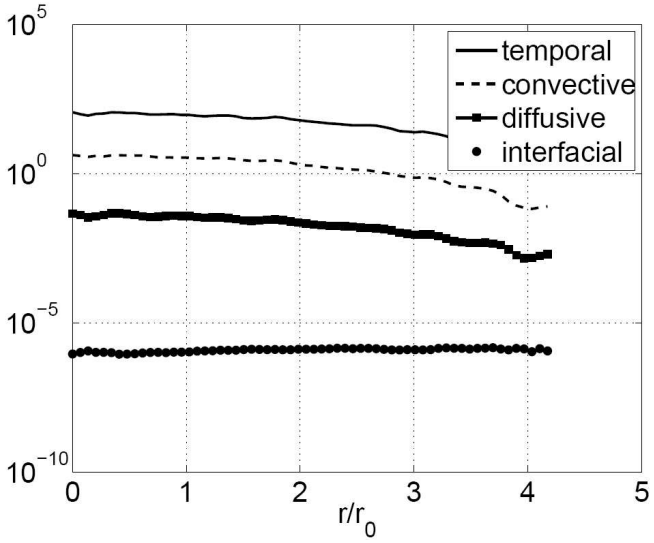

Figure 3 : Dimensionless Streamwise momentum, semilog scale.

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 [2]. Major improvement made recently by Germano [3] and modified by Lilly [4] gives good results when compared with experimentations or DNS in monophasic flows.
The tests we had conduct with the Smagorinsky/Lilly model did not entirely satisfy us in the case of primary atomization.
Another way is to use scale similarity assumption as Bardina modelling. More recent models combine the Smagorinsky model and scale similarity model. These models are named mixed models.
In this paper the scale similarity model is tested in the particular case of primary atomization.
In this section the model is developed for τ_{conv_ij} since the other terms can be obtained in the same manner.

Scale similarity model

Considering $\tau_{conv\_i} = \overline{\rho U_i U_j} - \overline{\rho U}_i \overline{U}_j$, the Leonard decomposition can be written [14]:

$$\tau_{conv\_ij} = Lij + Cij + Rij \quad , \tag{13}$$

With:

$$Lij = \overline{\overline{\rho U}_i \overline{U}_j} - \overline{\overline{\rho U}}_i \overline{\overline{U}}_j \quad ,$$

$$Cij = \overline{\rho' \overline{U}_i \overline{U}_j} - \overline{\rho' \overline{U}}_i \overline{\overline{U}}_j + \overline{\rho' U'_i \overline{U}_j} - \overline{\rho' U'}_i \overline{\overline{U}}_j + \ldots$$
$$\overline{\overline{\rho U}_i \overline{U}_j} - \overline{\overline{\rho U}}_i \overline{\overline{U}}_j + \overline{\rho' \overline{U}_i U'_j} - \overline{\rho' \overline{U}}_i \overline{U'}_j + \ldots$$
$$\overline{\overline{\rho U}_i U'_j} - \overline{\overline{\rho U}}_i \overline{U'}_j + \overline{\rho U'_i U'_j} - \overline{\rho U'}_i \overline{U'}_j \quad ,$$

$$Rij = \overline{\rho' U'_i U'_j} - \overline{\rho' U'}_i \overline{U'}_j \quad .$$

The model proposes to use only the Leonard term Lij in order to models the SGS terms.

Finally the SGS terms models are:

$$\tau^{mod\,el}_{int\,erf\_i} = \overline{\overline{U}_i \overline{\phi}} - \overline{\overline{U}}_i \overline{\overline{\phi}} \quad , \tag{14}$$

$$\tau^{mod\,el}_{conv\_ij} = \overline{\overline{\rho U}_i \overline{U}_j} - \overline{\overline{\rho U}}_i \overline{\overline{U}}_j \quad , \tag{15}$$

$$\tau^{mod\,el}_{temp\_i} = \overline{\overline{\rho U}_i} - \overline{\overline{\rho U}}_i \quad . \tag{16}$$

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 (14), (15) and (16). Tests are carried out far from the inlet of the liquid jet as shown on figure 4. The results are presented as scatter plots allowing to compare SGS contribution from against the models. It can be noticed that the filter length $\overline{\Delta}$ is expressed compared to the DNS mesh size δ_x.

