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Large eddy simulation of spray atomization with a probability density function method

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Abstract

Despite recent advances in numerical methods for multiphase flows, the complete simulation of a liquid spray is still an illusive goal. There are few models that can describe accurately both the primary and secondary atomization simultaneously. The biggest difficulty is the wide range of length scales involved; from millimetres in the largest liquid structures close to the smallest micron-size droplets. This wide range makes Direct Numerical Simulation of sprays very expensive all scales need to be resolved and expensive algorithms are required to reconstruct accurately the interface. Large Eddy Simulations are becoming increasingly popular in turbulent flows due to their better description of turbulence and the relative robustness of sub-grid stress models. Despite its advantages, Large Eddy Simulation cannot describe accurately fluid structures that occur at sub-grid levels. This paper presents a new model to describe the atomization process. The method consist of solving a joint sub-grid probability density function of liquid volume and surface using stochastic methods. The approach can simulate both dense and dilute regions of the spray. The proposed model can determine instantaneous

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sub-grid liquid structures (droplets) distributions as well as to capture the primary break-up. The results of the simulations are compared to a Direct Numerical Simulation of a Diesel Jet break-up. The mean liquid volume and surface density are well predicted; The modelling of the sub-grid scales is shown to be fundamental in the dilute regions of the spray.

Keywords: Spray Atomization, Probability Density Function, Large Eddy Simulations, Surface Density

1. Introduction

Liquid atomization is the process in which a liquid jet breaks-up or disintegrates into small fragments or droplets. Atomization a very complex phenomenon that has a deep impact in many engineering processes. It controls the size of the structures that define the spray properties; mostly droplets size distribution and droplets velocities. The atomization process depends on complex interactions between aerodynamic and capillary forces. Turbulence and shear deform the liquid-gas interface, while surface tension both promote and delay the instabilities. Liquid structures are shed from the dense spray core, forming ligaments that pinch-off and form droplets. The droplet break-up pattern in itself is also very complex, a droplet may break into few big droplets (vibrational break-up) or myriad of small droplets (bag break-up), among other possibilities. Pilch and Erdman (1987) showed the different break-up mechanisms based on the Weber, We , number (ratio of inertia to capillary forces).

The direct simulation of the atomization process is a difficult task in itself. The smallest liquid fragments have to be accurately resolved to capture the

formation of ligament-forming and droplet break-up. Unfortunately, the size of the smallest scale in atomization is not accurately characterised: there is no equivalent to a Kolmogorov scale in atomization. This size can be up to thousand times smaller than the characteristic nozzle length, depending on the bulk Weber Reynolds numbers.

Direct Numerical Simulations (DNS) of atomization are very sophisticated and include complex numerical methods: see recent works by Menard et al. (2007); Fuster et al. (2009); Tomar et al. (2010); Shinjo and Umemura (2010); Herrmann (2011). All these simulations are very expensive, with $\mathcal{O}(10^9)$ computational cells used. The simulation domain is reduced to a few tens of nozzle diameters. The simulations still depend on grid refinement and can create *artificial* droplets of the order of the mesh size. Based on the cost of DNS, direct numerical description of atomization remains impossible for realistic sprays, where the atomization process occurs over hundreds of nozzle diameters.

The alternative is to use models to describe the behaviour of the sub-grid scales. Commercial and industrial solver use models based on Reynolds Averaged Navier-Stokes (RANS) equations. However, the atomization process seems chaotic in nature and highly unsteady. Removing the temporal component increases the complexity of the model who has to account for both disparity of space and time scales. Moreover, there are some uncertainties in the turbulence modelling, in particular when dealing with highly three-dimensional flows (such as swirl injectors). Large Eddy Simulations (LES) has proven to be cost-effective and accurate way to model single phase turbulent flows. However its application to two-phase flows is still limited.

Numerical approaches for spray atomization are usually different depending on the spray region. In the primary break-up, where relatively few droplets are observed, an Eulerian-Eulerian formulation is used to represent accurately the interface dynamics. Turbulence effects may be included in the velocity description, but the fluid phase is described as exactly as possible. These simulations can be considered therefore under-resolved DNS, where the interface is resolved at LES grid level. Examples of primary atomization LES in the literature are Villier et al. (2004); Bianchi et al. (2007); Ishimoto et al. (2007, 2008); Srinivasan et al. (2008). All these simulations do not consider the sub-grid perturbations of the interface and neglect the effect of sub-grid turbulent fluctuations on it. The recent work of Chesnel et al. (2010, 2012), showed that this contribution is indeed important to accurately capture the primary atomization and it has to be included.

In the secondary break-up region, the spray can be considered as dilute and the droplets are small and quasi-spherical. In this region a Lagrangian approach is favoured, where the droplets are treated as point sources that exchange mass, momentum and energy with the Eulerian gas phase. The Lagrangian approach is simple to implement, albeit difficult to optimise for parallel computing. Gorokhovski and Saveliev (2003); Apte et al. (2003); Bini et al. (2009); Jones and Lettieri (2010) proposed stochastic break-up models in the Lagrangian framework to account for secondary atomization. These break-up models are based on different concepts: either maximum entropy principle, population balance or Kolmogorov's theory of fragmentation. All of them requires estimates for fragmentation rates and break-up frequencies.

The transition between the Eulerian and Lagrangian approaches of the

dilute region is not simple. Kim et al. (2007); Tomar et al. (2010) use hybrid Eulerian-Lagrangian approaches, where after the Eulerian solver determines the initial droplet structures; Lagrangian point droplets are injected into the flow. There is currently a trend Herrmann (2010); Gorokhovski et al. (2012); Hecht et al. (2013) to develop methods to treat this transition accurately and create numerical methods that can potentially describe the complete spray atomization process. See the review by Gorokhovski and Herrmann (2008) for details.

During the past two decades, a class of methods have arisen that can, a priori, describe the spray regions uniformly: Vallet and Borghi (1999); Vallet et al. (2001) proposed the Σ -Y model, which later was known as the Eulerian-Lagrangian Spray Atomization (ELSA) model. The ELSA approach solves a more general concept than droplet sizes, the surface density. The model solves, in an Eulerian sense, two equations: one corresponding to the liquid volume (or mass) and the other to the surface density. The model gives directly relevant quantities for spray characterisation such as Sauter Mean Diameter (SMD) and liquid dispersion based on simple relations between surface density and volume. The methodology has been used mostly in the RANS framework: Beheshti et al. (2007); Hoyas et al. (2011); Lebas et al. (2009) with good agreement compared with experimental data on dense and dilute sprays. Chesnel et al. (2012) formulated recently the ELSA variant in the LES framework. The model requires closure of the filtered surface density production and destruction. Shear-turbulence, droplet collision and breakup processes create and destroy surface and ultimately provide the sub-grid liquid structure sizes. These source terms are non-linear: they involved

(at least) quadratic closures on surface and complex dependencies on the liquid volume fraction.

From DNS atomization pictures, it is clear that there is a wide range of sub-grid liquid-structure sizes that interact in a complex form. A single filtered value of volume and surface per cell, cannot represent accurately all these structures. The ELSA method does not distinguish between two droplets and an equivalent filament with same volume and surface. To improve the sub-grid liquid structure description, a novel sub-grid formulation is presented in this paper. The formulation is based on the solution of a joint volume-surface density, sub-grid Probability Density Function (PDF) or Filtered Density Function (FDF). This LES-PDF solution accounts for sub-grid fluctuations of the surface and liquid volume, and therefore characterise sub-grid structures. In dilute sprays, the formulation can be seen as equivalent to the classical spray-PDF equation of Williams (1958) in LES context. The resultant PDF equation is solved using a Eulerian Monte-Carlo approach (the Stochastic fields). The model permits to describe sub-grid fluids structure and their interactions in both spray regions without the need of modelling transition. Although, this works restricts to incompressible, constant density, two-phase flows without phase change; The formulation can be rapidly extended to variable density, evaporating flows.

The paper is organised as follows: First, the fundamental multiphase equations will be presented together with conventional surface density equation closures. In the second section the LES-PDF methodology will be introduced, followed by the proposed implementation of the Stochastic Fields approach. Then the solved filtered momentum equations will be described

with the employed sub-grid models. Finally, LES-PDF predictions of volume fraction and surface density will be compared with the DNS results of Chesnel (2010).

2. Fundamental equations

2.1. Volume Fraction

In incompressible flows $\nabla \cdot \mathbf{u} = 0$, the continuity equations can be written as

$$\frac{\partial \rho}{\partial t} + u_j \frac{\partial \rho}{\partial x_j} = 0 \quad (1)$$

By definition, $\phi(\mathbf{x}, t)$ is the *liquid volume fraction*. In the present work $\phi = 0$ represents the gas phase (hereafter, subscript g) and $\phi = 1$ the liquid phase (subscript l). The fluid density can be then expressed as

$$\rho = (1 - \phi)\rho_g + \phi\rho_l \quad (2)$$

where ρ_g and ρ_l is the gas and liquid densities respectively. The equation to describe the evolution of ϕ , can be obtained directly by substitution from Eqn. (1), viz.:

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} = 0 \quad (3)$$

2.2. Surface Density

The three-dimensional liquid-gas interface $\mathbf{x}^I(t)$ can be defined by the zero of a smooth function $F(\mathbf{x}, t)$. The normal of the interface can be defined by $\mathbf{n} = -\nabla F/|\nabla F|$, where the normal points toward the gas by convention. The field F follows a convective equation with the interface velocity $\mathbf{u}^I$

$$\frac{\partial F}{\partial t} + u_j^I \frac{\partial F}{\partial x_j} = 0 \quad (4)$$

Any velocity field, $\mathbf{u}^I$, with the same normal velocity will give the same surface solution; the interface velocity is invariant over the choice of surface coordinates

$$\mathbf{u}^I \cdot \mathbf{n} = C = \frac{\partial F / \partial t}{|\nabla F|} \quad (5)$$

The *normal* velocity is the only one related to the movement of the surface. A phase indicator function, $\chi(\mathbf{x}, t)$ can be defined using a Heaviside function H

$$\chi = H(\mathbf{x} - \mathbf{x}^I) \quad (6)$$

The integral of χ over an infinitesimal δV return the volume fraction ϕ . The gradient of the indicator function is given by:

$$\nabla \chi = \nabla H(\mathbf{x} - \mathbf{x}^I) = \delta(F) \nabla F \quad (7)$$

Where the characteristic function δ has been introduced. Using the definition of $\mathbf{n}$, the gradient is rewritten, viz.

$$\nabla \chi = -\delta(F) \mathbf{n} |\nabla F| \rightarrow \mathbf{n} \cdot \nabla \chi = -\delta(F) |\nabla F| \quad (8)$$

The interface Dirac function or *fine-grained surface density* is defined as:

$$\delta_I \equiv -\mathbf{n} \cdot \nabla \chi \quad (9)$$

with units of inverse length, m^{-1} . The evolution equation of δ_I can be found from the knowledge of the flow field (see Marle (1982) and Lhuillier (2003), among others) and is given by

$$\frac{\partial \delta_I}{\partial t} + u_j \frac{\partial \delta_I}{\partial x_j} = -\delta_I n_i n_j \frac{\partial u_i}{\partial x_j} \quad (10)$$

The integral of δ_I over an infinitesimal δV gives the *surface density*, Σ ,

$$\Sigma(\mathbf{x}, t) = \frac{1}{\delta V} \int_V \delta_I dV = \frac{1}{\delta V} \int_I dS = \frac{\delta S^I}{\delta V} \quad (11)$$

