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### DNS STUDY OF COLLISION AND COALESCENCE OVER A WIDE RANGE OF VOLUME FRACTION

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#### ABSTRACT

Among the different processes that play a role during the atomization process, collisions are addressed in this work. Collisions can be very important in dense two-phase flows. Recently, the Eulerian Lagrangian Spray Atomization (ELSA) model has been developed<sup>1,2</sup>. It represents the atomization by taking into account the dense zone of the spray. Thus in this context, collisions modeling are of the utmost importance. In this model results of collisions are controlled by the value of an equilibrium Weber number,  $We^*$ . It is defined as the ratio between the kinetic energy to the surface energy. Such a value of  $We^*$  has been studied in the past using Lagrangian collision models with various complexity<sup>3</sup>. These models are based on analysis of collisions between droplets that have surface at rest<sup>4</sup>. This ideal situation can be obtained only if droplet agitation created during a collision has enough time to vanish before the next collision. For a spray, this requirement is not always fulfilled depending for instance on the mean liquid volume fraction. If there is not enough time, collisions will occur between agitated droplets changing the issue of the collision with respect to the ideal case.

To study this effect, a DNS simulation with a stationary turbulence levels has been conducted for different liquid volume fractions in a cubic box with periodic condition in all directions. For liquid volume fraction close to zero the spray is diluted and collisions between spherical droplets can be identified. For a volume fraction close to one, collisions between bubbles are found. For a middle value of the volume fraction no discrete phase can be observed, instead a strong interaction between both liquid and gas phases is taking place. In all this case the equilibrium value of the Weber number  $We^*$  can be determined. First propositions to determine  $We^*$  as a function of the kinetic energy, density ratio, surface tension coefficient and the volume fraction will be proposed.

#### INTRODUCTION

For many years research on atomization has been carried on to improve the characteristic and the control of sprays. This is particularly true as far as fuel injection is considered. In the context of the atomisation of Diesel jet several works have been proposed to improve the reliability of the modelling approach<sup>1,2,5,6</sup>. The modelling proposal, the so-called ELSA model is based on a realistic description of the dense zone of the spray. While

most of two phase flow approaches used for atomisation consider that the liquid phase is dispersed and composed of liquid parcels mainly isolated, in the ELSA approach no assumption is done on the topology of the interface. Instead the liquid-gas mixture is considered in the whole. Within the mixture, the liquid and the gas may evolve like standard species. The interfacial phenomena are then characterised mainly by the knowledge of an additional variable, the surface density. This model has been developed for flows with high value of the Reynolds number. Accordingly, corresponding velocity fields fell in the category of turbulent flows. However, this turbulence may differ from the classical turbulence encountered in single phase flows. These two points: surface density and turbulence in two-phase flows are the main subject of the present work. Because experiments are difficult for dense two-phase flows, they are completed here by a numerical approach. It is based on a DNS of well controlled two-phase flow. The classical homogeneous and isotropic turbulence configuration initially proposed by <sup>7</sup> to study scalar mixing is extended to two-phase flows. The DNS solver used in this study is presented first, and then the main features of the ELSA model are recalled. This show the importance for the surface density equation of terms like the equilibrium Weber number  $We^*$ . Finally first results are extracted from DNS test case.

## NOMENCLATURE

$k$	Kinetic turbulent energy
$\mathbf{n}$	Normal to the interface
$\mathbf{V}$	Velocity vector (ms <sup>-1</sup> )
$Y$	Species mass fraction
$Sc$	Schmidt number
$S_i$	Source term for surface density
$We$	Weber number

### Greek letters

$\phi$	Liquid volume fraction
$\kappa$	Main curvature (m <sup>-1</sup> )
$\lambda$	Level set function (m)
$\mu$	Dynamic viscosity (kgm <sup>-1</sup> s <sup>-1</sup> )
$\Omega$	Surface density per unit of mass (m <sup>2</sup> kg <sup>-1</sup> )
$\Psi$	Dense function indicator
$\rho$	Density (kgm <sup>-3</sup> )
$\Sigma$	Surface density per unit of volume (m <sup>-1</sup> )
$\sigma$	Surface tension coefficient

### Subscripts

G	Gas
L	Liquid
T	Turbulence

### Upper scripts

*	Equilibrium
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## DNS SIMULATION OF THE ATOMISATION

The proposed work concerns mainly the atomisation process that is relevant for Diesel spray, but it has certainly application for other injection devices. The main drawback for this kind of atomisation is the lack of experimental data in the vicinity of the injector tip. The high velocity and high density variation in this zone prevent to use classical measurement apparatus. In particular, the diffraction effect is the main reason of failure for optical diagnostic. Even if new measurement techniques have been developed <sup>8-11</sup>, DNS simulation is still a very interesting tools to explore the vicinity of the liquid jet exit.