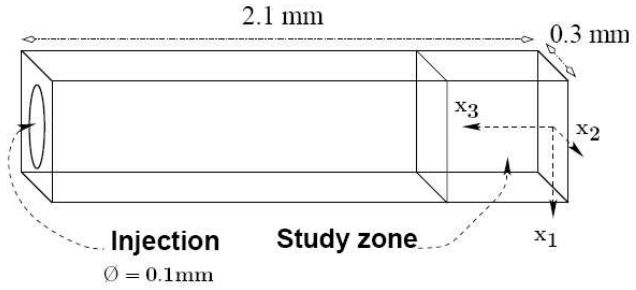

Figure 4 : DNS computationnal domain with dimensions, the a priori tests are conducted at the end of injection (Study zone)

Figures 5 and 6 confirm the potentiality of the model to represent the $\tau_{int\,erf\_i}$ of the phase function equation.

The figures 7 and 8 show the correlation between $\tau^{mod\,el}_{temp\_i}$ and $\tau^{mod\,el}_{temp\_i}$ for $\overline{\Delta} = 5\delta_x$. The model is well suited to represents this SGS term, since the scatter point are distributed around line plotted in these graphs. We can notice that for the injection direction U_3 the values are more sprayed around the fitting line, there are more velocity fluctuations in this direction.
Concerning the $\tau^{mod\,el}_{conv\_ij}$ term this is almost the same result, figure 9. The model well reproduces the real SGS terms.

