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MODELLING OF THE FRACTAL DIMENSION IN THE PRIMARY ATOMIZATION OF HIGH-SPEED LIQUID JETS

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ABSTRACT

The direct numerical simulations (DNS) performed to date for atomizing high-speed liquid jets do not fully resolve the small scale primary breakup dynamics at the liquid-gas interface. As such they rather represent “quasi-DNS”, or Large-Eddy Simulations (LES) with no model for the subgrid-scale effects on the interface. The present work attempts to improve the level of description of the unresolved subgrid-scale geometry of the interface by applying the concept of fractal analysis. The fractal nature of atomizing jets has been observed in several experiments [1,2], where the degree of tortuosity of the interface was measured in terms of a fractal dimension. In the present work, the fractal dimension is modelled using a dynamic procedure, which was originally introduced by Knikker *et al.* [3] to describe the highly wrinkled flame surfaces of premixed combustion in LES. The proposed approach is tested in LES of an atomizing jet, where two cases are considered – one with a very high, and one with a low Weber number. It is shown that the present concept based on a dynamic subgrid-scale model of the fractal dimension represents a simple, computationally feasible approach, which yields an appropriate measure for the unresolved small-scale structure of the interface.

INTRODUCTION

The strongly contorted surface occurring in the primary atomization of a liquid jet at high Reynolds and Weber numbers is characterized by a large variety of time and length scales. This strongly challenges any numerical simulation of this phenomenon. Particularly, when the topology of the interface changes, as it is the case in the pinch-off of a ligament from a jet or sheet and its subsequent contraction down to drop formation, the relevant length scale approaches zero. This makes the concept of direct numerical simulations (DNS), which by definition attempts to resolve all relevant length scales, unfeasible for simulating the process of primary breakup in full detail. Due to this fundamental problem and the excessive computational costs, the direct simulations performed to date basically represent under-resolved “quasi-DNS”, or Large-Eddy Simulations (LES) without modelling of the unresolved subgrid-scale dynamics at the liquid-gas interface. For the numerical tracking of the resolved interface contours, the simulations by Bianchi *et al.* [4] and Villiers *et al.* [5] used the Volume-of-Fluid (VoF) method combined with a surface reconstruction algorithm, while Desjardin *et al.* [6] and Menard *et al.* [7] applied conservative forms of the Level-Set method. Despite the very fine computational grids applied in all these simulations, the resolution appears to be still not sufficient to fully capture the small-scale topology, which results in a grid-dependent statistics for the small droplets.

The present work attempts to describe the unresolved small scale topology of the interface based on the concept of fractal analysis. The tortuosity of the interface is described in terms of a fractal dimension, computed with a dynamic modelling procedure (Germano *et al.* [8]). The two-phase flow field for the resolved large scales is obtained from an LES using the VoF method to track the resolved liquid-gas interface on the large scales.

GOVERNING EQUATIONS

The spatially filtered transport equations for mass, momentum, and the phase marker function solved by the LES are written as

$$\frac{\partial \tilde{u}_i}{\partial x_i} = 0, \tag{1a}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial\left(\bar{\rho}\tilde{u}_i\tilde{u}_j\right)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\bar{\tau}_{ij} + \bar{\tau}_{sgs,ij}\right) + \sigma\bar{\kappa}\frac{\partial \bar{\Theta}}{\partial x_i}, \tag{1b}$$

$$\frac{\partial \bar{\rho}\tilde{\Theta}}{\partial t} + \frac{\partial\left(\bar{\rho}\tilde{u}\tilde{\Theta}\right)}{\partial x_j} = 0, \tag{1c}$$

where a density-weighted filtering operation, which reads for an arbitrary quantity F

$$\tilde{F}\left(\boldsymbol{x},t\right) = \frac{\overline{\rho F}}{\bar{\rho}}\left(\boldsymbol{x},t\right) = \frac{1}{\bar{\rho}}\iiint_{\mathcal{D}} \rho F\left(\boldsymbol{x}-\boldsymbol{\xi},t\right)G\left(\boldsymbol{\xi}\right)d\boldsymbol{\xi} \tag{2}$$

is used. The phase marker function Θ is by definition unity in the liquid and zero in the gaseous phase. Its filtered representation $\bar{\Theta}$ denotes volumetric liquid fraction, which is related to the density-weighted filtered counterpart by

$$\bar{\Theta} = \frac{\bar{\rho}}{\rho_\ell}\tilde{\Theta}. \tag{3}$$

The last term on the rhs of the momentum equation represents the resolved surface tension force, which is computed based on the Continuous Surface Force method introduced by

Brackbill *et al.* [9]. It involves the resolved mean curvature given by

$$\bar{\kappa} = \nabla \cdot \vec{\boldsymbol{n}}, \; \vec{\boldsymbol{n}} = -\frac{\nabla \bar{\Theta}}{\left\| \nabla \bar{\Theta} \right\|}. \tag{4}$$

The subgrid-scale transport of momentum $\bar{\tau}_{sgs,ij}$ is modelled using the Smagorinsky model with the model constant C_S = 0.1. In the present work, the dynamics of the large scales is assumed to be unaffected by the unresolved, subgrid-scale topology of the interface. The modelling of the small-scale interface structures is therefore not incorporated in the present formulation for the resolved field. A two-way coupling of the proposed subgrid-scale model with the large-scale field is subject of future work.

