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A LES SIMULATION OF ATOMISATION

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ABSTRACT

Large Eddy Simulation has been used with a lot of success for single phase flows. Its extension to multiphase flows is underway. As far as liquid-gas flows are concerned, two limit cases have been addressed: In one hand, if the liquid phase corresponds to a set of droplets with diameters smaller than the LES filter size, a subgrid spray is described. In the other hand, if the characteristic sizes of the surface wrinkles are greater than the LES filters size, the surface is resolved and LES models concern the velocity field. An example of the first approach is a dilute spray¹ and an example of the second approach is waves at ocean surface².

The issue with LES simulation of atomization is that a surface resolved LES is expected close to the injector together with a subgrid sprays LES far from the injector when the spray is finally formed. If only a resolved LES is used, the drop diameter cannot be smaller than the LES filter size. It follows that smaller diameters cannot be described and the breakup process is blocked numerically at a size related to the filter size

³. At the contrary if a subgrid spray LES is used a model is necessarily used that is accurate only for given type of injector

⁴. The present work addresses the problem induced by this transition between resolved and unresolved spray. A first approach is proposed that is able to reach both limits⁵. The transition is performed using a filtered surface density equation to avoid the assumption that ligaments, sheets and other surface topologies becomes spherical droplet abruptly at the subgrid level. Results will be shown to demonstrate the ability of the model to recover the essential characteristics of a spray in a Diesel like application.

INTRODUCTION

For many years research on atomization has been carried on to improve the characteristic and the control of sprays. This is particularly true as far as fuel injection is considered. Because the finale combustion is directly dependant on the characteristics of the spray, for instance to reduce pollutant emission, a special attention has been spend on the design of fuel injector. As a consequence for injector manufacturers the time needed to

develop a new injector has been reduced and the requirements are more drastic. To face this challenging task, numerical simulations of flow inside the injector has been developed, see for instance ^{6,7}. In the other hand simulations of two phase flow with vaporisation and combustion have been used extensively to improve internal combustion engine (ICE) for many years ⁸. New models of atomisation able to represent the dense zone at the exit of the injector ⁹ have build a bridge between in injector flow simulations and simulations of the whole combustion process. Since phenomena involved in this kind of applications are very complex the direct numerical simulation (DNS) is still out of reach. Thus, most of the studies devoted to injection and combustion in ICE have been done in the Reynolds average Navier-Stokes (RANS) context. Because the power of computer has been growing fast, large eddy simulation appears as a solution to benefit of the new computational possibilities to improve the reliability of RANS simulation and to explore new ways of using numerical simulation. The LES approach initially developed for single non reactive flows has been applied recently and successfully for ICE engine ¹⁰. The possibility of using LES for simulation inside the injector and potential gains have just been explored ¹¹. Therefore a strong interest exists in prolonging the ability of LES to deal with complex flows to the field of atomisation. The present work is a step forward in this direction.

NOMENCLATURE

\mathbf{n}	surface normal vector
v_α	velocity component
\mathbf{V}	velocity vector (ms^{-1})

Greek letters

φ_l	liquid volume fraction
ϕ	distance function (m)
κ	surface curvature (m^{-1})
ρ	density (kgm^{-3})
σ	surface tension coefficient (Nm^{-1})
τ_{φ_l}	subgrid scale term for φ_l

Subscripts

l	liquid
g	gas

OVERVIEW OF LES FOR TWO PHASE FLOWS

To address the problem of LES of atomisation it is useful to overview the possible approach used in the context of LES for two phase flows. LES is originally developed to deal with turbulence in single phase flows. Here, two phase flows are considered only as liquid-gas flows. Compare to single phase flows, the complexity is amplified mainly because of three phenomena:

- The presence of important density variations requires a robust computational code.
- The surface that separates the two phases is the place of jump for several quantities such as the density, the viscosity and the pressure.
- The surface tension force appears as an additional force inside the flow that requires a good representation of the interface geometry, to be reliably estimated.

To address this complexity in the context of LES two main approaches have been proposed.