The above surface density can be understood as the amount of spatial surface per unit volume at a given time and spatial position. This concept was introduced by Candel and Poinot (1990) in premixed combustion context to define a volumetric flame surface density. The convolution of the δ_I with any smooth function f gives

$$\frac{1}{\delta V} \int_V \delta_I f(\mathbf{x}, t) dV = \frac{1}{\delta V} f(\mathbf{x}_I, t) \delta S^I \equiv f^I \Sigma \quad (12)$$

where the subscript I indicates evaluated at the interface. The evolution equation for the interfacial surface density can be derived by integrating (10) over a small volume and using (12)

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial u_j^I \Sigma}{\partial x_j} = -\frac{1}{\delta V} \int_V \delta_I n_i n_j \frac{\partial u_i}{\partial x_j} dV \quad (13)$$

The integral term in the right-hand side (RHS) of the Eqn. (13) describes the stretching of the surface due to velocity gradients and curvature effects. As the interface normal is not a continuous function, if the integral were to be over a large volume the integral would have to be split. The discontinuity of the normal, will appear in break-up processes and surface intersections; including fragmentation or coalescence of surfaces. As the integral is performed over an infinitesimal δV , the velocity has no sub-volume scales. If the interface is considered a material interface without mass transfer then the interface velocity is just the fluid velocity $\mathbf{u}^I = \mathbf{u}$. The final equation for the

flame surface density is the one presented by Pope (1988) and Vervisch et al. (1995) among others:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial u_j \Sigma}{\partial x_j} = -\Sigma n_i n_j \frac{\partial u_i}{\partial x_j} \quad (14)$$

The above equation together with the Eqn. (3) form the fundamental equations to be solved in the present paper. The term in the RHS of (14) can be positive or negative depending on the flow field and interface orientation. However, Batchelor (1952) showed that its average contribution will be positive. In the absence of surface tension, in a isotropic homogenous turbulent flow the spatially-averaged equation (14) reduces to

$$\frac{\partial \hat{\Sigma}}{\partial t} = -\overline{\Sigma n_i n_j} \frac{\partial u_i}{\partial x_j} \quad (15)$$

Where the operator $\hat{\cdot}$ indicates spatial average. The RHS term in (15) is highly anisotropic at low Reynolds numbers, but it becomes isotropic at high Reynolds numbers where the mean orientation of the surface is lost. At high Reynolds numbers, the term can be simplified to $\hat{\Sigma} \times \tau_t$ with $\tau_t > 0$ and the solution is:

$$\hat{\Sigma} = \hat{\Sigma}_0 \exp(t/\tau_t) \quad (16)$$

Where Σ_0 is the initial surface density. The solution corresponds to the classic result of Batchelor (1952) of the evolution of a interface length-scale $\mathcal{L}$ of initial size $\mathcal{L}_0$ in a turbulent flow given, whose evolution is given by

$$\mathcal{L} = \mathcal{L}_0 \exp(-t/2\tau_K) \quad (17)$$

Where the decay timescale is half the Kolmogorov time-scale, $\tau_K \propto (\varepsilon/\nu)^{1/2}$, where ε is the energy dissipation and ν the kinematic viscosity.

Equation (14) has been derived using surface kinematic arguments. The restorative surface forces act through the interface jump condition , which can be written following Kataoka (1986) as

$$\sigma \kappa n_i + \llbracket p n_i - n_j \tau_{ij} \rrbracket = 0 \quad (18)$$

where σ is the surface tension and p is the pressure and τ_{ij} the viscous stress. The interface forces due to the disjoining pressure and the Marangoni effect have been neglected. κ is the local curvature, which can be related locally to the surface density by $\kappa = dS^I/dV_l \approx \Sigma/\phi$. The above equation couples the momentum equation with the surface density through the jump in normal stresses. The surface pressure $\sigma \kappa$ controls the dynamics of the interface at moderate Weber numbers and/or small scales.

Equations (3) and (14) are point *micro-scale* equations and there are no *fluid scales*. Characteristic scales (droplets, filaments), can only be described when the equations are integrated over a control volume, V , much larger than the support kernel $V \gg \delta V$. Similarly, the surface corrugation by turbulence or *sub-grid wrinkling*, see Hawkes and Cant (2000), only appears when V is finite. The closure problems of the surface equations was largely summarised by Delhay (2001). Integrating directly Eqn. (10) over a control volume V do not reduce the uncertainties. A new spatial average surface density $\hat{\Sigma}$ equation will appear where the interface velocity $\mathbf{u}^I$ is unclosed (or the velocity-surface density correlations $\widehat{u_j \Sigma}$).

Using non-equilibrium thermodynamic arguments, Séro-Guillaume and

Rimbert (2005) postulate a closure for the interface velocity of the form

$$u_j^I = u_j - \frac{\sigma}{T} V \mathcal{L} \frac{\partial \hat{\Sigma}}{\partial x_j} \quad (19)$$

Where T is the temperature and $\mathcal{L}$ an unknown Onsanger kinetic coefficient between thermodynamic forces and fluxes, see Callen (1985). The last term in the RHS represents a *restorative* velocity $\mathbf{u}^s = K \nabla \hat{\Sigma}$, where $K = \sigma V \mathcal{L} / T > 0$. This velocity *diffuses* surface density similarly to a turbulent diffusion process. The velocity $\mathbf{u}^s$ vanish if the interface moves uniformly or if the system is locally in thermodynamic equilibrium (minimum free energy).

Some simplifications can be introduced in very dilute flows, where droplet or bubble scales are typically much smaller than the volume size: usually the cell-size $h \sim V^{1/3}$. Kocamustafaogullari and Ishii (1995); Morel (2007); Kataoka et al. (2012) proposed several formulations in this context which are limited to high Weber numbers. Regardless the simplifications, the use of the spatial averaging operator $\hat{\cdot}$ introduces models in the averaged surface density equation to account for droplet break-up/bubble coalescence. Nearly all the models in the literature have the same general formulation, originally proposed by Ishii (1975) and also adopted by Vallet and Borghi (1999) formulations, viz.

$$\frac{\partial \hat{\Sigma}}{\partial t} + \bar{u}_j \frac{\partial \hat{\Sigma}}{\partial x_j} = \mathcal{S}_{gen} - \mathcal{S}_{dest} \equiv \mathcal{S} \quad (20)$$

Where $\mathcal{S}_{gen}$ is the generation of surface (due to turbulence and break-up) and $\mathcal{S}_{dest}$ is the destruction of surface density due to droplet collisions, etc. The modelling of the source term $\mathcal{S}$ is often phenomenological, and involves correlation of turbulence and droplet time scales. Jay et al. (2006) expressed

the source term in quadratic form

$$\mathcal{S} = a\hat{\Sigma} - b\hat{\Sigma}^2 \quad (21)$$

where the inverse time-scales a and coefficient b , depend on the flow field, volume and orientation. In a primary atomization process, the first term can be understood as the surface generation due to the growth of fluid instabilities (i.e. Kelvin-Helmholtz) followed by a non-linear saturation process Jay et al. (2003, 2006). In a dispersed flow, the second term would be the destruction of surface due to droplet coalescence, see Lebas et al. (2009). The most common form for the term (21), introduced by Vallet and Borghi (1999) and other ELSA works, see Beheshti et al. (2007); Lebas et al. (2009) is the restoration to equilibrium:

$$\mathcal{S} = \frac{\hat{\Sigma}}{\tau} \left(1 - \frac{\hat{\Sigma}}{\hat{\Sigma}_{eq}} \right) \quad (22)$$

Where Σ_{eq} is an equilibrium or critical surface density and τ and associate time-scale. To estimate the equilibrium surface density, the surface energy is assumed locally at dynamic equilibrium with the local kinetic energy. Neglecting the viscous stresses and assuming isothermal flows, a local equilibrium condition can be expressed as

$$\Sigma_{eq} = \frac{\rho k \phi}{\sigma} \quad (23)$$

where $k = \mathbf{u} \cdot \mathbf{u}/2$ is the kinetic energy. The deviation from local equilibrium can be characterised by a critical Weber number $We^* = \rho k \phi / \sigma \Sigma_{eq}$. The original formulations of Vallet and Borghi (1999) as well as the dense flows of Lebas et al. (2009) assume $We_{den}^* \approx 1$, which correspond to the equilibrium

condition Eqn. (23). Luret et al. (2010) and the DNS studies of Duret et al. (2013), suggest that values can oscillate in a range $We_{den}^* \approx 1 - 3$.

In dilute flows, the term (22) involves surface generation by droplet break-up and surface destruction by droplet collision and an associated We_{bkp}^* is required. Reitz and Bracco (1982) found that the We_{bkp}^* is approximately constant $We_{bkp}^* \approx 12$ at low values of liquid Ohnesorge numbers ($Oh < 1$)

The critical Weber number due to droplet collision We_{coll}^* can be obtained based on an *equilibrium* Sauter mean diameter d_{32} , viz $We^* = We_{coll}(d_{32}^*)$ Lebas et al. (2009). From evaluation of several Lagrangian droplet collision models, Luret et al. (2010) found a range of critical numbers $We_{coll}^* \approx 12 - 15$. However, Luret et al. (2010) suggests that We_{coll}^* may be as small as 3.5 when non-spherical collision are considered. Chesnel et al. (2012) showed a dependency of surface density values to We^* , and a definitely single value is to be established.

Each term, S_{den} , S_{coll} and S_{bkp} have an associated time-scale, τ , in (22). Time scales associated to turbulent break-up are usually k_t/ϵ in RANS or $||\bar{S}_{ij}||^{-1}$ in LES. Collision time scales models, τ_{coll} , are based on particle collision theory, see Vallet et al. (2001), while the droplet break-up time-scale, τ_{bkp} , is obtained from Pilch and Erdman (1987). In the conventional ELSA-RANS spray formulation Beheshti et al. (2007); Lebas et al. (2009), the dense, break-up and collision surface terms must be included. To incorporate all three terms in a single formulation, the terms are weighted by an indicator function to distinguish between dilute and dense flows based on a linear function on ϕ . Duret et al. (2013) proposed instead to combine the We^* to incorporate both dilute and dense flows.

The surface equilibrium model (22) is not well defined when the surface is at rest. Under this conditions, from (23), the equilibrium surface is 0 and surface will be destroyed infinitely fast (unless $\tau \rightarrow \infty$). The existence of a liquid-gas interface implies the existence of a *minimum* surface even at rest. From (11), it can be shown that the minimum surface density is inversely proportional to the size of the integration kernel h , i.e. $\Sigma_{min} \propto 1/h$. A expression of $\Sigma_{min} \approx 1/h$ was used to define the surface boundary conditions by RANS simulations of Vallet and Borghi (1999) and Beheshti et al. (2007). Lebas et al. (2009) defined $\Sigma_{min} \approx \phi(1 - \phi)/l_t$, with l_t is a turbulent length scale and include a extra source term, $\mathcal{S}_{init}$, to generate surface at the boundaries. Chesnel et al. (2012) proposed $\Sigma_{min} \propto \sqrt{\phi(1 - \phi)}/h$ and use the decomposition $\Sigma = \Sigma' + \Sigma_{min}$ to avoid the need of using $\mathcal{S}_{init}$. The final equilibrium expression for the modified would be $\Sigma_{eq}^* = \Sigma_{eq} + \Sigma_{min}$. In the case of dense flows and using Chesnel et al. (2012) formulation, Σ_{eq}^* is:

$$\Sigma_{eq}^* = \frac{\rho k \phi}{\sigma} + C_{\Sigma} \sqrt{\phi(1 - \phi)}/h \quad (24)$$

Chesnel (2010) proposed $C_{\Sigma} = 2.4$ based on DNS results and simple geometries. Rewriting the above expression, it can be seen that $\Sigma_{min} > \Sigma_{eq}$ when the local Weber number $We_h = \rho k h / \sigma$ is smaller that a critical mesh Weber, $We_{h,crit}$

$$We_{h,crit} = C_{\Sigma} \sqrt{\frac{1 - \phi}{\phi}} \quad (25)$$

which results in $We_{h,crit} \approx 7$ in non-dilute flows, $\phi > 0.1$. In LES and RANS simulations of atomization problems, $We_h \gg We_{h,crit}$ and the results are relatively insensitive to the form of Σ_{min} . However, in very dilute flows at

lower Weber numbers, the form of Σ_{min} may be important. In principle the difficulties of using Σ_{min} could be avoided by reformulating (14) in terms of interface surface S^I , following Séro-Guillaume and Rimbart (2005), however the resultant expression would be an integro-differential equation instead of a simpler partial differential equation. In such case, the following analysis of Section 3 would not be possible, although theoretically an alternative formulation could be proposed.