MODELLING OF THE SMALL SCALE STRUCTURES

The present approach parameterizes the small scale interfacial structures in terms of the so-called fractal dimension δ. The fractal dimension basically describes the degree of tortuosity of a surface. It varies between $\delta = 2$, in the case of a smooth Euclidean plane, and $\delta = 3$, in the case of a surface which fills the considered volume completely. The fractal nature of the interface in the primary breakup region of atomizing liquid jets has been observed in various experimental investigations by Shavit *and* Chigier [1] and Dumouchel *et al.* [2].

The present work extends an ansatz from the literature due to Knikker *et al.* [3], who proposed the concept of fractal analysis to model the filtered flame surface density in premixed combustion. Using the phase marker function Θ as a quantity analogous to the progress variable in premixed flames, the filtered surface density $\bar{\Sigma}$ in two-phase flows is written as

$$\bar{\Sigma}\left(\boldsymbol{x},t\right) = \iiint_{\mathcal{D}} \left\| \nabla \Theta\left(\boldsymbol{x}-\boldsymbol{\xi},t\right) \right\| G_{\Delta}\left(\boldsymbol{\xi}\right) d\boldsymbol{\xi}. \tag{5}$$

The so defined filtered surface density $\bar{\Sigma}$ is modelled introducing the ansatz

$$\bar{\Sigma}\left(\boldsymbol{x},t\right) \cong \left\| \nabla \bar{\Theta} \right\| \Xi, \tag{6}$$

where the wrinkling factor Ξ accounts for the unresolved contribution of the subgrid scales. This factor is modelled as

$$\Xi = \left(\frac{\bar{\Delta}}{h_c} \right)^{\delta-2}, \tag{7}$$

involving the grid-filter width $\bar{\Delta}$, as the outer cut-off scale, and a characteristic length scale h_c, as the inner cut-off scale. Assuming similarity between the fractal topology on the grid-filter level $\bar{\Delta}$ and larger test filter level $\hat{\bar{\Delta}} > \bar{\Delta}$, the fractal dimension δ is obtained using a dynamic procedure [8] to read finally

$$\delta = 2 + \frac{\log\left(\left\langle \widehat{\left\| \nabla \bar{\Theta} \right\|} \right\rangle \Big/ \left\langle \left\| \nabla \hat{\bar{\Theta}} \right\| \right\rangle \right)}{\log\left(\hat{\bar{\Delta}} \big/ \bar{\Delta} \right)}. \tag{8}$$

The angular brackets denote the spatial average in the homogeneous direction. Rewriting the filtered interfacial surface density $\bar{\Sigma}$ as a composition of a resolved and an unresolved contribution

$$\bar{\Sigma} = \left\| \nabla \bar{\Theta} \right\| + \left(\overline{\left\| \nabla \Theta \right\|} - \left\| \nabla \bar{\Theta} \right\| \right) = \Sigma_{res} + \Sigma_{sgs}, \tag{9}$$

the unresolved component reads

$$\Sigma_{sgs} = \left\| \nabla \bar{\Theta} \right\| \left(\Xi - 1 \right). \tag{10}$$

The characteristic length scale h_c in Eq. (7) basically represents the interface thickness. It is assumed here as the critical (maximum stable) radius r_{cr} for the breakup of a droplet exposed to the dynamic forces of the ambient turbulent gas flow. As such, r_{cr} is obtained by balancing the disruptive dynamic inertial and capillary forces as

$$r_{cr} = \frac{We_{cr}\, \sigma}{\rho_g \left\langle u'^{\,2}_{rel} \right\rangle} = h_c. \tag{11}$$

The turbulent velocity scale u'_{rel} in Eq. (11) is estimated following Kuznezov *and* Sabel´nikov [10]

$$\left\langle u'^{\,2}_{rel} \right\rangle \cong \left\langle \varepsilon \right\rangle t_{st}, \qquad t_{st} = \frac{2\, r_{cr}^{\,2}\, \rho_l}{9\, \mu_g}. \tag{12}$$

dependent on the mean viscous dissipation rate and Stokes time scale.