The first one applies to two-phase flows where a continuous carrier phase and a discrete phase can be defined (CD-LES). As for RANS approach, in LES this simplified representation of the spray can be useful for many problems. It consists to assume that the liquid part is only composed by spherical droplets that are mainly isolated from each other. Then, the flow inside the droplet does not need to be computed integrally. They can be considered at a subgrid scale level as a set of particles that are characterised by a reduce number of parameters such as position, velocity and diameter. Of course, an important effort on modelling may be require to describe the evolution of the spray and its interaction with the carrier phase ^{1, 12, 13}. However, this formulation can be analysed thanks to DNS simulations based on a similar description of the spray, for phenomenon as complex as the effect of preferential concentration on the vaporisation process ¹⁴.

At the opposite when no discrete phase can be defined both phases have to be considered continuously this the continuous-continuous LES of two phase flows (CC-LES). In this case the flow is resolved for both phases and special numerical methods have been developed to describe the interface. In the first step the flow is supposed to be completely resolved like in DNS. Numerical methods dedicated to liquid gas flows with an interface include front tracking methods ¹⁵, boundary integral methods ¹⁶, volume-of-fluid methods ¹⁷, level set methods ¹⁸. Each method has his own advantages and drawbacks, the last development in this fields proposed to combine different numerical approaches. The resulting approaches are able to simulate completely complex flows such as the atomisation of a high-speed liquid jet ¹⁹. However their extension to LES simulation is not straight forward expect in a special case where the interface wrinkles are resolved at the LES filter size. This is the case for instance of waves in oceans. The characteristic size of waves can be one order of magnitude bigger, or even more, than the smallest sizes of the turbulent structures in the air. In this case the LES modelling concerns only the dynamic of each phase from each side of the interface. For such methods, generally, a modelling of the subgrid stress tensor is applied for the velocity very similarly than those used for single phase flows ². Because the interface geometry is resolved at the LES filter level, the treatment of the interface is done like in DNS, though special modifications have been proposed to the Smagorinsky model to represent the turbulence decay close to the interface ²⁰.

In the case of atomization it is expected to use CC-LES approach with a filter size allowing the interface scales to be resolved close to the injector exit. This is necessary to capture the first instabilities that promote the breakup of the jet. However, most of the injectors produce shortly a dilute spray with very small droplets. The interface resolved CC-LES approach would be far to consuming in term of computational resources. Indeed, once the spray is formed such an approach would be comparable to a DNS approach which is unaffordable because the droplet size decrease as large scales of the flow increase following the expansion of the spray. Once the spray is formed the appropriate numerical approach should be the CD-LES that considers the spray at a subgrid level. Thus, the challenge, as far as LES of atomisation is concerned, is to proposed a method that include CC-LES and CD-LES approaches and able to represent the transition between both approaches in a realistic way.

DNS SIMULATION OF THE ATOMISATION

The proposed work concerns mainly the atomisation process that is relevant for Diesel spray, but it has certainly application for other injection devices. The main drawback for this kind of atomisation is the lack of experimental data in the vicinity of the injector tip. The high velocity and high density variation in this zone prevent to use classical measurement apparatus. In particular, the diffraction effect is the main reason of failure for optical diagnostic. Even if new measurement techniques have been developed²¹⁻²⁴, DNS simulation is still a very interesting tools to explore the vicinity of the liquid jet exit.

We use for this work a DNS code "ARCHER" developed at the CORIA laboratory^{19, 25}. It has been used already to collect statistical information in the dense zone of the spray where nearly no experimental data are available. These simulations are sufficiently predictive and quantitative to be used for validation of modelling proposals⁹.

The numerical method describes the interface motion precisely, handles jump conditions at the interface without artificial smoothing, and respect mass conservation. Accordingly, the interface tracking is performed by a Level Set method. The Ghost Fluid Method is used to capture accurately sharp discontinuities. The Level Set and VOF methods are coupled to ensure mass conservation. A projection method is used to solve the incompressible Navier-Stokes equations that are coupled to a transport equation for level set and VOF functions.

Level Set methods are based on the transport of a continuous function ϕ , which describes the interface between two phases^{18, 26}. This function is defined by the algebraic distance 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 allows to determine the evolution of the interface in a given velocity field \mathbf{V} ²⁶:

$$\frac{\partial \phi}{\partial t} + \mathbf{V} \cdot \nabla \phi = 0 \quad (1)$$

Particular attention must be paid to this transport equation. Problems may arise when the level set method is developed: a high velocity gradient can produce wide spreading and stretching of the level sets, such that ϕ no longer remains a distance function. Thus, a re-distancing algorithm¹⁸ is applied to keep ϕ as the algebraic distance to the interface.