2.3. The Navier-Stokes

For completeness the one-fluid incompressible Navier-Stokes equations are presented

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \sigma \kappa n_i \delta_I \quad (26)$$

In Newtonian fluids the viscous stress is $\tau_{ij} = 2\mu S_{ij}$, where the strain-rate tensor is $S_{ij} = 1/2(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$. Gravity and external forces have been discarded. In the one-fluid formulation the surface forces, $\mathbf{f}_\sigma = \sigma \kappa \mathbf{n} \delta_I$ appear explicitly in the momentum equations. The viscosity, μ , is assumed to depend linearly on ϕ , similarly to ρ , see Eqn. (2).

3. The Probability Density Function Method

3.1. The sub-grid PDF

The spatial filter of a function $f = f(\mathbf{x}, t)$ is defined as its convolution with a filter function, G , according to:

$$\bar{f} = \int_V f(\mathbf{x}', t) G(\mathbf{x} - \mathbf{x}', t; \Delta) dV' \quad (27)$$

Δ is the filter width associated with G and the filter function G is taken positive definite in order to maintain positive filtered values of positive definite functions f . A fine-grained characteristic function can be defined following Klimenko and Bilger (1999)

$$\psi(\mathbf{x}, t; \underline{\theta}) = \delta [\theta_1 - \phi(\mathbf{x}, t)] \delta [\theta_2 - \Sigma(\mathbf{x}, t)] \quad (28)$$

Where $\underline{\theta} = (\theta_1, \theta_2)$ is the sample space vector for the liquid volume ϕ and surface density Σ respectively. By using the filtering operation (27), a sub-grid (or filtered) joint *Probability Density Function*, or P_{sgs} , of fluid volume and surface density can be obtained

$$P_{sgs}(\mathbf{x}, t; \underline{\theta}) = \int_V \psi(\mathbf{x}', t; \underline{\theta}) G(\mathbf{x} - \mathbf{x}', t; \Delta) dV' \quad (29)$$

The quantity $P_{sgs}(\theta_1, \theta_2) d\theta_1 d\theta_2$ represents the probability of $\theta_1 < \phi < \theta_1 + d\theta_1$ and $\theta_2 < \Sigma < \theta_2 + d\theta_2$ to exist within a filter-width at a given position in space and time. If a solution of P_{sgs} (29) exists, the complete sub-grid size distribution of liquid structures could be described independently of the type of sub-structures (droplets or filaments) or regime (dense or dilute).

An evolution equation for the PDF can be derived from equations (3) and (14) using the rule of differentiation of generalised functions, see Gao and O'Brien (1993); Vervisch et al. (1995). The resultant sub-grid PDF equation is then

$$\frac{\partial P_{sgs}}{\partial t} + \frac{\partial \overline{u_j | \underline{\theta}} P_{sgs}}{\partial x_j} + \frac{\partial \mathcal{S}_k(\underline{\theta}) P_{sgs}}{\partial \theta_k} = 0 \quad (30)$$

where the source terms are obtained from Eqn. (14)

$$\mathcal{S}_1 = 0 \quad \mathcal{S}_2 = \mathcal{S}_{gen} = -\theta_2 n_i(\theta_1) n_j(\theta_1) \frac{\partial \tilde{u}_i}{\partial x_j} \quad (31)$$

The PDF equation (30) requires a closure model for the *conditionally filtered* velocity $\overline{\mathbf{u}|\underline{\theta}}$. This velocity is divided into a three contributions *main, turbulence* and *surface*.

$$\overline{u_j|\underline{\theta}} P_{sgs} = \bar{u}_j P_{sgs} - D_{sgs} \frac{\partial P_{sgs}}{\partial x_j} - u_j^s(\theta_2) P_{sgs} \quad (32)$$

Herrmann and Gorokhovski (2009) proposed a similar velocity decomposition for the sub-grid velocity in multiphase flows LES. The first term in (32) corresponds to the PDF transport by the filtered velocity $\bar{\mathbf{u}}$. In the second term a gradient model Schmidt and Schumann (1989) is used to represent PDF transport by sub-grid turbulent fluctuations, with a sub-grid diffusivity coefficient. This is a standard procedure in LES-PDF for combustion, see Jones and Navarro-Martinez (2009). The gradient model may not be accurate in the presence of sub-grid counter-gradient transport, however no simple alternatives exist in the PDF context. The term accounts for scalar transport by sub-grid fluctuations and its role is similar to the terms $\overline{\mathbf{u}\phi} - \bar{\mathbf{u}}\bar{\phi}$. Labourasse et al. (2007) showed that Smagorinsky-type closures may not be adequate close to the interface and a scale similarity model is preferred in the work of Chesnel et al. (2012). The implementation of a scale similarity model in a PDF context is complex and in the present work a Smagorinsky-type model is retained. The sub-grid diffusivity is then proportional to the

turbulent viscosity (see Section 4)

$$D_{sgs} = \frac{\nu_{sgs}}{Sc_{sgs}} \quad (33)$$

Where in analogy to the RANS mass-weighted model, the sub-grid Schmidt number takes a value of ρ_g/ρ_l , which corresponds to a value of $Sc_{sgs} = 1$ in the gas phase.

The last term in (32) represents the restorative velocity, which is assumed to depend only on surface density, similarly to the second term in Eqn. (19). Assuming that $\mathbf{u}^s \approx K \vec{\nabla} \Sigma$ and that K is weakly dependent on position, it can be shown that:

$$\frac{\partial u_j^s P_{sgs}}{\partial x_j} \approx \frac{\partial \mathcal{S}_{des} P_{sgs}}{\partial \theta_2} \quad (34)$$

where $\mathcal{S}_{des} = K \nabla \Sigma \nabla \Sigma$ is an unclosed positive term, which destroys surface density. This term has similarities to the micro-mixing or scalar dissipation, which arise from the molecular diffusion term, see Pope (1981). The term in Eqn. (34) vanishes if the surface is at equilibrium, which not necessary imply a zero gradient in surface density. In the present work a phenomenological model is assumed for $\mathcal{S}_{des}$ in the same shape as the models used for the $\Sigma - Y$ or ELSA models, see Equation (22), viz:

$$\mathcal{S}_{des}(\theta_2) = \frac{1}{\tau} \left(\frac{\theta_2}{\Sigma_{eq}^*} \right) \theta_2 \quad (35)$$

The model is directly applied to the sample space θ_2 , and therefore there are no physical scales; the phase space can be considered to be always "dense" and the corresponding critical Weber number is taken as $We^* \approx 1$ (Σ_{eq}^* is taken from Eqn. 24). Sub-grid scales effects, collisions and sub-grid droplets

appear indirectly through their effects in the PDF. The equilibrium time-scale τ is assumed to be the same as $\mathcal{S}_{gen}$ and is taken as $1/\tau = |\mathcal{S}_{gen}|/\theta_2$. Both $\mathcal{S}_{gen}$ and $\mathcal{S}_{des}$ can only exist if there is certain liquid volume $\theta_1 > 0$ and surface density $\theta_2 > 0$. The Σ_{min} needed in Σ_{eq}^* is taken from the empirical definition of Chesnel (2010).

The final closed sub-grid joint PDF transport equation is

$$\begin{aligned} \frac{\partial P_{sgs}}{\partial t} + \frac{\partial \bar{u}_j P_{sgs}}{\partial x_j} = \frac{\partial}{\partial x_j} \left[D_{sgs} \frac{\partial P_{sgs}}{\partial x_j} \right] \\ - \frac{\partial \mathcal{S}_{gen}(\underline{\theta}) P_{sgs}}{\partial \theta_2} + \frac{\partial \mathcal{S}_{des}(\underline{\theta}) P_{sgs}}{\partial \theta_2} \end{aligned} \quad (36)$$

In the present work, a joint-scalar PDF approach has been followed. It would be theoretically possible to use a joint velocity-scalar PDF, $P_{sgs}(\underline{\theta}, \underline{U})$, following for example Gicquel et al. (2002). The conditional filtered velocity (32) in this case would be closed and there would be no need of model (35). Nevertheless, extra unclosed terms will appear in the modelling of the conditional stress and pressure terms, with all the known drawbacks of joint velocity scalar methods, see Haworth (2010). In the case of variable density flows, a similar formulation (36) could be obtained by introducing a density weighted PDF $\overline{\rho\psi} = \bar{\rho}\tilde{P}_{sgs}$. Similarly, in the case of evaporating flows, a term should be added in the RHS of the transport equations (3) and (14), that would results in new terms added to the PDF equation (36). These terms would account for the volume of liquid lost by evaporation (a term proportional to Σ) and the associated surface destruction.

3.2. The Stochastic Fields Formulation

The transport equation (36) is a Fokker-Planck equation. It is possible to solve directly this equation using Eulerian methods, see for example Fox (2003), and solve only a small set of moments using a Direct Quadrature Method of Moments (DQMOM) approach. The most common method is to solve an equivalent system of Stochastic Differential Equations (SDE) based on Lagrangian particles. This system of "notional" particles has the same moments that the original PDF equation. Such system scales linearly with the number of independent variables, unlike deterministic methods, and therefore permits to solve Eqn. (36) at a reasonable cost.

An alternative to Lagrangian particles is the Eulerian Stochastic Fields method proposed by Valiño (1998). The Stochastic Fields solution is based on deriving an equivalent system of Stochastic Partial Differential Equations (SPDE) equivalent to the PDF transport equation. The Eulerian field solution for the system of SPDEs is defined in the whole space and does not correspond to any "realisation" of the system. The fields solution represent an equivalent system with the same moments as Eqn. (36). The Stochastic Fields formulation was extended to LES by Mustata et al. (2006) and has been applied successfully to a large number of problems in turbulent reacting flows in this context: see Jones and Navarro-Martinez (2007); Jones et al. (2012); Bulat et al. (2013); Dodoulas and Navarro-Martinez (2013); Dumond et al. (2013) among others.

