

## A DNS database to improve atomization modeling

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### Abstract

Recent advances in interface tracking method allows us to use them as a tool to study primary atomization. Some recent works have performed accurate Direct Numerical Simulation of turbulent liquid jets which are very promising. Unfortunately, these simulations have shown that, even with a high resolved DNS of 6 billions points [1], the finest scales of the flow are not resolved. This issue shows that subgrid models are necessary to modelize the physics under this particular scale.

In order to improve modeling, it is useful to study simpler configurations which allows us to solve all relevant scales of the flow. In single-phase flows, DNS of Homogeneous Isotropic Turbulence (HIT) is still used to study scalar mixing and the Kolmogorov theory. Extension of this configuration to two-phase flows to characterize important processes (for example turbulence/interface interactions, vaporization) is emerging in recent DNS studies. The aim of this work is to pursue these studies by analyzing the interface behaviour of two-phase flows in a forced HIT. This analysis is performed over a large range of liquid volume fractions. From these results we can extract useful informations in order to improve modeling of primary atomization.

Both phase are resolved in DNS, the interface tracking method used is a coupled Level Set/VOF method. High density ratio between the two phases is chosen to simulate realistic engine conditions. Quantitative and qualitative aspects are analyzed, with a main focus on interfacial quantities (equilibrium interface density and Weber number), which are key parameters for primary atomization modeling.

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### Introduction

Combustion of liquid fuel remains one of the major source of energy. The injection phase is a critical step for mixture preparation and the induced combustion. Hence, many works have been devoted to the description of the injection process and its influence on the vaporisation and mixing. However, experiments allowing these processes to be studied are difficult in particular close to the dense zone of the spray. The last decade has seen the appearance of numerical method devoted to two-phase flows with an accurate description of the interface. These interface tracking methods like the Volume of Fluid method, Level Set method and Front-tracking method are the most common strategy used for Direct Numerical Simulation (DNS). Discontinuities at the interface have to be treated carefully. To do this, numerical methods like the delta function method [2] and the ghost fluid method [3] were developed. The last one made possible to apply sharp jump conditions at the interface. As far as atomization is concerned, successful studies have emerged to describe the primary atomization of liquid jets ([4], [1]).

Unfortunately, these simulations have shown that, even with a resolution of 0.35 micrometers [1], the finest scales of the flow are not resolved. To optimize the computational cost, some studies use an adaptive mesh refinement [5] [6], but there is still a numerical cutoff scale. It is possible that in few years, improvement of numerical methods and computational efficiency will permit to solve the finest scale of two-phase flows. Furthermore, the finest scale in multiphase flows remains unknown, contrary to the Kolmogorov and the Bachelor scale in single phase flows.

This issue shows that subgrid models are necessary to modelize the physics under this particular scale, like the Large Eddy Simulation (LES) of single phase flows. LES of two phase flows have been investigated in few studies. A first approach consist in keeping interface tracking methods to solve the interface, but without solving the finest scales of wrinkling ([7] for example). Another approach, more phenomenological, is to describe continuously the transition between a well resolved interface and structures smaller than the cell size. This approach introduces the interface density area, which indicate the quantity of interfacial area in each cell, but without indications on the shape of the structures [8]. These approaches give interesting statistical results, independant of the mesh size and in accordance with two-phase flow DNS.

In order to improve LES modeling, it is useful to study simpler configurations which allows us to solve all relevant scales of the flow. In single-phase flows, DNS of Homogeneous Isotropic Turbulence (HIT) is still used to study scalar mixing and the Kolmogorov theory. Extension of this configuration to two-phase flows to characterize

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interface/turbulence interactions is emerging in recent DNS studies : with a freely decaying turbulent two-phase flow [9], with a forced HIT [10] [11] [12], with solid particles in an HIT [13], and with a downward turbulent flows for bubbly flows [14].

The aim of this paper is to pursue these studies by analyzing statistical quantities extracted from a validated two-phase flows DNS database [12], with a main focus on interfacial quantities. From these results we can extract useful informations in order to improve modeling of primary atomization, like the equilibrium Weber number used in the ELSA model [15].

Both phases will be resolved in DNS; the interface tracking method that has been used is a coupled Level Set/VOF method. A high density ratio between the two phases is chosen to simulate realistic engine conditions. Both quantitative and qualitative aspects are analyzed.