We use for this work a DNS code "ARCHER" developed at the CORIA laboratory <sup>12, 13</sup>. It has been used already to collect statistical information in the dense zone of the spray where nearly no experimental data are available. These simulations are sufficiently predictive and quantitative to be used for validation of modelling proposals <sup>2</sup>.

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

Level Set methods are based on the transport of a continuous function  $\lambda$ , which describes the interface between two phases <sup>14, 15</sup>. This function is defined by the algebraic distance between any point of the domain and the interface. The interface is thus described by the 0 level of the Level Set function. Solving a convection equation allows to determine the evolution of the interface in a given velocity field  $\mathbf{V}$  <sup>15</sup>:

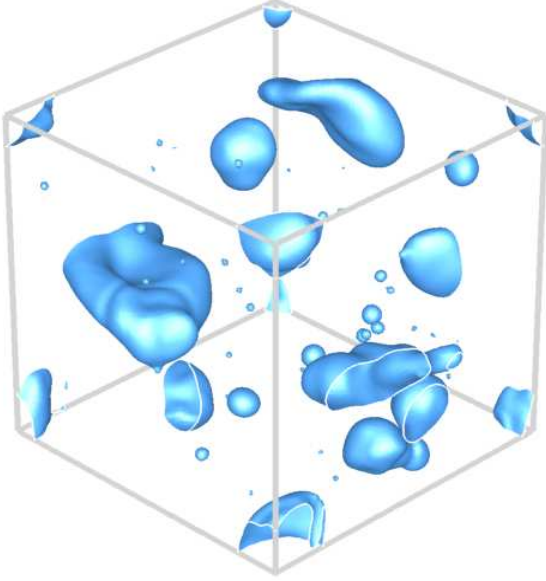
$$\frac{\partial \lambda}{\partial t} + \mathbf{V} \cdot \nabla \lambda = 0 \quad (1)$$

Particular attention must be paid to this transport equation. Problems may arise when the level set method is developed: a high velocity gradient can produce wide spreading and stretching of the level sets, such that  $\lambda$  no longer remains a distance function. Thus, a re-distancing algorithm <sup>14</sup> is applied to keep  $\lambda$  as the algebraic distance to the interface.

To avoid singularities in the distance function field, a 5<sup>th</sup> order WENO scheme has been used for convective terms <sup>16</sup>. Temporal derivatives are computed with a third order Runge Kutta scheme. One advantage of the Level Set method is its ability to represent topological changes both in 2D or 3D geometry quite naturally. Moreover, geometrical information on the interface, such as normal vector  $\mathbf{n}$  or curvature  $\kappa$ , are easily obtained through:

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

It is well known that numerical computation of equation (1) and a redistance algorithm can generate mass loss in under-resolved regions. This is the main drawback of Level Set methods. However, to improve mass conservation a coupling between VOF and Level Set<sup>17</sup> method has been performed.



**Figure 1:** Instantaneous snapshot of the surface for the reference case

This DNS approach is applied in a cubic domain with periodic conditions. The amount of liquid can be prescribed and the total turbulence energy is kept constant thanks to a linear forcing<sup>18</sup>. The figure 1 present a snapshot of the liquid interface after that a constant state has been achieved in average. This configuration is of upmost interest to get data for modelling in a relatively dense zone of the two phase flow. The mean liquid volume fraction is for this case:  $\bar{\phi}_l = 5\%$ . It is clear that a direct application of an optic diagnostic in such a media will suffer multiple scattering of the light. Here, the DNS approach is clearly a very efficient tool, though the numerical convergence is still an issue. While for single phase flows the smallest length scales can be estimated (Batchelor for the scalar and Kolmogorov for the velocity) this is not anymore the case as far as liquid gas flows are concerned. The diffusive effect that limits the size of the smallest inclusion for classical scalar field does not act on this immiscible mixture. The diffusion is replaced by the surface tension force. But as long as the main curvature remains small the surface tension force does not act. This is the case for liquid sheets than can become very thin. Moreover due to the important density ratio between gas and liquid, the smallest scale of the liquid scalar