To avoid singularities in the distance function field, a 5th order WENO scheme has been used for convective terms²⁷. Temporal derivatives are computed with a third 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 \mathbf{n} or curvature \mathcal{K} , are easily obtained through:

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \quad \kappa(\phi) = \nabla \cdot \mathbf{n} \quad (2)$$

It is well known that numerical computation of equation (1) and a redistance algorithm can generate mass loss in under-resolved regions. This is the main drawback of Level Set methods. However, to improve mass conservation a coupling between VOF and Level Set²⁸ method has been performed.

APPLYING RESOLVED INTERFACE CC-LES METHOD TO THE ATOMISATION

The resolved interface CC-LES approach consists in using a DNS approach with interface capturing ability in such conditions that all scales of the velocity field are not completely resolved but where all interface wrinkles are resolved. A LES model is applied for the subgrid Reynolds stress in order to represent the subgrid scale motion. Applying such an approach for atomisation³ is appealing but rises some problems. The front tracking methods need at less one mesh cell to represent a liquid parcel. One quality of the numerical method is to conserve the liquid mass, as a consequence the method prevent any further breakup of the liquid parcels as soon as their sizes become comparable to the mesh size. This numerical artefact can be considered qualitatively as an additional numerical surface tension force. When using this method for atomisation the sizes of the droplets form during the atomisation are numerically controlled. Such behaviour is demonstrated on figure 1 where the DNS code ARCHER is used to represent the atomisation of a Diesel jet. The inlet diameter is $D_i = 100 \mu m$.

The gas density is $\rho_g = 25\text{kg}\cdot\text{m}^{-3}$ and the liquid density is $\rho_l = 696\text{kg}\cdot\text{m}^{-3}$. The surface tension coefficient is set to $\sigma = 0.06\text{N}\cdot\text{m}^{-1}$. The inlet liquid velocity is equal to $U_i = 79\text{m}\cdot\text{s}^{-1}$.

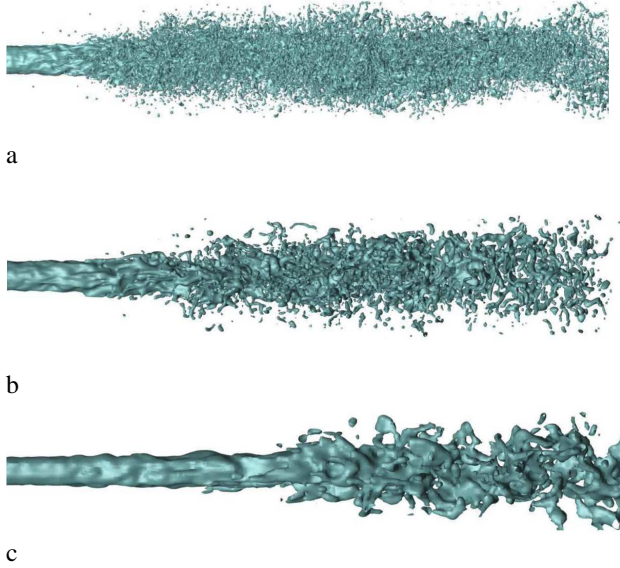


Figure 1: Numerical simulation of a Diesel injection for three different mesh refinements. a-128-128-1024 b-64x64x512 c-32x32x256

The figure 1 represents three instantaneous snapshots obtained with the code ARCHER for three different mesh refinements. The interface geometries are very different, as expected the more the mesh is refined the smaller are the liquid parcels. What is more surprising is that the mesh size effect act not only on the smallest scales of the surface but also on all scales of the surface. It may be due to the model used for injecting a synthetic turbulence²⁹. Depending on the mesh cell size the spatial behaviour of the turbulence can be affected. However, increasing the mesh cell size has an effect very similar to an increase of the surface tension coefficient.