In the present work, the equivalent PDF can be defined from N stochastic fields as:

$$P_{sgs} = \frac{1}{N} \sum_{\alpha=1}^N \delta[\theta_1 - \phi^\alpha(\mathbf{x}, t)] \delta[\theta_2 - \Sigma^\alpha(\mathbf{x}, t)] \quad (37)$$

Each stochastic field, α , would have its own liquid volume fraction and surface density, ϕ_α and Σ_α . To derive the equivalent SPDE equation two approaches exist depending on the interpretation of the stochastic integral: Valiño (1998) following Ito and Sabel'nikov and Soulard (2005), following Stratonovich. In the Ito formulation, the transport equations for the stochastic fields are

$$\begin{aligned} \frac{d\phi^\alpha}{dt} + \bar{u}_j \frac{\partial \phi^\alpha}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[D_{sgs} \frac{\partial \phi^\alpha}{\partial x_j} \right] \\ &\quad + \sqrt{2D_{sgs}} \frac{\partial \phi^\alpha}{\partial x_j} dW_j^\alpha \\ \frac{d\Sigma^\alpha}{dt} + \bar{u}_j \frac{\partial \Sigma^\alpha}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[D_{sgs} \frac{\partial \Sigma^\alpha}{\partial x_j} \right] \\ &\quad + \sqrt{2D_{sgs}} \frac{\partial \Sigma^\alpha}{\partial x_j} dW_j^\alpha + \mathcal{S}_{gen}^\alpha - \mathcal{S}_{des}^\alpha \end{aligned} \quad (38)$$

Where $d\mathbf{W}^\alpha$ is a Wiener term of 0 mean and variance $\sqrt{dt}$. The notation $d\phi^\alpha$ indicates that the stochastic fields are differentiable in space but discontinuous in time. The solutions of equations (38) preserve the boundedness of the scalar as the gradient of the fields vanish as the scalars approach extrema values. In a very fine LES, where $\Delta \rightarrow 0$, D_{sgs} would disappear (as well as $\mathcal{S}_{des}$, through $\Sigma_{min} \rightarrow \infty$) and all the fields will collapse towards the Eqns. (3) and (14).

The first-moments (or filtered values) can be obtained by averaging the stochastic fields solution

$$\bar{\phi} = \frac{1}{N} \sum_{\alpha=1}^N \phi^\alpha \quad (39)$$

Similarly, sub-grid higher moments of ϕ and Σ can be obtained. Applying the averaging operator to Eqns (38) over a large number of fields we obtained Chesnel et al. (2012) equations for filtered volume and surface density.

$$\begin{aligned}\frac{\partial \bar{\phi}}{\partial t} + \bar{u}_j \frac{\partial \bar{\phi}}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[D_{sgs} \frac{\partial \bar{\phi}}{\partial x_j} \right] \\ \frac{\partial \bar{\Sigma}}{\partial t} + \bar{u}_j \frac{\partial \bar{\Sigma}}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[D_{sgs} \frac{\partial \bar{\Sigma}}{\partial x_j} \right] + \overline{\mathcal{S}_{gen}} - \overline{\mathcal{S}_{des}}\end{aligned}\quad (40)$$

The equivalent SPDE transport equations for the stochastic fields in Stratonovich interpretation are

$$\begin{aligned}\frac{d\phi^\alpha}{dt} + (\bar{u}_j + u_j^{g,\alpha} + u_j^d) \frac{\partial \phi^\alpha}{\partial x_j} &= 0 \\ \frac{d\Sigma^\alpha}{dt} + (\bar{u}_j + u_j^{g,\alpha} + u_j^d) \frac{\partial \Sigma^\alpha}{\partial x_j} &= \mathcal{S}_{gen}^\alpha - \mathcal{S}_{des}^\alpha\end{aligned}\quad (41)$$

Where $\mathbf{u}^{g,\alpha}$ and $\mathbf{u}^d$ are the Gaussian and drifts velocities respectively given by:

$$\begin{aligned}u_j^{g,\alpha} &= \sqrt{2D_{sgs}} \circ \frac{dW_j^\alpha}{dt} \\ u_j^d &= -\frac{1}{2} \frac{\partial D_{sgs}}{\partial x_j}\end{aligned}\quad (42)$$

Where $\circ$ denotes Stratonovich interpretation of the stochastic integral, which preserves the results of classical calculus. By using the Ito-Stratonovich transformation Gardiner (1983) it can be shown that the systems (38) and (41) are equivalent. Both formulations are relatively easy to implement in existent CFD code as they are fully Eulerian and there is not any restriction on the type of spatial discretization schemes to be used. The Ito equations(38)

form a system of convection-diffusion equations and therefore it is not possible to define an sharp interface between liquid and gas in every stochastic field. The Stratonovich equations, (41), are hyperbolic in nature. The solution of the system propagates information along stochastic characteristic paths Jones and Navarro-Martinez (2009). The stochastic fields can be therefore discontinuous in space and a sharp interface could exist at field level. High-resolution schemes, such as level-set, could then be used to solve the stochastic field equation for volume of fluid.

Once the stochastic field equations have been advanced, all relevant parameters can be obtained directly. Being an Eulerian approach, a geometric normal per field can be defined $\mathbf{n}^\alpha = -\vec{\nabla}\phi^\alpha$ despite not being an interface in the physical sense. A characteristic length per stochastic field, $\mathcal{L}_{32}$ which would be the corresponding Sauter Mean Diameter (SMD) in mono-dispersed sprays ($\mathcal{L}_{32} \equiv d_{32}$) can be defined as

$$d_{32}^\alpha = \frac{6\phi^\alpha}{\Sigma^\alpha} \quad (43)$$

where the relevant filtered moments, $\bar{d}_{32}$ could be obtained directly by (39). The Eulerian nature of the method allows to obtain directly the instantaneous sub-grid droplet size distribution $DSD(\mathbf{x}, t; d_{32})$, by directly sampling the results of Eqn. (43).

Computing the filtered moments from a stochastic calculation (either particles or fields) introduces an error proportional to the sub-grid variance and inversely proportional to the square root of the number of samples $\sim \text{Var}_{sgs}/\sqrt{N}$. Sub-grid variances of instantaneous distributions are much smaller than time-average DSDs, especially if Δ is small. The statistical er-

ror may still be significant for instantaneous filtered moments at low number of fields, however its effects will be relatively small in large scale droplets distributions or in stationary flows, which involve calculations over thousands of time steps. In spray simulations where secondary atomization (mostly a sub-grid phenomenon) is important, the number of fields will need to be increased.

4. Large Eddy Simulations

Using the filter definition (27) the following set of equations are obtained from the Navier-Stokes equations (26):

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0 \quad (44)$$

$$\begin{aligned} \bar{\rho} \frac{\partial \bar{u}_i}{\partial t} + \bar{\rho} \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = & -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (2\bar{\mu} \bar{S}_{ij}) \\ & + \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \bar{f}_{\sigma,i} + f_{\rho,i}^{sgs} + f_{\mu,i}^{sgs} \end{aligned} \quad (45)$$

Where $\tau_{ij}^{sgs} = \overline{\rho u_i u_j} - \bar{\rho} \bar{u}_i \bar{u}_j$ is the unknown sub-grid stress. The sub-grid trace free stress is assumed proportional to the strain rate in a standard Smagorinsky (1963) model, viz:

$$\tau_{ij}^{sgs} - \frac{1}{3} \tau_{kk}^{sgs} = 2\bar{\rho} \nu_{sgs} \bar{S}_{ij} \quad (46)$$

where the proportionality constant has units of the kinematic viscosity and is often referred to as a turbulent (or sub-grid) kinematic viscosity ν_{sgs} and is modelled as

$$\nu_{sgs} = (C_S \Delta)^2 ||\bar{S}_{ij}|| \quad (47)$$

Where $||\bar{S}_{ij}|| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$ is the Frobenius norm of the filtered strain rate. The Smagorinsky Constant, C_S , is obtained using the Dynamic approach of Piomelli and Liu (1995). In incompressible flows, the trace of the sub-grid stress is absorbed into the pseudo-pressure $\bar{p}^* = \bar{p} - \tau_{kk}^{sgs}/3$

The filtered surface forces can be decomposed, following Herrmann and Gorokhovski (2009) in:

$$\overline{f_{\sigma,i}} = \sigma \bar{\kappa} \bar{n}_i \bar{\delta}_I + f_{\sigma,i}^{sgs} \quad (48)$$

Where the first term represent the surface forces at resolved scale and the second term represent the effect of capillary forces on sub-grid scales. The numerical modelling of the first term is not trivial as there is no clear interface at the filtered field $\bar{\phi}$. Chesnel et al. (2012) defined the filtered normal $\bar{\mathbf{n}} = -\nabla \bar{\phi}$ and a mean curvature $\bar{\kappa} = -\nabla \cdot \bar{\mathbf{n}}$. It is common to neglect $\mathbf{f}_{\sigma}^{sgs}$ in atomization problems, arguing that their effect would be negligible at the high Weber numbers expected: See the works by Villier et al. (2004); Bianchi et al. (2007); Ishimoto et al. (2008); Chesnel et al. (2012). Nevertheless, curvature is largest at the smallest scales and sub-grid surface tension forces must play a dominant role there. Models for $\mathbf{f}_{\sigma}^{sgs}$ are relative new, see Herrmann and Gorokhovski (2009), and difficult to implement in a general form. Chesnel et al. (2010) performed a budget analysis of this term in a atomization DNS and the results showed that $\mathbf{f}_{\sigma}^{sgs}$ to be much smaller than the large scale contribution and other terms in momentum equation. In this work $\mathbf{f}_{\sigma}^{sgs} \approx 0$ and the surface tension forces in the largest scales has been

implemented using the Continuum Surface Force approach Brackbill et al. (1992) with a mean curvature.

The use of conventional filtering instead of density weighting creates sub-grid interphase forces that arise from the large variation of density and viscosity, see formulations by Liovic and Lakehal (2007); Labourasse et al. (2007)

$$f_{\rho,i}^{sgs} = \frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i - \overline{\rho u_i}) \quad (49)$$

$$f_{\mu,i}^{sgs} = \frac{\partial}{\partial x_j} 2 (\overline{\mu S_{ij}} - \bar{\mu} \bar{S}_{ij}) \quad (50)$$

The modelling of the $\mathbf{f}_\rho^{sgs}$ could be avoided by using a density weighted filter $\overline{\rho f} = \bar{\rho} \tilde{f}$. However this will involve to use a general continuity equation as $\nabla \cdot \tilde{\mathbf{u}} \neq 0$, which can cause instabilities in pressure-based methods with large density variation. The behaviour of this term is not clear and a-priori DNS tests of Labourasse et al. (2007) showed its contribution to be non-linear with filter width; Chesnel et al. (2010)'s study found the term to be significant and its contribution up to 30 % the resolved part depending on filter width and flow region. Chesnel et al. (2010) proposed a scale similarity model, viz :

$$\mathbf{f}_\rho^{sgs} = \frac{\partial}{\partial t} [C_\rho (\widehat{\widehat{\rho \mathbf{u}}} - \widehat{\widehat{\rho}} \widehat{\widehat{\mathbf{u}}})] \quad (51)$$

where in this context $\widehat{\cdot}$ is a test-filter. However, there are uncertainties on the choice of C_ρ . Due to this uncertainties the sub-grid force $\mathbf{f}_\rho^{sgs}$ has been neglected in this study. Errors can then be expected in regions with large sub-grid velocity and density variations.

The closure of the term $\mathbf{f}_\mu^{sgs}$ does not depend largely on the filter-type and a-priori always need modelling The budget balance of Chesnel et al. (2010)

suggest that on average $\langle \nabla \tau^{sgs} \rangle \gg \langle \mathbf{f}_\mu^{sgs} \rangle > \langle \mathbf{f}_\sigma^{sgs} \rangle$. Similar results were obtained by Vincent et al. (2008), where the term was found to be less than 0.5 % compared to the other terms in Eqn (46) , and Labourasse et al. (2007) who found the contribution to be "small". Accordingly in this work, $\mathbf{f}_\mu^{sgs}$ has been neglected.