field should modify also the smallest scale of the velocity field. Despite these drawbacks, we consider that this DNS configuration is able to give interesting information to improve modelling in dense two phase flow. The next section overviews the ELSA model that contains a modelling description of dense two phase flows.

## DESCRIPTION OF THE ELSA MODEL

The goal of the ELSA model is to describe realistically the dense zone of the spray. Based on the assumption of a high Reynolds and injection Weber number values, the ELSA model is naturally well adapted to Diesel Direct Injection conditions. This assumption corresponds to an initial atomization dominated by aerodynamic forces. The global behaviour of the model and its ability to describe Diesel injection have been checked out by Lebas et al.<sup>2</sup>.

A liquid-gas flow is considered as a unique flow with a highly variable density  $\bar{\rho}$  which can be determined thanks to the following equation:

$$\frac{1}{\bar{\rho}} = \frac{\tilde{Y}_l}{\rho_l} + \frac{1 - \tilde{Y}_l}{\rho_g} \quad (3)$$

$\tilde{Y}_l$  corresponds to the mean liquid mass fraction. While,  $\rho_g$  and  $\rho_l$  are respectively the gas and the liquid densities. Considering the two-phase flow as a unique mixture flow with a highly variable density implies that the transport equation for the mean velocity does not contain any momentum exchange terms between the liquid and the gas phases. This ‘‘mixture’’ approach has to be combined with a turbulence model. The (k- $\epsilon$ ) model is generally used even if other models have been tested<sup>6</sup>. A regular transport equation for the mean liquid mass fraction  $\tilde{Y}_l$  can be written in the complete case with a source term representing the effect of vaporization:

$$\frac{\partial \bar{\rho} \tilde{Y}_l}{\partial t} + \frac{\partial \bar{\rho} \tilde{Y}_l \tilde{u}_i}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{Sc_{t,l}} \frac{\partial \tilde{Y}_l}{\partial x_j} \right) - \bar{\rho} \dot{m}_{v,ELSA} \tilde{\Omega} \quad (4)$$

$\tilde{\Omega}$  is the liquid-gas interface density per unit of mass and  $\dot{m}_{v,ELSA}$  represents the vaporization rate per unit of mass<sup>19,20</sup>.

To determine the amount of surface between the two phases, classical approaches consist in considering spherical liquid drops and using the diameter as geometrical parameter. But a more general parameter has to be used where a diameter of droplet cannot be defined: the liquid-gas interface density, noted  $\bar{\Sigma}$  when expressed per unit of volume or  $\tilde{\Omega}$  when given per unit of mass. The following equation relates both definitions:

$$\bar{\rho}\tilde{\Omega} = \bar{\Sigma} \quad (5)$$

The transport equation for this variable is postulated. In the latest version of the ELSA model, it takes the following form <sup>2</sup>:

$$\begin{aligned} \frac{\partial \bar{\rho}\tilde{\Omega}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j \tilde{\Omega}}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{Sc_{t,\Omega}} \frac{\partial \tilde{\Omega}}{\partial x_j} \right) \\ + \Psi(S_{init.} + S_{turb.}) & \quad (6) \\ + (1 - \Psi)(S_{coll./coal.} + S_{2ndBU} + S_{vapo.}) & \end{aligned}$$

This equation must be applicable from the dense zone up to the dispersed spray where droplets are eventually formed. In this latter case, an equivalent diameter of Sauter can be defined using the liquid-gas interface density and the mean liquid mass fraction :

$$D_{32} = \frac{6\tilde{Y}_l}{\rho_l \tilde{\Omega}} \quad (7)$$

Each source term  $S_i$  (equation 6) models a specific physical phenomenon encountered by the liquid blobs or droplets.