The dependence of the result on the mesh refinement rises two questions:

1. Is mesh convergence achieved in DNS?
2. Does that have an effect on mean behaviour of the liquid jet?

Concerning the first question, the problem is that for liquid gas flow the smallest sizes of the flow are not known in contrary to single phase flows. There is no equivalent to the Kolmogorov length scale. Because there is no diffusion of the scalar (liquid concentration) even at small scales (inviscid flows) the Batchelor scale is not defined. The mechanism that prevents the

existence of very small scales is based on surface tension force. But it does act only for strong curvatures. Thus liquid sheets can be very thin as soon as their curvature remains small. Finally this possibility to have very small dimension for the scalar field as also an effect on the dynamic at small scales of the flow because the density is linked to the scalar field.

To address the second question statistical results have been extracted from the previous simulation.

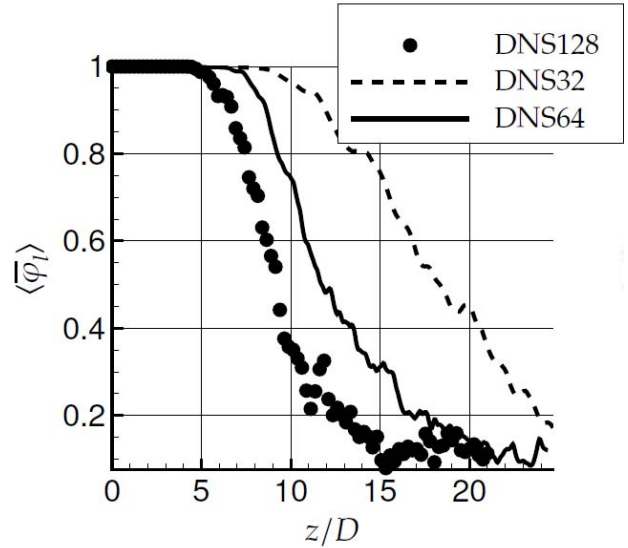


Figure 2: Mean liquid volume fraction along the main axis of injection obtained with DNS code ARCHER for three different refinements. DNS128 (128x128x1024) DNS64 (64x64x512) DNS32 (32x32x256)

The mean liquid volume fraction obtained for three mesh refinements is represented on figure 2. Clearly, different mesh sizes lead to different liquid penetrations. For the less refined mesh the numerical method introduces an additional surface tension force that prevents the spray to be atomized. As a consequence the liquid jet penetrates further. It is interesting to test the resolved interface CC-LES. This is done here by adding a Smagorinsky model to filtered velocity equations. The corresponding results are represented on figure 3.

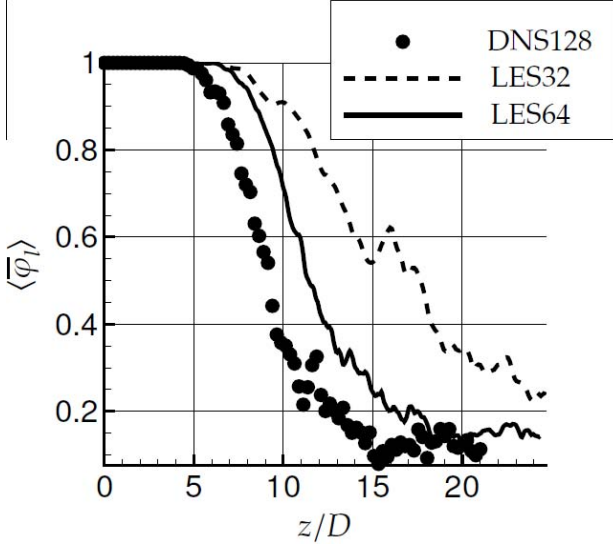


Figure 3: Mean liquid volume fraction along the main axis of injection obtained with code ARCHER, LES simulation corresponds to simulation with a Smagorinsky model for velocity equation. DNS128 (same as figure 2) LES64 (64x64x512) LES32 (32x32x256)

The effect of introducing a LES model for the velocity equation does not bring a clear improvement. The liquid penetrations remind strongly affected by the mesh size. Partial conclusions at this point is that resolved surface CC-LES approaches are not sufficient to represent the atomisation process; first because they do not lead to a subgrid spray that can be described by a CD-LES approach; second even the initial behaviour of the spray is affected by the mesh cell size.