The one-field LES formulation (46) does not have information about the relative velocity between liquid and gas (the slip velocity). The slip velocity may affect the vaporisation rate and cause that large sub-grid drops have higher fluctuations than small ones Beheshti et al. (2007). In a RANS context, Beheshti and Burluka (2004) solved an additional transport equation for the slip velocity. However, Beheshti et al. (2007) suggests that variable density effects are more important to jet spreading than slip velocity. In LES, the slip velocity has a much lower effect, as its effects are limited to instantaneous sub-grid scales. In the present study, no attempt has been done to include these effects. A large-scale time-average slip velocity could be then estimated by $\langle \langle \bar{\mathbf{u}} | \phi_{den} \rangle - \langle \bar{\mathbf{u}} | \phi_{dil} \rangle \rangle$.

In order to close the momentum equation and link it with the PDF solution, the filtered density and viscosity are obtained from:

$$\bar{\rho} = (1 - \bar{\phi})\rho_g + \rho_l\bar{\phi} \quad (52)$$

and

$$\bar{\mu} = (1 - \bar{\phi})\mu_g + \mu_l\bar{\phi} \quad (53)$$

where $\bar{\phi}$ is obtained from the stochastic field solutions using the average (39).

5. LES of liquid atomization

5.1. Test Case

The model presented in sections 3 and 4 is compared with DNS results of primary atomization. The test case is based on a set-up by Menard et al. (2007) and it was computed by Chesnel et al. (2010). The configuration is a relatively simple liquid jet issuing into a quiescent air and is characteristic of a moderate Pressure Diesel injector. The database have time-averaged results of Σ and ϕ and is a good test to asses the model. The same configuration was studied previously using RANS by Beau et al. (2005) and Lebas et al. (2009); and using LES by Chesnel et al. (2012). The physical parameters are shown in Table 1.

The DNS results showed a very complex pattern of atomization, with droplets and ligaments shedding from the main liquid core jet. The core liquid jet is surrounded by a cloud of small fragments/droplets. The definition of the minimum mesh size in a multiphase flow DNS is not clear and there is not clear consensus in the literature, see Shinjo and Umemura (2010) and Duret et al. (2012). Menard et al. (2007) assumed that no secondary break-up was occurring at scales below the DNS resolution; The simulations showed that the local Weber number was $We_h < 10$. Gorokhovski and Herrmann (2008) suggest that the results were not a "true" DNS as $We_h > 1$, and artificial droplets were present.

5.2. Numerical Implementation

The in house code BOFFIN created by Jones et al. (2002) was used for the present LES computations. The present version used comprises a second-

order-accurate finite volume method, based on a fully implicit low-Mach-number formulation using a staggered storage arrangement. Spatial derivatives for the momentum equation are approximated by standard second-order central differences. The momentum equations are integrated using a second-order Crank-Nicholson scheme.

In this work, the Ito formulation (38) is retained, the comparison of stochastic fields implementation is beyond the scope of this work Jones and Navarro-Martinez (2009) showed little difference in the context of turbulent combustion. The stochastic field are solved using an operator-splitting technique: The *convective* step uses a modified CICSAM scheme Ubbink and Issa (1999) using the field-normal $\mathbf{n}^\alpha$ to minimise numerical diffusion, while the *diffusive* step uses central derivatives. An alternative scheme, a 5th order WENO scheme from Jiang and Peng (2000), was implemented. However the advantage of locally refining the mesh by the CICSAM approach out-weights the higher accuracy obtained by the more expensive WENO scheme. As mentioned in Section 4, there is no limitation to the schemes to be used as long as they are bounded. The spatial gradient appearing in the stochastic term (38) in the Ito formulation is approximated using central differences.

The time difference of the Ito process is discretized using the Euler-Maruyama scheme from Kloeden and Platen (1992). The Wiener process (or random walk) is modelled with a weak approximation, $dW_j^\alpha = \sqrt{dt}\eta_j^\alpha$, where η_j^α is a $\{-1, 1\}$ dichotomic random vector, see Gardiner (1983) for details. This approximation reduces the error from random number generators when a small number of samples are used. The resultant scheme is *weakly* consistent of order $\sqrt{dt}$ in the sense of Kloeden and Platen (1992).

Two grids were tested: a $256 \times 64 \times 64$ cells, on a domain of $5 \text{ mm} \times 2 \text{ mm} \times 2 \text{ mm}$ this grid will be hereafter denoted LES-COARSE. A secondary mesh of $256 \times 128 \times 128$ was used on a shorter domain of $2.5 \text{ mm} \times 2 \text{ mm} \times 2 \text{ mm}$ (hereafter LES-FINE). The computational domains are larger than the original DNS calculations, the grids are stretched towards the shear of the jet at $r = D/2$. The relative mesh-size ratio between coarse and fine mesh is 2. The smallest cells in the fine mesh are $5 \text{ }\mu\text{m}$ cells in y and z with $10 \text{ }\mu\text{m}$ in x (axial direction). The number of cells within the jet is 10 for LES-COARSE and 20 for LES-FINE. While adequate LES resolution in multiphase flows is difficult to define, both meshes will resolve the largest part of the energy spectrum in an equivalent, single-phase, simulation of a jet. The filter width, Δ , used in the LES is taken as the cubic root of the local volume cell. The cell expansion ratio is small (3.5%) to minimise commutative errors in the filtering of the derivatives. The local Weber numbers are in average $We_{\Delta} > We_{h,crit}$. The DNS simulation use a digital inflow generator from Klein et al. (1998) with an turbulent length scale of $\mathcal{L}_t = 10 \text{ }\mu\text{m}$ and an inflow with a turbulence intensity of 5 %. In the present LES, nor the fine or the coarse mesh, have enough resolution to accurately capture such small turbulent fluctuations as $\Delta \sim \mathcal{L}_t$. To simplify the inflow conditions, simpler axial and azimuthal perturbations are superimposed to mean profile, following the implementation of Navarro-Martinez et al. (2005).

The system of equations (38) need appropriate boundary conditions. In the absence of more knowledge about the sub-grid inlet conditions, the boundary conditions are assumed to be known with negligible sub-grid variance: $\phi^{\alpha}(0, t) = \bar{\phi}(0, t)$ and $\Sigma^{\alpha}(0, t) = \bar{\Sigma}(0, t)$. The incoming surface is

defined at the inflow interface cell as $\bar{\Sigma}(0, t) = 1/\Delta \equiv \Sigma_0$

The number of fields chosen in the simulation is $N = 16$, which is double the typical number used in LES-PDF simulations of reactive flows. Jones and Navarro-Martinez (2007) stochastic field simulations, showed small differences in time-averaged moments between $N = 8$ and $N = 16$. A compromise must be established in practical simulations between reducing Δ and improve the *instantaneous* PDF resolution (increase N). The cost of the simulation is cubic with the number of grid points, while grows linearly with N . The present calculation where performed in a 8-core personal workstation and the fine mesh solution took approximately 3 days for converged statistics.

5.3. Results

The surface density equation results are very sensitive to the initial and boundary conditions. A finer mesh would produce higher values of surface density even in DNS. In dense regions, the values of Σ predicted by LES will scale with $1/\Delta$, while in diluted regions where only sub-grid structures are present Σ will scale with $1/\Delta^3$. In order to compare directly between the LES and the DNS results, both solutions are normalized by their respective Σ_0 .

The qualitative behaviour of the surface density evolution can be seen in Figure 1, where an instantaneous snapshot is shown. Surface density grows along the interface, as the surface wrinkles. After 5-10 jet diameters, the jet starts to break and the surface density quickly increases. In the downstream region there are severe intermittency in the surface generation. In Fig. 1, the iso-contour $\bar{\phi} = 0.5$ gives an approximation of the spray penetration and the convolution of the surface

The mean liquid dispersion results can be seen in Figures 2 and 3. The LES-COARSE results show a rapid decay of the volume fraction, while LES-FINE predictions indicate a much better agreement on liquid penetration and primary break-up. Both grid show a similar level of mean volume of fluid at $x/D > 15$. The early break-up of the coarse mesh can be attributed to insufficient grid resolution; LES-COARSE does not capture accurately the inflow fluctuations and the mesh is much larger than $\mathcal{L}_t$ in the jet core. Nevertheless, the LES-FINE results showed a much better agreement with the DNS database (see Fig. 3), with acceptable results at all stations, despite an over-prediction in the centreline at $x/D = 10$ and a larger spreading at $x/D = 20$, where LES overestimates the DNS by approximately 30 % at $r/D = 1$. The quality of predictions is similar to the LES of Chesnel et al. (2012) , despite using different meshes and sub-grid closures. The reasons of the discrepancy in the liquid volume fraction predictions at the point of jet-break-up are not known and Chesnel et al. (2012) showed similar effect. Overall, the average dispersion is well captured; the spray angle is approximately $17^\circ - 20^\circ$ (obtained from iso-contour $\bar{\phi} = 0.01$) which agrees well to the spray angle of 19.2° obtained with Reitz and Bracco (1982) correlation.

In Figure 4, the mean surface density profiles are shown along the centreline. The position of the maximum surface density, at approximately 10 nozzle diameters, is correctly captured as well as levels far downstream, suggesting that the main surface growth and destruction mechanisms are captured correctly. The error in the dispersion of the liquid fraction in the LES-COARSE is carried out, and the surface density spreads excessively in the coarsest mesh.

Chesnel et al. (2012) showed variations of maximum Σ of 50%, depending on the values of We^* used (6 and 15) despite the simulation been mostly a dense flow. The present LES-PDF results showed a closer agreement to DNS data using effectively a $We^* = 1$. No conclusions can be directly inferred between models, as the results of Chesnel et al. (2012) were obtained with a filtered surface equation, with different τ . In dense flows the present formulation may be advantageous as the generation/destruction term depends on the surface orientation through $\mathbf{nn} : \nabla \bar{\mathbf{u}}$. A simulation neglecting the surface destruction term $\mathcal{S}_{des} = 0$, lead to surface density values more than 100 times larger after 10 jet diameters and therefore 100 times smaller structures. This suggests that the $\mathcal{S}_{des}$ term plays a key role in spray atomization and accurate modelling is key.

In Figure 6, a snapshot of LES-FINE in the dilute part of the spray is shown. Surrounding the jet core, turbulence stripes small-scale structures (of the order of 2-4 μm) After 10-15 jet diameters, larger structures of 5-8 μm are observed. It is to know the detail of the structures generated and distinguish if they are droplets or liquid ligaments; only knowledge of its characteristic length $\mathcal{L}$ (and its moments) is possible. In the 25 jet diameters computed in the LES-FINE and original DNS calculations, is not possible to observe a large dilute region. However, the picture is qualitatively similar to the experimental observations of Mayer and Branam (2004) where droplets were quickly formed without a coaxial flow. In Figure 7, the structures formed in the dilute region in the LES-COARSE simulation are shown with a domain extending 50 diameters. The behaviour is qualitatively similar to the LES-FINE at $x < 25D$ with a larger dilute region with structures

between 2 and 6 μm

In Figure 8, the instantaneous normalised sub-grid DSD over a 3Δ region close to the end of the domain ($x = 48D$) is shown. The DSD (or PDF) showed a relatively wide range of structure with sizes from 2.5 to nearly 10 μm , whereas the minimum droplet diameter in the DNS calculations was estimated at 2.4 μm . The cell under consideration has a filtered mean $\bar{d}_{32} = 5.26 \mu\text{m}$ with a sub-grid root mean square of $\bar{d}''_{32} = 1.33 \mu\text{m}$. The time-averaged SMD at the same location is $\langle d_{32} \rangle = 8.08 \mu\text{m}$ with a time root mean square of $\langle d'_{32} \rangle = 2.33 \mu\text{m}$. As expected, the sub-grid fluctuations of droplets sizes are of the order of temporal fluctuations, $\bar{d}'' \sim \langle d' \rangle$. Without any more detailed information on the size of the structures from the DNS (the DNS domain was shorter) it is impossible to validate the actual distribution observed in Fig. 8. However it should be possible, even if the surface density scaled with Δ , to compare characteristic lengths $\mathcal{L}$ as they should be independent on mesh spacing. There are significant large fragments even at 50 jet diameters and the regime locally can be defined in transition: the droplets cannot be assumed to be spherical and certainly not mono-dispersed.