## Numerical methods

### Navier-Stokes equation

The joint Level Set/VOF method is coupled with a projection method to carry out the direct numerical simulation of incompressible Navier-Stokes equations:

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} = -\frac{\nabla p}{\rho} + \frac{1}{\rho} \nabla \cdot (2\mu \mathbf{D}) + \mathbf{g} + \mathbf{f} + \frac{1}{\rho} \sigma \kappa \delta(G) \mathbf{n} \quad (1)$$

where  $p$  is the fluid pressure,  $\mathbf{V}$  the velocity vector,  $\mathbf{g}$  the gravity vector,  $\mu$  the dynamic viscosity, and  $\mathbf{D}$  the viscous deformation tensor. At the interface, the surface tension force can be considered based on the Dirac function  $\delta(G)$ :  $\sigma$  is the surface tension,  $\mathbf{n}$  the normal unit vector,  $\kappa$  is the curvature computed from the Level Set function  $G$ . The gravity term is neglected in this study. To solve the derivatives, a fifth-order scheme, WENO 5 ([16]), is used for convective terms, and a second-order central finite difference scheme is chosen for diffusive terms. (See [4] for further details concerning the numerical procedure.) A forcing method is necessary to maintain the turbulent kinetic energy at a prescribed level. This is achieved through the source term  $\mathbf{f}$ , which induces linear forcing ([17]). It results in  $\mathbf{f} = A\mathbf{v}'$  where  $A$  is the forcing coefficient,  $\mathbf{v}'$  represents velocity fluctuations, and  $\bar{\mathbf{v}}$  is the mean flow velocity. In this paper,  $\overline{(\cdot)}$  refers to volume averaging. A Reynolds decomposition has been applied to the velocity field  $\mathbf{V}$ . The evolution equation of the turbulent kinetic energy  $k = \frac{1}{2} \overline{\mathbf{v}'^2}$  may be written:

$$\frac{\partial k}{\partial t} + \nabla \cdot (\bar{\mathbf{v}} k) = C_k + 2Ak \quad (2)$$

where  $C_k$  regroups the typical energetic contributions (i.e. without forcing) for the sake of clarity. The estimation of  $C_k$  involves a liquid-gas interface. It is therefore complex to estimate  $A$  directly from equation 2, thus, the following two-stage procedure has been set up :

Stage 1 - Estimation of  $C_k^{n-1}$  based on the  $A^{n-1}$  constant value :

$$C_k^{n-1} = \frac{k^n - k^{n-1}}{\Delta t} - 2A^{n-1}k^{n-1} \quad (3)$$

Stage 2 - Computation of the forcing constant  $A^n$  based on  $C_k^{n-1}$  :

$$2A^n k^n = \frac{k_c - k^n}{\tau_f} - C_k^{n-1} \quad (4)$$

where  $k_c$  is the chosen level of kinetic energy,  $\tau_f$  is a characteristic relaxation time ( $\tau_f = 3\Delta t$  has been retained in this study) to avoid a sharp forcing term. Thus, the force coefficient  $A$  is computed at each time step to introduce the forcing term  $\mathbf{f}$  in the Navier-Stokes equations.

This method maintains a statistically stationary Homogeneous Isotropic Turbulence (HIT) in the whole domain.

However this kind of forcing have some drawbacks : energy is added at all scales, contrary to usual spectral forcing where the forcing is applied at a chosen wavenumber. But applying a spectral forcing in interface tracking DNS is rather complex due to discontinuities across the interface, and also leads to much higher computational cost (by using FFT transform). The choice of a linear forcing have been made for its simplicity and because there is a lack of studies concerning forcing method in interface tracking DNS. A better forcing method, preferably in physical space, will be a major improvement for future works.