TEST CASES

LES of high-speed atomizing jets are carried out, considering two test cases with liquid injection conditions representative for Diesel engines. The Reynolds number based on the bulk liquid inflow at the nozzle is $\mathrm{Re} = U_\ell D / \nu_\ell$ =15500 in both cases. The liquid phase Weber number, $We = \rho_\ell U_\ell^{\,2} D / \sigma$, is set to a realistically high value in the first case $We = 1.4 \cdot 10^6$. In the second case, it is set to a low, arbitrary value We = 1000 in order to examine the effect of a higher surface tension on the resolved interface structures.

The liquid inflow boundary conditions are obtained from an LES solution of a fully developed turbulent pipe flow for the given liquid Reynolds number. The axially symmetric computational domain extends over 20 nozzle diameters in the streamwise, and 10 nozzle diameters in the cross-stream direction. The numbers of grid points in the streamwise/cross-stream/azimuthal directions are 150 x 150 x 64, respectively.

RESULTS: LARGE-SCALE TOPOLOGY

The liquid core lengths x_ℓ obtained for both cases are shown in Fig. 1. They are determined by the maximum axial extension of the region, where the instantaneous values of the resolved marker function $\bar{\Theta}$ is always greater than 0.5 (denoted by the red-coloured areas in Fig. 1).

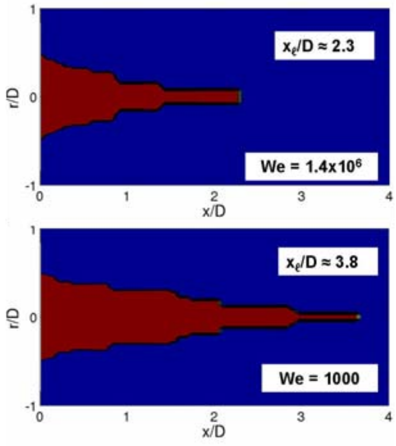

Figure 1: Liquid core length x_ℓ.

The higher surface tension associated with the lower Weber number obviously has a stabilizing effect on the resolved interface leading to a longer liquid core length x_ℓ. Previous simulations performed by Villiers *et al.* [5] for the same test case with the higher Weber number revealed the comparable results $x_\ell / D \approx 3.5$ and $x_\ell / D \approx 2.0$ for two different liquid inflow conditions they applied.

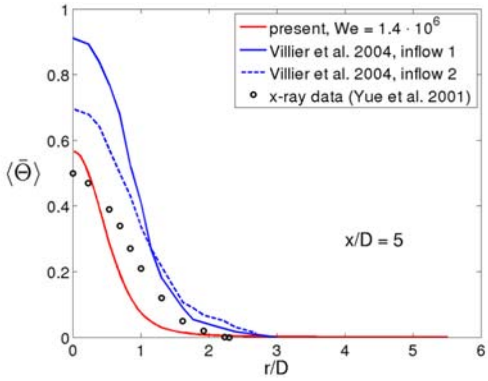

Figure 2: Radial profiles of the averaged liquid volume fraction at the downstream position x/D = 5.

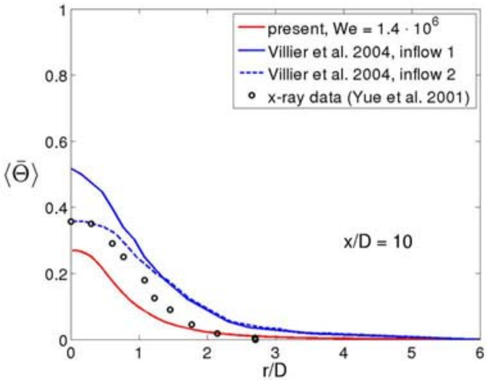

Figure 3: Radial profiles of the averaged liquid volume fraction at the downstream position x/D = 10.

Figures 2 and 3 show the results for the radial profiles of the averaged liquid volume fraction $\langle\bar{\Theta}\rangle$ at two selected positions downstream. The corresponding profiles obtained by Villier *et al.* [5], and experimental data measured at comparable conditions by Yue *et al.* [11] are shown as well. The results of the present simulations agree remarkably well with the experiments.