To understand the effects of the sub-grid model, a simulation was carried out neglecting the sub-grid modelling of surface density and liquid volume by using one field only $N = 1$. This will assume that $\bar{\mathcal{S}} = \mathcal{S}(\bar{\phi}, \bar{\Sigma})$ and the governing equations would be (40). The results are shown in Figure 9. In the region before jet break-up, both simulations predict similar levels of surface density, suggesting that sub-grid fluctuations are small in that region. This regions correspond to the initial DNS domain. After approximately 20 diameters, the sub-grid effects become relevant. Without any sub-grid model

the average surface is destroyed too quickly and structure predicted and 5 times larger. The LES-PDF suggest that the mean surface density stabilises after 50 diameters, suggesting than characteristic sizes become more uniform.

6. Conclusions

This paper presents a novel method to compute spray atomization using a LES-PDF approach with Stochastic Fields. To the author's knowledge this is the first implementation of LES-PDF for spray atomization. The method permits to obtain instantaneous sub-grid characteristic length distributions. The PDF treatment of the equation, allows to simplify the modelling of the surface density source term. Uncertainties in the definition of We^* are reduced as sampling space is always dense. The Eulerian nature of the stochastic field method allow the model to be easily implemented in CFD codes using high-order numerical schemes and with structures or unstructured approaches. The model does not need coupling with a secondary Lagrangian LES as smallest scales are represented. The method can be extended to evaporating and reacting flows by adding species and energy equations to the model. Preliminary results showed the ability of the model to reproduce DNS results, regarding the dispersion of the liquid phase and the surface density. The method naturally allows for break-up of sub-grid scales. It is very difficult to any practical computation to capture exactly the detailed inflow conditions, especially with small, high-frequency fluctuations. There are uncertainties in the sub-grid closures, especially in the momentum equations. This are not exclusive of this approach but of all LES model of multiphase flows. A full joint velocity-scalar PDF may potentially reduce

uncertainty. Sub-grid droplet fluctuations are of the same order of the time counterparts, suggesting that sub-grid modelling is necessary for accurate results and it becomes more relevant in secondary atomization. Although the present paper show results with primary atomization; the RANS results of Beheshti et al. (2007) of air-blast atomization using the $\Sigma - Y$ model suggest that the model can be used to simulate secondary atomization and consequently all spray regions: from nozzle, to the secondary atomization. The model does not need coupling with a secondary Lagrangian LES as smallest scales are represented. Extensions to evaporating and reacting flows could be implemented very simply by adding species and energy equations to the model.

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Gas density	25 kg m^{-3}
Liquid density	696 kg m^{-3}
Gas viscosity	10^{-5} Pa s
Liquid Viscosity	$1.18 \times 10^{-3} \text{ Pa s}$
Surface tension	0.06 N m^{-1}
Injection diameter (D)	$100 \text{ }\mu\text{m}$
Bulk flow velocity	79 m s^{-1}
Liquid Reynolds	4659
Liquid Weber	7239

Table 1: Physical Parameters from Chesnel et al. (2012)

Figure 1: Snapshot of $\bar{\Sigma}/\Sigma_0$ in the centre-plane at $z = 0$ (LES-FINE). The black line indicates iso-contour of $\bar{\phi} = 0.5$

Figure 2: Axial distribution of liquid volume fraction. Symbols indicate DNS data from Chesnel et al. (2012)

Figure 3: Radial distribution of liquid volume fraction along. Legend as in Fig 2

Figure 4: Axial distribution of liquid surface density Σ/Σ_0 . Legend as in Fig 2

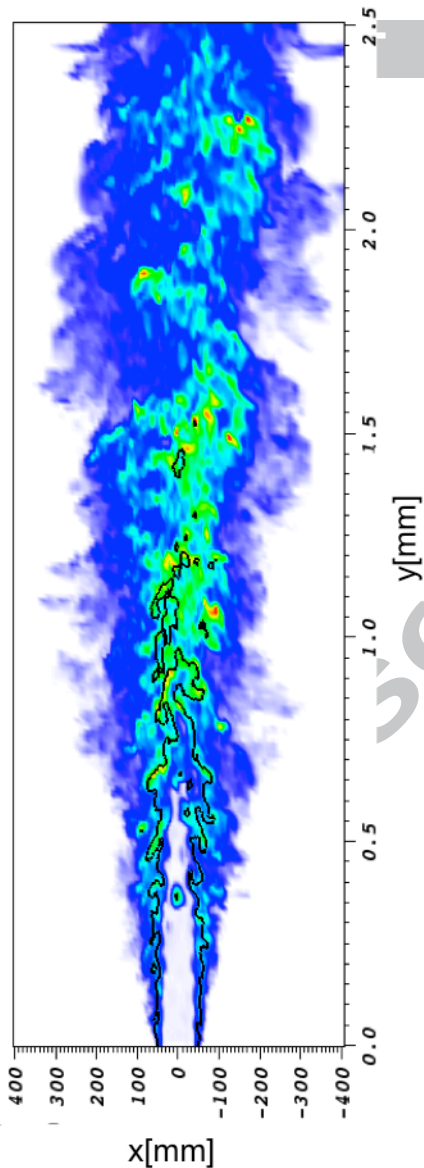
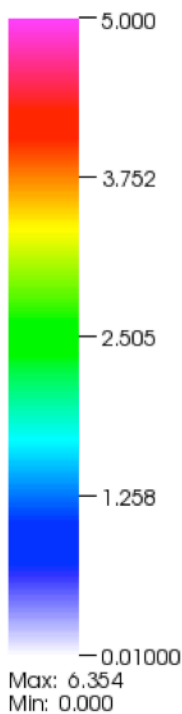
Figure 5: Radial distribution of liquid surface density Σ/Σ_0 . Legend as in Fig 2

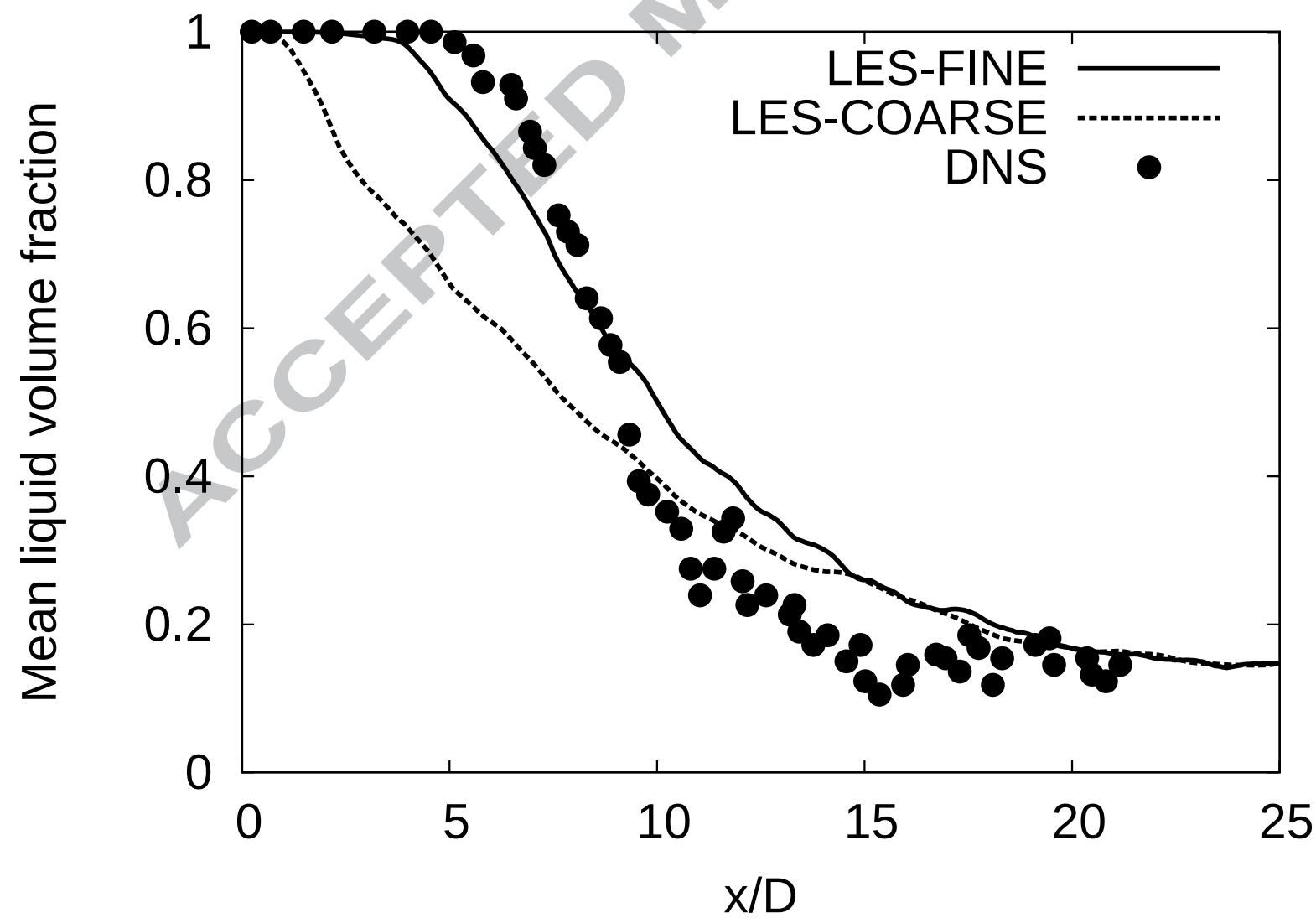
Figure 6: Snapshot of $\bar{d}_{32}$ in the centre-plane at $z = 0$ (LES-FINE). The values shown are in the dilute region of $\bar{\phi} < 0.1$. The black line indicates the iso-contour $\bar{\phi} = 0.1$