### Interface tracking method

In the following, the interface tracking method and the treatment of discontinuities are recalled. More details can be found in the work of [4]. Level Set methods use a continuous function to describe the interface ([18], [19]). This function is defined as the signed distance between any points of the domain and the interface. The 0 level curve of that function therefore provides the interface location. The convection equation to describe the motion of the interface in a given velocity field  $\mathbf{V}$  reads:

$$\frac{\partial G}{\partial t} + \mathbf{V} \cdot \nabla G = 0 \quad (5)$$

Eq. (5) is the hyperbolic type, and the discretization method must combine a high convergence order and robustness. Thus, for the distance function field, a 5th-order WENO scheme ([16]) is used for convective terms. The normal unit vector  $\mathbf{n}$  and the curvature of the interface  $\kappa(G)$  are evaluated based on the Level Set function by :

$$\mathbf{n} = \frac{\nabla G}{|\nabla G|}, \quad \kappa(G) = \nabla \cdot \mathbf{n} \quad (6)$$

The Level Set method  $G$  no longer remains a distance function when solving Eq. (5) because of the velocity gradients. A redistancing algorithm ([20]) is thus applied to keep  $G$  as the signed distance to the interface. A numerical resolution of Eq. (5) combined with the redistancing algorithm can induce mass loss in under-resolved regions. This loss is the main drawback of Level Set methods. To improve mass conservation, extensions of the method have been proposed ([21], [22], [23]). Specific studies have been developed to evaluate some of these methods ([4]). It has been found that the Coupled Level Set and Volume-of-Fluid method (CLSVOF, see [21]) is well adapted to capture atomization processes ([4], [15]). The main concept of this method is to benefit from the advantage of both Level Set and VOF strategies: mass loss is limited through the VOF method, and a fine description of interface properties is kept with the Level Set. The Level Set permits the reconstruction of an accurate interface in each cell and helps in the transport of the liquid volume fraction. The location of the interface is slightly modified to retain an amount of liquid in a computational cell that corresponds to the liquid volume fraction determined by the VOF approach. This displacement is used to ensure mass conservation.

Fluid dynamics equations are solved in the context of a low Mach number approach, based on a projection method for the direct numerical simulation of incompressible Navier-Stokes equations (detailed in [24]). The density and the viscosity depend on the sign of the Level Set function according to each phase (liquid and gas). To finalize the description of the two-phase flow, jump conditions across the interface are taken into account with the Ghost Fluid (GF) method. In the GF method, ghost cells are defined on each side of the interface ([25], [26]). This prolongs each phase in order to allow smooth derivatives in the vicinity of the interface. As defined previously, the interface is characterized through the distance function, and jump conditions are extrapolated on a few nodes on each side of the interface. Further details on implementing the GF method to solve the Poisson equation with discontinuous coefficients can be found in the literature ([26], [24]).

### Numerical configuration

The solution is carried out in a 3D cubical domain with periodic boundaries similar to the study of [12]. This configuration extends previous numerical studies on mixing in single-phase flows ([27]) to two-phase flows with a fully resolved liquid-gas formulation. To accurately control the various inputs of the simulation, a three-dimensional forced homogeneous turbulence of a gas / liquid flow is considered with a liquid volume fraction ranging between 5% to 95%. The liquid gas interface is represented in Figure 1 to illustrate the numerical configuration for a liquid volume fraction of 5%. To define a configuration with effective interactions between the liquid-gas interface and the turbulence, the following dimensionless parameters have been retained: gaseous Weber number  $We_g = \rho_g \bar{k} L / (\sigma) = 1$ , liquid Weber number  $We_l = \rho_l \bar{k} L / (\sigma) = 30$ , liquid based Reynolds number  $Re_l = \sqrt{\bar{k}} L / \nu_l = 310$ , liquid Ohnesorge number  $Oh_l = \sqrt{We_l} / Re_l = 1.77 \cdot 10^{-2}$ . Where  $\bar{k}$  is the mean kinetic energy (usually equal to  $k_c$ ),  $\sigma$  the surface tension,  $\nu$  the kinematic viscosity in the appropriate phase,  $\rho$  the density and  $L$  the box length.

Two mesh resolution are studied to analyze the influence of the mesh size on results ( $128^3$  and  $256^3$ ). The corresponding set of fluid parameters is summarized in Table 1.