RESULTS: SMALL-SCALE TOPOLOGY

Figure 4 shows the streamwise variation of the cross-sectional averages of the fractal dimension δ obtained with the proposed dynamic model in both cases. In the high Weber number case, the effect of surface tension forces appears to be negligibly small. The turbulent fluctuations in the liquid bulk inlet stream together with the highly strained boundary layer evolving from the lid of the nozzle lead to a strongly contorted interface right from the entry of the liquid. This can be clearly seen from the rapid increase of the fractal dimension δ immediately downstream from the nozzle. In the low Weber number case, the surface tension forces evidently lead to a smoother interface topology in the inflow region. Accordingly, the fractal dimension δ starts from a comparably low value at the inlet and increases gradually further downstream. It finally reaches the same level as in the high Weber number case, which indicates that the considerable differences in the small-scale topology of the inflow region vanish downstream. Experimental measurements by Dumouchel *et al.* [2] at a comparable low liquid Weber number We = 2000 are depicted as well. The experimental data also exhibit an approximately linear increase with the downstream distance from the nozzle, which is well in line with the present model predictions for the lower Weber number case.

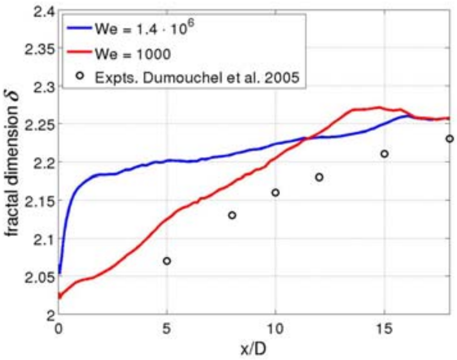

Figure 4: Axial profiles of the averaged fractal dimension δ.

The spatial distribution of the unresolved component Σ_{sgs} relative to the total filtered surface density $\bar{\Sigma}$, given by Eqs. (9)-(10), is shown in Fig. 5. The relative unresolved contribution evidently reaches considerably higher levels in the high Weber number case. It becomes highest (> 60%) particularly in the outer, off-centre regions, where the liquid mass per volume tends to be small. This indicates a highly diluted state of the liquid phase being dispersed into many small droplets, which are not resolved by the LES. The indicated transition into a diluted state of the liquid also suggests the use of a Lagrangian description of the motion of the liquid phase rather than an Eulerian description. The ratio $\Sigma_{sgs}/\bar{\Sigma}$ obtained from the present model can evidently serve as a useful criterion for such a change of the computational frame of reference.

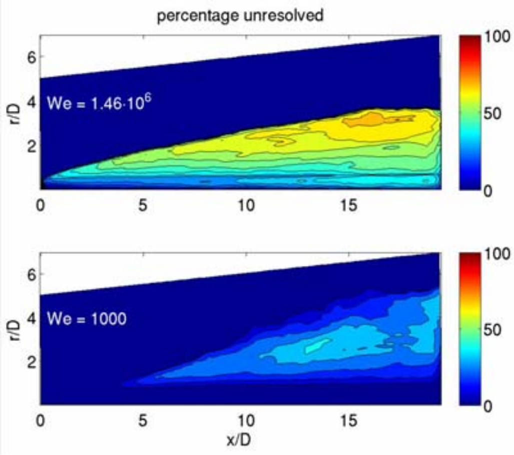

Figure 5: Unresolved subgrid-scale contribution in percent.

CONCLUSIONS

Numerical simulations of the atomization of high-speed liquid jets face the fundamental problem of insufficiently resolved small-scale structures of the interface. The present work attempts to describe this unresolved topology based on a fractal dimension model.

The approach is tested in Large-Eddy Simulations of atomizing high-speed liquid jets at two different Weber numbers. The large-scale characteristics, such as the liquid core lengths and radial profiles of the averaged liquid volume fraction, are compared with experiments and other numerical simulations from the literature. It is shown that the present VoF-based LES captures the large-scale characteristics of the interface remarkably well.

The fractal dimension predicted by the proposed dynamic model exhibits a realistic behaviour in terms of magnitude and downstream variation when compared to experimental measurements. The present modelling of the fractal dimension is proven to be a computationally feasible and simple approach, which provides a valuable estimate for the unresolved contribution to the interface density.

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NOMENCLATURE

Symbol	Quantity	SI Unit
D	orifice diameter	m
G	spatial filter function	m^{-3}
h_c	length scale	m
$\vec{n}$	unit normal vector	-
p	pressure	kg/ms^2
r_{cr}	critical radius	m
t	time variable	s
U	bulk inlet velocity	m/s
u	velocity	m/s
We_{cr}	critical Weber number	-
x	space variable	m
Δ	filter width	m
δ	fractal dimension	-
ε	dissipation rate	m^2/s^3
Θ	phase marker	-
κ	local surface curvature	m^{-1}
μ	dynamic viscosity	kg/ms
ν	kinematic viscosity	m^2/s
Ξ	wrinkling factor	-
ξ	space variable	m
ρ	density	kg/m^3
Σ	interface density	m^{-1}
σ	surface tension coefficient	kg/s^2
τ	stress tensor	kg/ms^2

Subscripts	Quantity
g	gas
ℓ	liquid
sgs	subgrid-scale

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