$S_{init.}$  is an initialization term, taking high values near the injector nozzle, where the mass fraction gradients take its highest values. It corresponds to the minimum production of liquid-gas interface density necessarily induced by the mixing between the liquid and gas phases <sup>21</sup>.

$$S_{turb.} = \frac{\bar{\rho}\tilde{\Omega}}{\tau_t} \left( 1 - \frac{\tilde{\Omega}}{\tilde{\Omega}^*} \right) \quad (8)$$

$S_{turb.}$  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 supposed to be driven by a kind of turbulent time scale  $\tau_t$ . This production/destruction term is defined to reach an equilibrium liquid-gas interface density  $\tilde{\Omega}^*$ . It corresponds to the quantity of surface obtained at equilibrium under given flow conditions. Several formulations can be proposed. Without any additional information the equilibrium Weber number has been taken as <sup>2</sup>:

$$We_{dense}^* = \frac{\bar{\rho}\tilde{k}\tilde{Y}_l}{\rho_l \sigma_l \tilde{\Omega}^*} = 1 \quad (9)$$

Once the equilibrium Weber number is given the corresponding equilibrium surface density is given by:

$$\tilde{\Omega}_{dense}^* = \frac{\bar{\rho}\tilde{k}\tilde{Y}_l}{\rho_l \sigma_l We_{dense}^*} \quad (10)$$

Where  $\sigma_l$  is the surface tension of the liquid phase.

$S_{coll./coal.}$  models the production/destruction of liquid-gas interface density due to the effects of collision and coalescence in the dilute spray region. Various forms of this term have been proposed <sup>3</sup>. One is compatible to the production term used in the dense zone of the spray (equation 8). But the others are based on binary collisions between droplets and take forms that are not similar to the one propose in equation (8). However, they all predict an equilibrium state if the liquid volume fraction remain constant in a flow with a constant turbulent agitation. This equilibrium state can be characterized by a Weber number. The proposed equilibrium Weber numbers have different values depending on the model. Weber numbers have many definitions depending on the phenomenon under study. In the context of collision, it takes the following form:

$$We^* = \frac{4\tilde{Y}_l \bar{k}_l}{\sigma \tilde{\Omega}} = 12 \leftrightarrow 15 \quad (11)$$

This definition of Weber number will be kept in the following.

$S_{2ndBU}$  deals with the production of liquid-gas interface density due to the effects of secondary breakup in the dilute spray region. This source term is derived from the work of Pilch and Erdman <sup>22</sup>. It enables the estimation of the breakup time scale  $\tau_{2ndBU}$  accordingly to the Weber number of the gas phase  $We_g$ , thanks to empirical correlations.

Vaporisation is characterized thanks to  $S_{vapo.}$ . It comes from a classical adaptation of the ‘‘D<sup>2</sup>’’ law of vaporization models for droplets and deals with the effects of destruction of liquid-gas interface density due to vaporization.

The transport equation of  $\tilde{\Omega}$  takes into account several physical phenomena encountered by the liquid phase. Some of them are specifically observed in the dense zone of the spray and other are dedicated to dispersed spray regions. A function  $\Psi$  has been introduced to switch from the dense formulation to the dispersed formulation continuously and linearly in term of liquid volume fraction <sup>2</sup>.

This description of the ELSA model show how an Eulerian method can be derived to deal with atomisation. Though it has been shown <sup>2</sup> that the presented form of the model is able to capture the global features of the atomisation of a Diesel jet, more detailed studies are still required. In the following the DNS configuration previously described will be used to scrutinize the flows for various liquid volume fractions varying from dilute to very dense spray.

## BEHAVIOUR LIQUID-GAS FLOWS IN STATISTICALLY CONSTANT ENVIRONMENT

The motivation of this study is to scrutinize a part of a liquid jet during its atomization. The test case is based on previous calculation of Diesel jet <sup>2</sup>. This is why the following test conditions have been retained:

$\rho_g$ (kg/m <sup>3</sup> )	25.0
$\mu_g$ (kg/m/s)	1.879 10 <sup>-5</sup>
$\rho_l$ (kg/m <sup>3</sup> )	753.6
$\mu_l$ (kg/m/s)	1.337 10 <sup>-3</sup>
$\sigma$ (N/m)	2.222 10 <sup>-2</sup>
$\rho_l / \rho_g$	30.14

**Table 1:** Fluids properties

They correspond to an injection of Diesel like liquid in air at a pressure of about 25 bars. Concerning the resolution there is mainly two opposite constraints: in one hand the smallest scales of the flow have to be resolved and in other hand the total size of the domain must be big enough to prevent any bias due to forced periodic conditions.