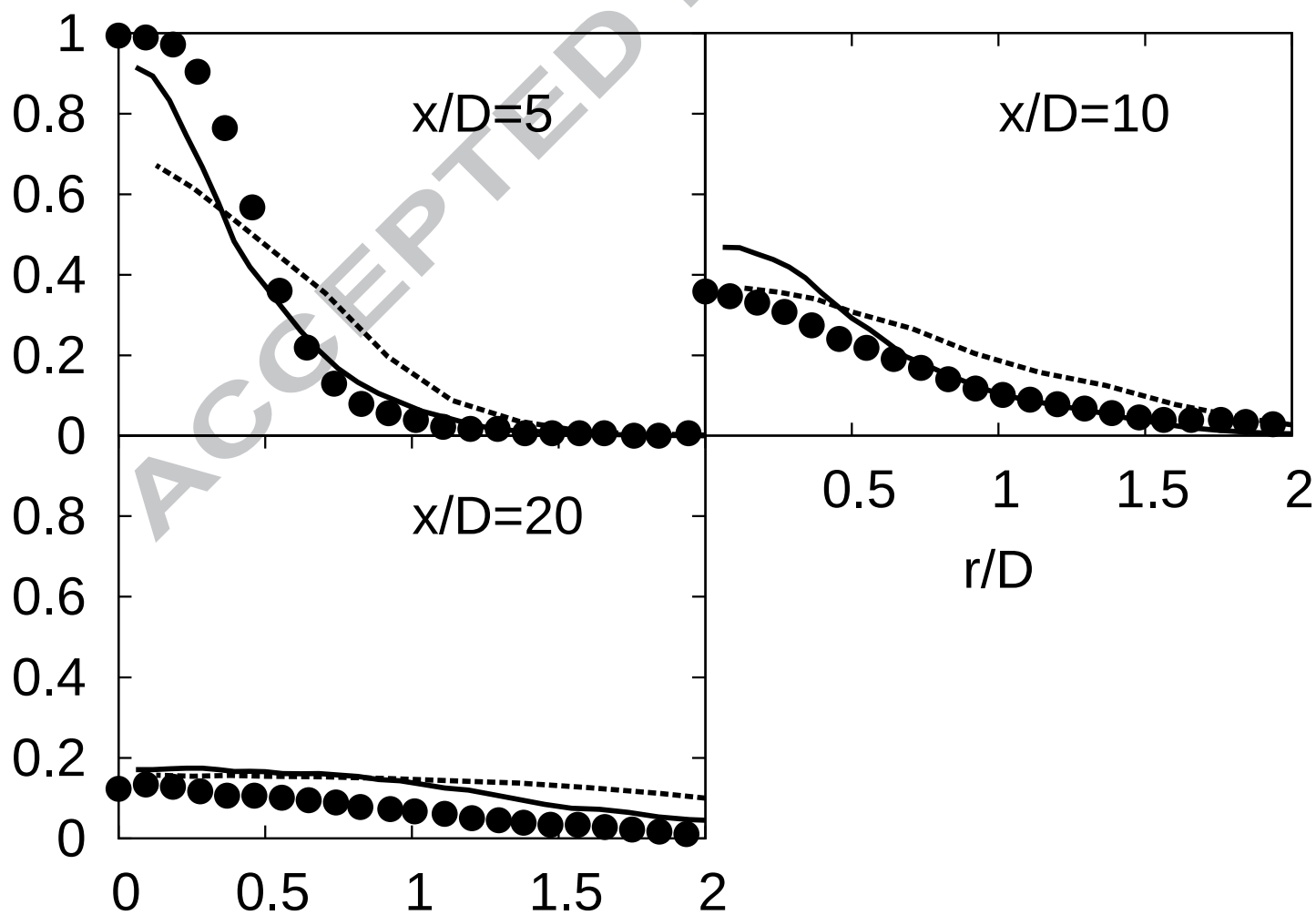
Figure 7: Snapshot of $\bar{d}_{32}$ in the centre-plane at $z = 0$ over a longer domain. The values shown are in the dilute region of $\bar{\phi} < 0.1$. The black line indicates the iso-contour $\bar{\phi} = 0.1$

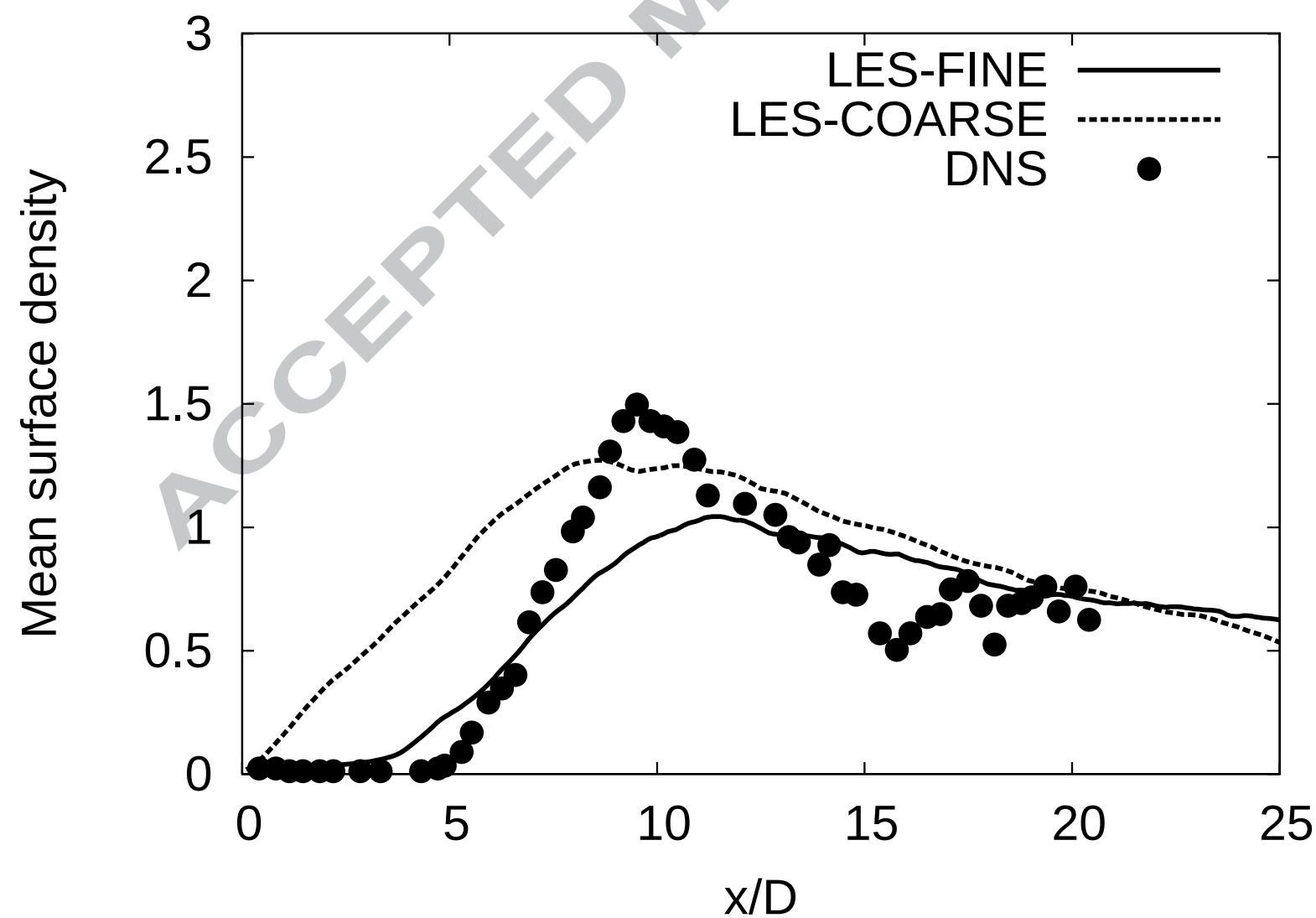
Figure 8: Instantaneous of sub-grid PDF of d_{32} at $(48D, 0, 0)$

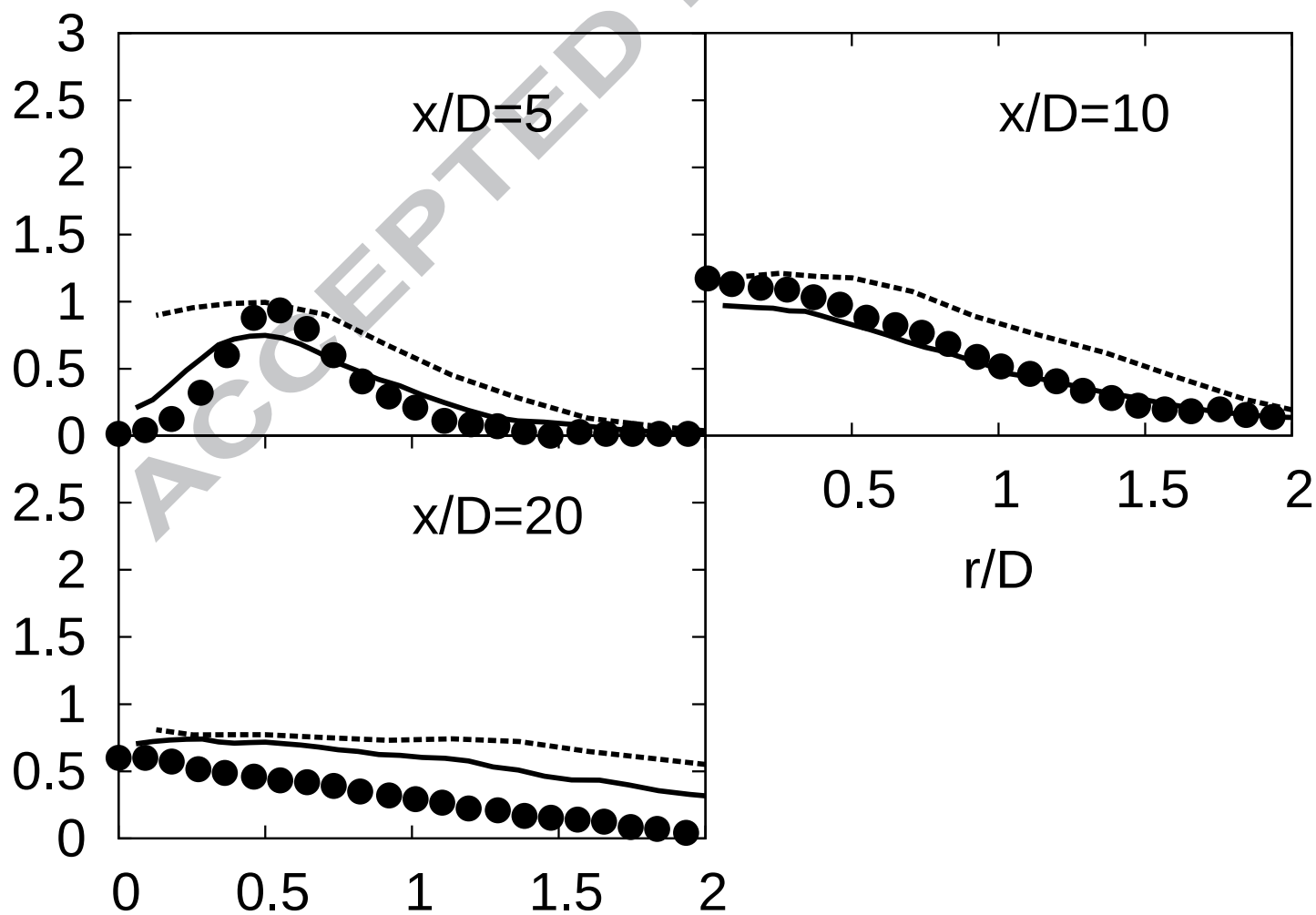
Figure 9: Mean liquid surface density Σ/Σ_0 along centreline. The plot shows the effect of sub-grid modelling in LES-COARSE