A PRIORI ANALYSIS OF DNS TO BUILD A SUITABLE LES OF ATOMISATION

To improve LES modelling it is useful to analysis a filtered field of a reference DNS simulation^{30, 31}. The filtered liquid volume fraction equation can be written as:

$$\frac{\partial \overline{\varphi}_l}{\partial t} + \frac{\partial v_\alpha \overline{\varphi}_l}{\partial x_\alpha} = \frac{\partial \tau_{\varphi_l}}{\partial x_\alpha} \quad (3)$$

Where the subgrid scale term is:

$$\tau_{\varphi_l} = \overline{v_\alpha \varphi_l} - \overline{v_\alpha} \overline{\varphi}_l \quad (4)$$

Here the upper line refers to a filtered variable. Previous studies, based on a priori analysis of a well resolved LES, have shown that this subgrid term is negligible by comparison of the other terms of the equation (3). But this a priori analysis can only be used to evaluate an instantaneous contribution. Even if

this term is small instantaneously, its cumulous effect all along the time may produce a visible effect. To explore this possibility a Bardina model of the subgrid scale term τ_{φ_l} has been used to compare with resolved surface CC-LES, for this later approach τ_{φ_l} is set to zero.

The figure 4, demonstrates the effect of this subgrid term. Even if this term is small and has negligible effect at the beginning of the spray (zone 1), its cumulative effect induced a clear difference depending on the model retained for τ_{φ_l} .

When this term is not neglected the iso-surface $\overline{\varphi}_l = 0.5$ does not represent the mean position of the interface in zone 2 as it is the case in zone 1. As the spray is transferred at the subgrid scale level this iso-surface corresponds only to a mean concentration of liquid and not any more to an approximation of the liquid surface. In contrary to the DNS approaches used in resolved interface LES, the amount of liquid enclosed in the iso-surface $\overline{\varphi}_l = 0.5$ is not conserved. Indeed, the atomisation of the liquid surface induces a flux of small liquid parcels out of this iso-surface. Similarly, gas inclusions go inside the liquid zone. Conclusion of this section is that the transfer of the liquid phase from a resolved interface area to a subgrid spray is driven by this subgrid term τ_{φ_l} .

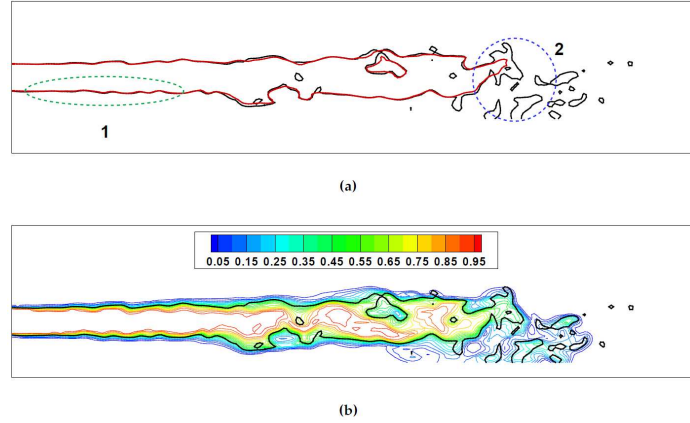


Figure 4: (a) comparison of iso-surfaces $\overline{\varphi}_l = 0.5$; in black the subgrid scale term τ_{φ_l} is neglected; in red τ_{φ_l} is replaces by a model of Bardina. (b) iso-surface of the filtered liquid volume fraction with the latter modelling of τ_{φ_l}

FIRST LES OF ATOMISATION

In this section we test a first LES model of atomisation satisfying the requirement of a possible transition between resolved interface CC-LES and subgrid spray CD-LES. The

model is based on the equation (3) where the subgrid term τ_{ϕ_l} is not neglected and replaced by a Bardina model. Additionally a Smagorinsky model is used for velocity equations similarly to previous LES simulation of figure 3.