Table 1: Parameters of the simulation (S.I. units)

$\rho_l / \rho_g$	$\sigma$	$\mu_g$	$\mu_l$	$k_c$	$L$	$\bar{\phi}$
30	0.0135	$1.879 \cdot 10^{-5}$	$5.65 \cdot 10^{-4}$	3.6	$1.5 \cdot 10^{-4}$	1 – 5 – 10 – 50 – 90 – 95%

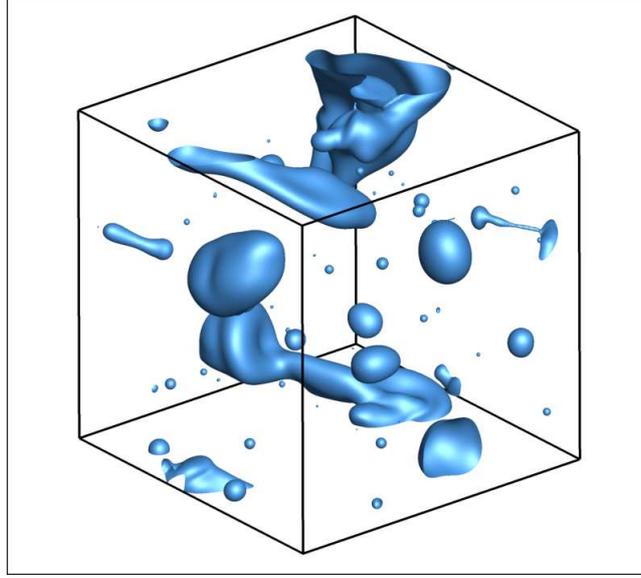


Figure 1: Interface visualization, liquid volume fraction  $\phi = 5\%$

### Primary atomization modeling

#### Equilibrium interface density

There are few modeling strategy to consider primary atomization. One of them is to use an interface density equation with appropriate source terms, to take into account effects of surface tension, vaporization, turbulence and coalescence. This is the ELSA model, initially proposed by Vallet et al. [28] and improved by Lebas et al [15] recently. The latest equation of the interface density is :

$$\frac{\partial \bar{\Sigma}}{\partial t} + \frac{\partial \bar{\Sigma} \tilde{u}_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\nu_t}{S_{C_t}} \frac{\partial \bar{\Sigma}}{\partial x_i} \right) + \Phi (S_{init} + S_{turb}) + (1 - \Phi) (S_{coll/coal} + S_{2ndBU}) + S_{vapo} \quad (7)$$

Where  $\bar{\Sigma}$  is the mean interface density,  $\Phi$  is a repartition function used to share out dense ( $\Phi = 1$ ) and dilute source terms ( $\Phi = 0$ ). In the DNS configuration (HIT, and no phase change) this equation is reduced to :

$$\frac{\partial \bar{\Sigma}}{\partial t} = S_{turb} \quad (8)$$

The turbulence source term is defined by :

$$S_{turb} = \frac{\bar{\Sigma}}{\tau_t} \left( 1 - \frac{\bar{\Sigma}}{\bar{\Sigma}^*} \right) \quad (9)$$

Where  $\bar{\Sigma}^*$  is the "equilibrium" interface density,  $\tau_t$  a turbulent timescale.

This term corresponds to the production/destruction of liquid-gas interface density due to the turbulent flow stretching and the effects of collision and coalescence in the dense part of the spray. It is assumed to be driven by a turbulent time scale  $\tau_t$ . This production/ destruction term is defined in order to reach an equilibrium value of the surface density  $\bar{\Sigma}^*$ . It corresponds to the quantity of surface that would be obtained by keeping constant the total mixture turbulent kinetic energy and the liquid volume fraction.

Usually, a equilibrium Weber number  $We^* = \frac{\phi \bar{k}}{\sigma \bar{\Sigma}^*}$  is used in primary atomization modeling to determine  $\bar{\Sigma}^*$ , most of the time the assumption  $We^* = 1$  is made. This means that the total energy is equally distributed between the kinetic energy and the surface energy. With this Weber number it is then possible to compute  $\bar{\Sigma}^*$  and finally  $S_{turb}$ . In this work, it is possible to extract the equilibrium surface density and the Weber number from the DNS and verify if this definition is adequate. This is done for two mesh resolutions.

Another comparison is performed by analyzing the work of Luret et al. [10] [11], who performed similar simulations but the turbulence was not fully resolved at small scales (contrary to the presented one which was validated [12]), because the main objective was to study droplets collision.