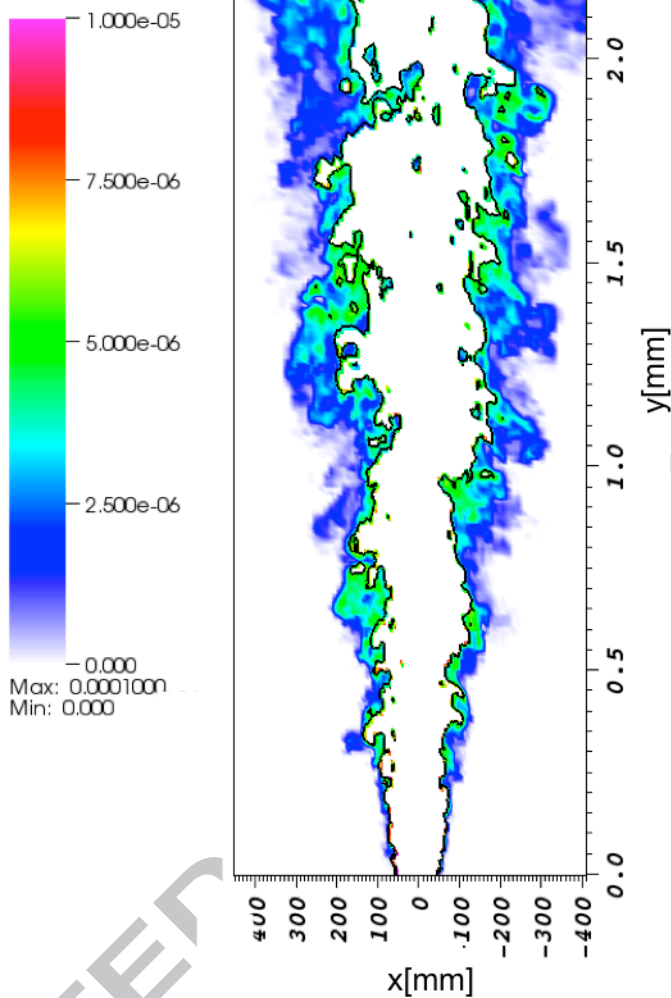


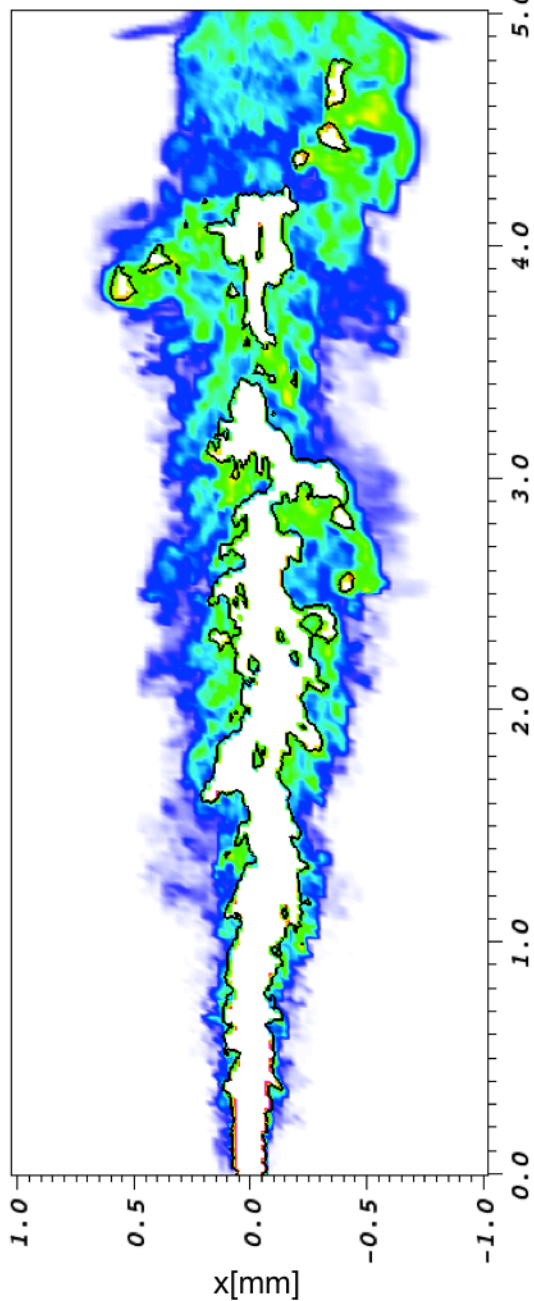
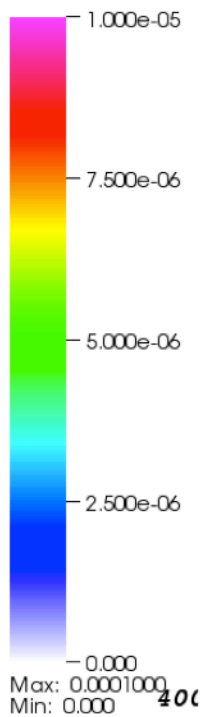


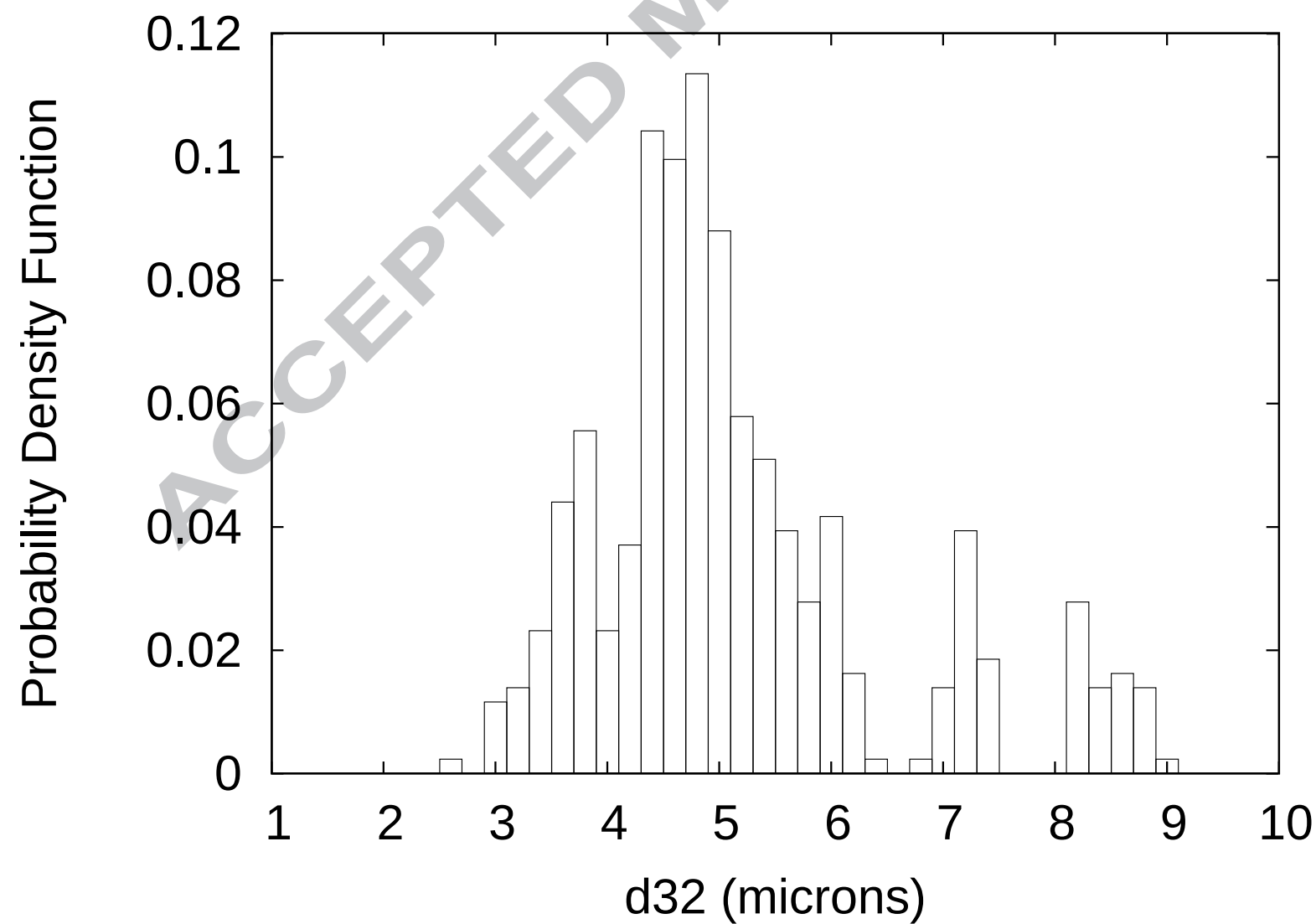


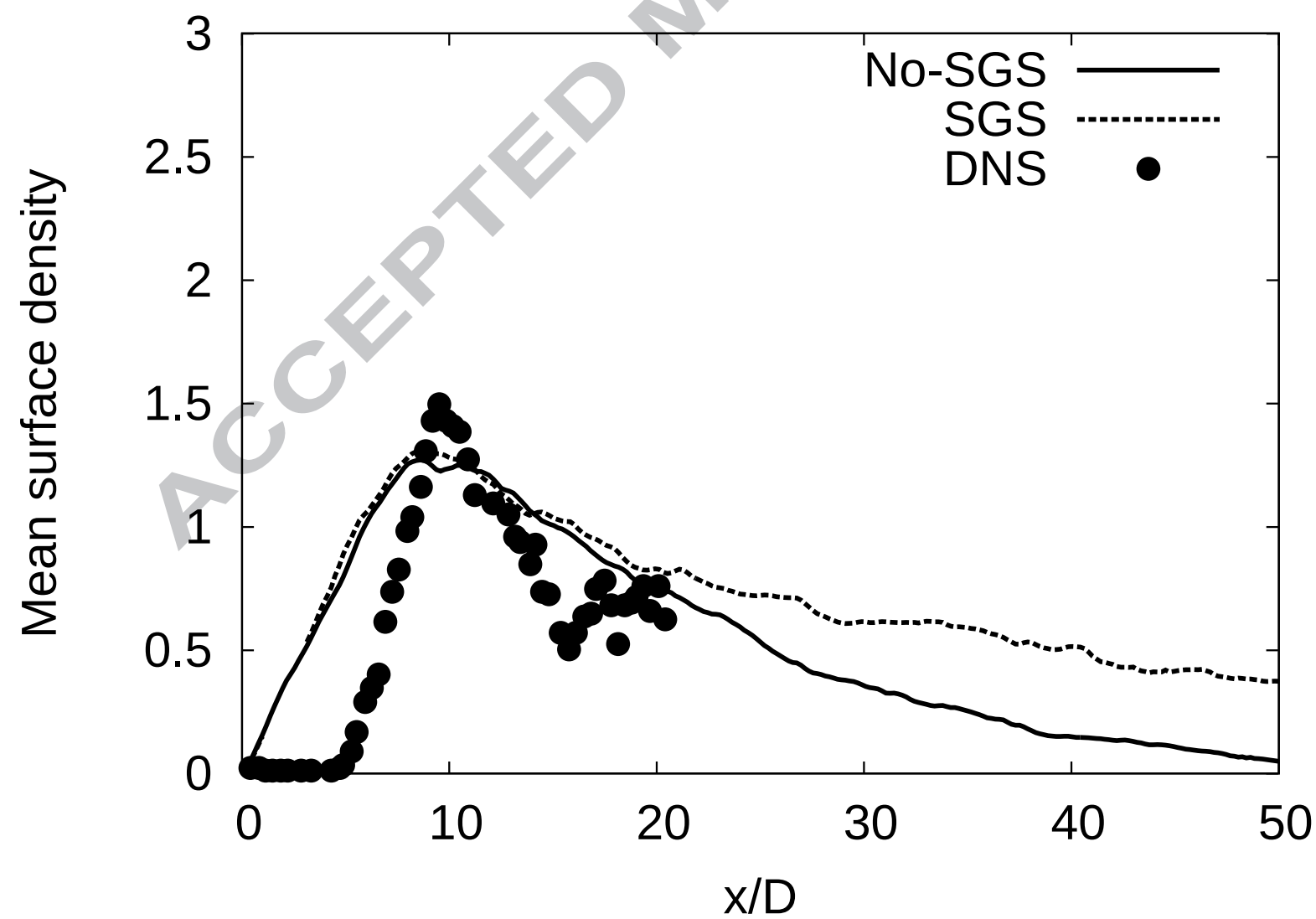












Highlights

- New LES-PDF model for atomization using liquid volume and surface density
- The model uses an Eulerian Monte Carlo approach
- The method resolves both dense and dilute regions of spray.
- The solution provides instantaneous sub-grid droplet size distribution.
- Surface density and liquid dispersion results are in good agreement with DNS