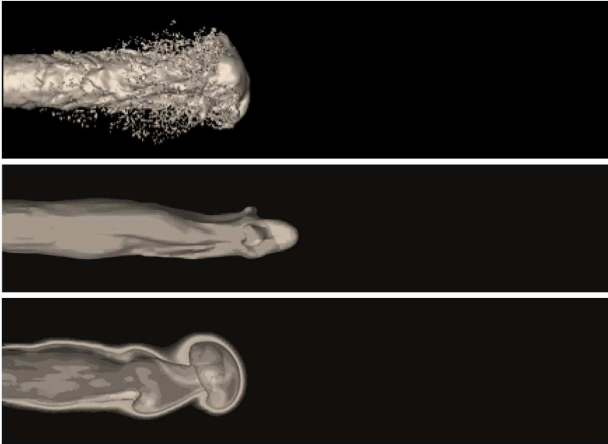


Figure 5: Iso-surfaces $\overline{\phi_l} = 0.5$ at the beginning of the injection. From top to bottom: DNS, resolved interface CC-LES ($\tau_{\phi_l} = 0$); LES of atomisation (τ_{ϕ_l} approximated by a Bardina model)

The figure 5 shows the iso-surfaces $\overline{\phi_l} = 0.5$ for a DNS test case and the two LES approaches at the beginning of the injection. As previously mentioned the resolved surface CC-LES prevent atomization of the liquid jet inducing a greater liquid penetration. At the contrary the modeling proposal of τ_{ϕ_l} allow for a transition of the spray from the resolved scale to the subgrid scale. The smooth contours around the iso-surface represent the filtered liquid volume fraction in a cut plane passing through the middle of the jet. The liquid volume fraction outside the iso-surface $\overline{\phi_l} = 0.5$ corresponds to liquid parcels detached from the main jet. This gives an encouraging qualitative result. To go further statistic are extract from this latter LES simulation of the atomisation to represent the profile of the mean liquid volume fraction along the main axis, see figure 6.

Comparisons of results presented in figure 3 and 6 show a real improvement when applying the new LES models that takes into account the subgrid term τ_{ϕ_l} . It is now possible to recover the axial profile of the mean liquid volume fraction obtained with the most refined DNS despite the lower mesh resolution. The apply model compare favourably for a computational mesh reduced by a factor height (New LES64) and even with mesh reduced by a factor 64 (New LES32). With the present test case it is not possible to go further because 10 mesh cells are at least

necessary to represent the injection profiles through the diameter of the jet.

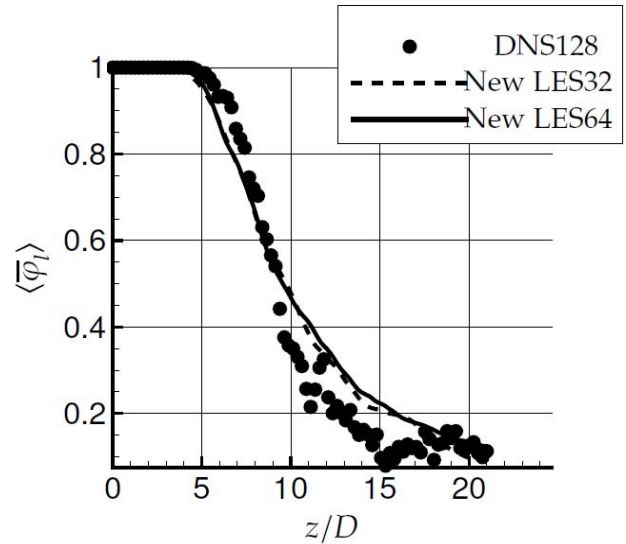


Figure 6: Mean liquid volume fraction along the main axis for the reference DNS case (DNS-128) and the new LES of atomisation

CONCLUSIONS

The present study proposed an original method to model the atomisation in the context of an LES approach. The main issue is the transfer of the spray from the resolved scale to the subgrid scale. The modelling proposal consists in taking into account of an additional subgrid term for the liquid volume fraction that is generally neglected. This term represents the effect of subgrid surface wrinkles that leads to the atomisation of the liquid jet. The model is tested by comparison to a refined DNS. Results are encouraging even if the model needs more complete validations to be definitely assessed. It is possible, for instance, that the resolution of the reference DNS should not be high enough to capture the smallest scales of the spray. However, the interest of this LES approach is its ability to find similar mean results with a smaller resolution. In a second step with this approach, we will determine the characteristic length scales of the subgrid liquid parcels. This information will eventually be equivalent to a liquid droplet distribution of diameter. This last step is underway thanks to a modelled equation for the surface density equation. First results will be shown during the oral presentation.

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