A new definition of the equilibrium Weber number is proposed to avoid that the variable tends to infinity or zero when  $\phi \rightarrow 0$  or 1 :

$$We^* = 4 \frac{0.5(\rho_l + \rho_g)\phi(1-\phi)\tilde{k}}{\sigma\bar{\Sigma}^*} \quad (10)$$

This definition may look surprising but it is one way to keep the same formulation of the Weber number for a large range of liquid volume fractions encountered in atomization (from dispersed spray to dense spray).

Results are shown in Figure 2. All variables are volume averaged in the whole domain and then time averaged over at least 50 eddy turnover times ( $\tau_t$ ) for the computation of the Weber number to assure proper statistical convergence.

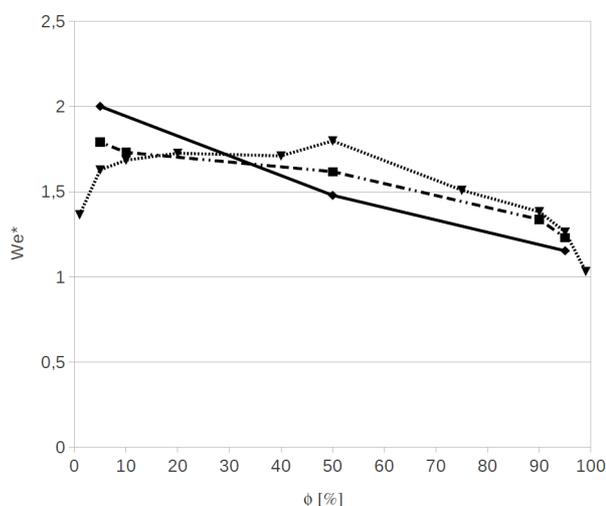


Figure 2: Equilibrium Weber number for various liquid volume fractions. Plain line :  $256^3$  configuration, dashed-dotted line :  $128^3$  configuration, dotted line : Results from Luret et al. [10] [11].

It is impressive that for these three configurations, the value of the Weber number is always ranged between  $We^* = 1$  and  $We^* = 2$ , even with a coarse grid and a turbulence not fully resolved. This can be very handy when using primary atomization model, because all variables are known in Equation 10 except  $\bar{\Sigma}^*$ , this last can be computed by assuming a Weber number equal to approximately 1.5 for example, accordingly to our results.

A better definition of the Weber number may be to take into account the "true" kinetic energy  $\overline{k_\Gamma}$  at the interface. This quantity is also available thanks to DNS.  $\overline{k_\Gamma}$  is computed by extracting velocities in cells that contains an interface, and then averaged in space and time. It should be recalled that the velocity is continuous across an inert interface, as in this study, allowing us to do this approximation of  $\overline{k_\Gamma}$ .

An interesting point is that the Favre averaged turbulent kinetic energy  $\tilde{k}$  ( $\tilde{k} = \frac{\rho k}{\rho}$ ) is very close to the one of the interface  $\overline{k_\Gamma}$  when  $\phi > 50\%$ . For example for the 50% case  $\overline{k_\Gamma} = 2.62$  and  $\tilde{k} = 2.55$ , and for the 95% case  $\overline{k_\Gamma} = 3.41$  and  $\tilde{k} = 3.58$ . Obviously, the liquid turbulent kinetic energy  $\tilde{k}_l$  is very close to  $\tilde{k}$  in dense case, because the liquid phase have a much higher density than the gas phase. However, for dispersed case ( $\phi = 5\%$ ), it seems that  $\tilde{k}$  is less relevant to characterize the kinetic energy at the interface :  $\overline{k_\Gamma} = 6.66$ ,  $\tilde{k} = 5.20$ . The liquid turbulent kinetic energy seems closer to  $\overline{k_\Gamma}$  :  $\tilde{k}_l = 6.33$ .

This means that the interface velocity is directly managed by the liquid phase, independently from the liquid volume fraction, between 5% and 95 %. This is not so surprising because of the liquid high density compared to the gas phase. Consequently, for atomization modeling it seems that taking  $\overline{k_\Gamma}$  is more relevant than  $\tilde{k}$  for the computation of the equilibrium Weber number.

### Definition of $S_{turb}$

The previous section assumed that the definition of  $S_{turb}$  (Eq. 9) is adequate. Unfortunately, this equation was postulated and not verified experimentally or numerically to the author's knowledge. Here we propose to verify this definition by changing the surface tension  $\sigma$  between two computations.