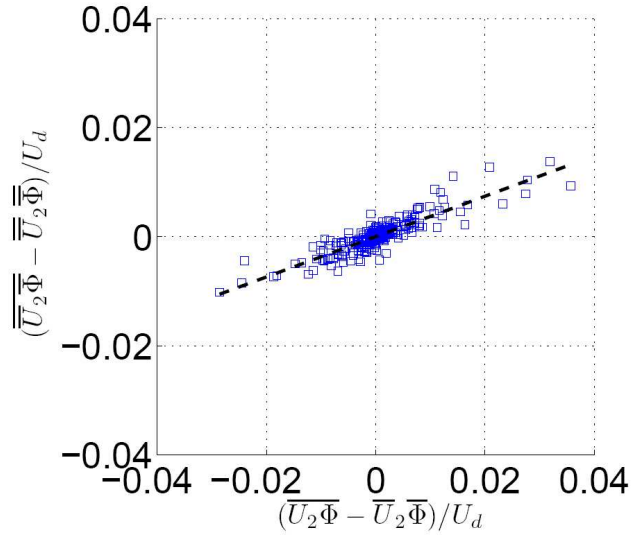

Figure 5 : Comparison DNS vs model for $\tau_{\text{int}\,erf\_2}$

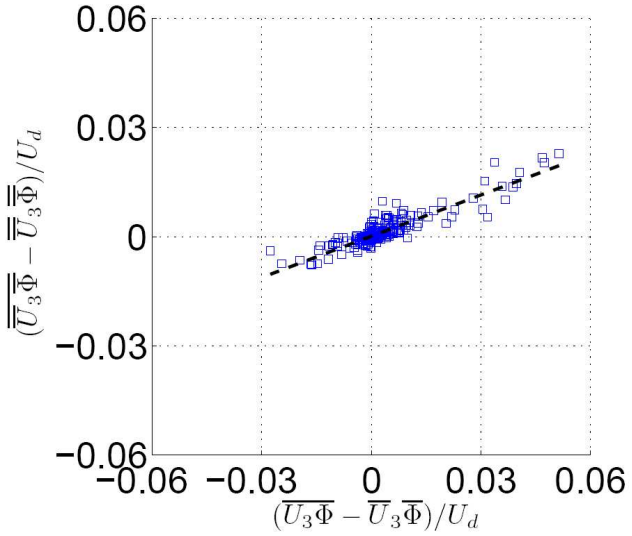

Figure 6 : Comparison DNS vs model for $\tau_{\text{int}\,erf\_3}$

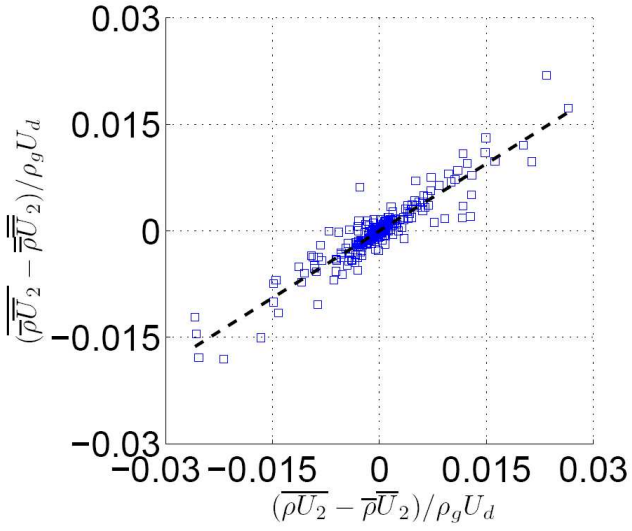

Figure 7 : Comparison DNS vs model for τ_{temp_2}

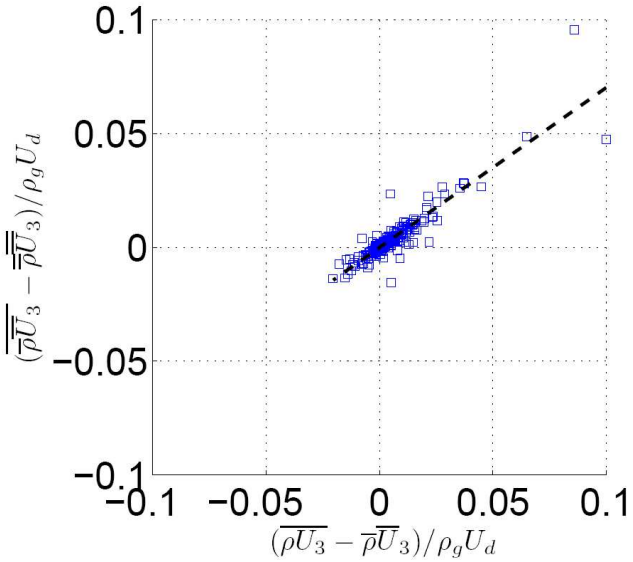

Figure 8 : Comparison DNS vs model for τ_{temp_3}

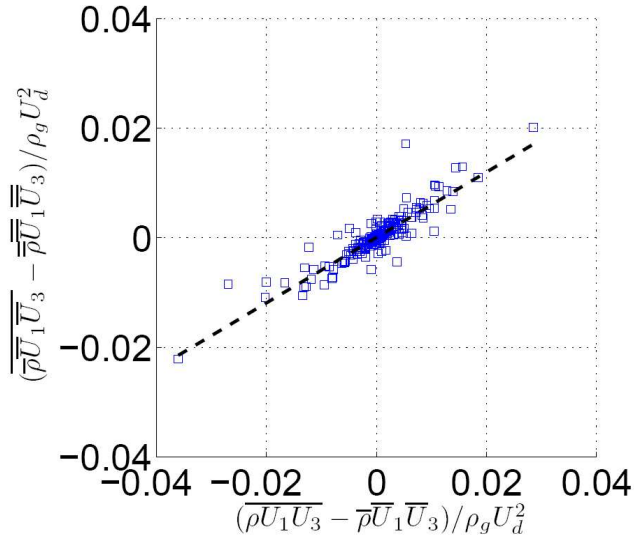

Figure 9 : Comparison DNS vs model for τ_{conv_13}

CONCLUSION

This study constitutes a preliminary work to test the phase functions as well as the SGS models usable in LES of primary liquid jet atomisation.

Primary atomisation is a particular flow where spatial scales vary strongly, both for turbulence and interface. The multiphasic aspect also adds difficulty in the description of this type of flow especially from an LES point of view.

We have developed the two-phase governing equations in a monofluid way, then also the filtered equations and exhibit all the SGS terms for the phase function transport equation and momentum equation. Specific SGS terms related to multiphasic flows have been extracted. Then we tested closure by using a classical model used in monophasic LES.

We tested "scale similarity" SGS models with an *a priori* procedure by using instantaneous fields resulting from a liquid jet primary atomisation DNS. We were able to compare the

real contribution extracted from the DNS with 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 and convective term.

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