A reference case is computed where  $\sigma = \sigma_1$  and  $\overline{\Sigma}_1$  is sufficiently converged to assume that the equilibrium is reached ( $\overline{\Sigma}_1 = \overline{\Sigma}_1^*$ ), restarts file from this case are stocked each  $5 \tau_t$ . Then, new computations are made with  $\sigma = \sigma_2$  starting from restart files created by the reference case. Changing the surface tension induce a new equilibrium interface density  $\overline{\Sigma}_2^*$ . From these computations, an ensemble averaging over all runs (where  $\sigma = \sigma_2$ ) is performed to extract the transient behaviour of the interface density (before reaching the new equilibrium  $\overline{\Sigma}_2^*$ ).

This procedure allows us to visualize the transient behaviour between two equilibrium interface density :  $\overline{\Sigma}_1^*$  and  $\overline{\Sigma}_2^*$ . To illustrate this in a simple way, a numerical resolution of the equation 9 is shown in Figure 3.

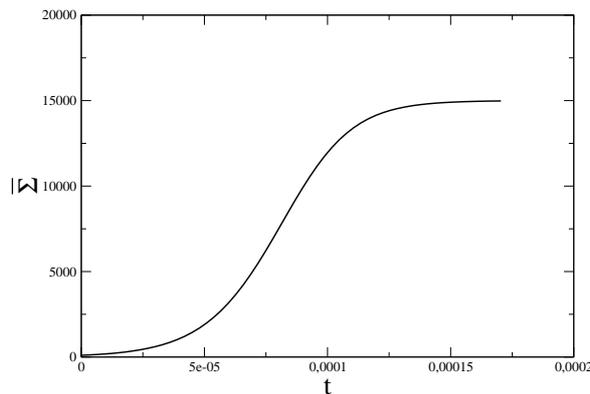


Figure 3: Numerical resolution of the equation 8. Initial condition :  $\overline{\Sigma}_0 = 100$ , and  $\overline{\Sigma}^* = 15000$ .

This work is currently in progress. The statistical convergence is difficult to reach with this configuration since we are focusing to the transient part of the interface density time evolution. The length of the transient part is unknown, this is an issue because a good estimation of  $\overline{\Sigma}_2^*$  is necessary to compare the model and the DNS. To have this estimation a splitting of the evolution of the interface density is performed to compute  $\overline{\Sigma}_2^*$  after the transient part. It is also difficult to change strongly the surface tension since mass loss occurs when  $\sigma$  is set to a small value, because it increases the fragmentation of liquid structures. Instead of affect  $\sigma$ , one can change the turbulent kinetic energy because this variable also have a major role in the Weber number. But as mentions in Duret et al. [12], validation of the turbulence with dissipative numerical schemes (used generally in interface tracking solver) is not straightforward. Resolution of small scales must be checked at each change in  $k$ . Furthermore, mass loss will remains an issue because it increases the Weber number.

18 simulations was performed to compute the transient part of the interface density evolution, but it seems that it is not sufficient to converge properly. Improvements of the method and more runs will be performed to improve the statistical convergence. This last result will be presented at the ICLASS conference.

### Conclusion

This paper present a way to improve primary atomization modeling by using two-phase flows DNS. Here, a comparison between the transport equation of the interface density in the ELSA model and the interface density behaviour with a full resolution of both phases and interface. Focusing on the turbulence source term, an improvement of the definition of the equilibrium Weber number is proposed based on DNS results. The turbulent kinetic energy used in the equilibrium Weber number should be the kinetic energy at the interface, but in modeling this information is not available. Instead, we proposed to used the liquid kinetic energy or the favre averaged kinetic energy in the equilibrium Weber number, because their value are closer to the kinetic energy at the interface. It seems that the liquid kinetic energy is the closest, this means that the interface velocity is directly managed by the liquid phase, independently from the liquid volume fraction in the considered range.

The interface density time evolution is also discussed. The surface tension is changed between two simulations and we observe how the interface density reach an equilibrium. This will be checked if the equation used for the turbulent source terms in the transport equation of the interface density in the ELSA model is adequate. The

difficulty to reach statistical convergence when focusing of the transient time evolution of the interface density is pointed out.

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