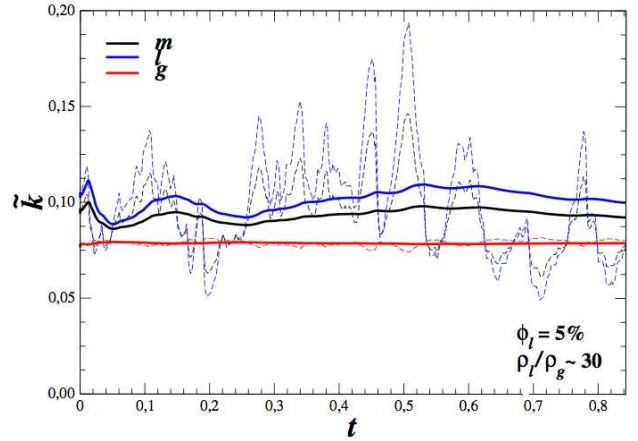
The smallest sizes of the flow could be the Kolmogorov scales, however the viscosity is different between the gas and the liquid. Moreover, as outlined before the Kolmogorov scales should be perturbed by the scalar field. Because of the inertia small liquid structures may produce in the gas smaller scales. On the contrary surface tension force tends to promote a coherent motion inside a liquid parcel or gas parcel. Clearly, all requirements cannot be satisfied at the same time. Thus a kind of arbitrary choice has prevailed when determining the following reference case:

Volume (m <sup>3</sup> )	0.01 <sup>3</sup>
Mesh (-)	128 <sup>3</sup>
$\phi_l$ (%)	5
$\bar{k}$ (m <sup>2</sup> /s <sup>2</sup> )	0.08

**Table 2:** Reference test case

To maintain a constant turbulence level a linear forcing procedure has been used. A snapshot of the liquid surface is presented once the flow has been established in figure 1. The figure 2 presents the turbulent kinetic energy obtained for the mixture, the liquid and the gas phase.

Turbulent kinetic energies presented on figure 2 are average spatially over the whole computational domain. They are drawn as functions of time (dashed line). Clearly, the mixture and liquid kinetic energy are not constant because there is not enough statistical convergence using only spatial averaging. Consequently we compute also the mean value in time of these spatial averaging (solid line).

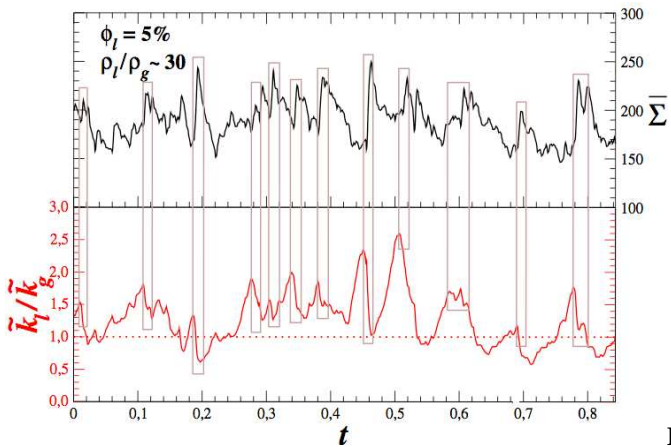


**Figure 2:** Turbulent kinetic energy over the time for the reference test case: dashed line spatial average - solid line spatial and time average; : complete mixture, l:liquid, g:gas.

Additionally Reynolds or Favre averaging can be used. They are equivalent when considering only one phase. Indeed, for this conditioned mean the density is constant. Presented results are Favre averaging, this choice is important for the mixture: by using Favre averaging, the average is mass weighted. Thus, the Favre averaging is mainly driven by the liquid average. On the contrary Reynolds average is volume weighted, hence the mixture Reynolds average kinetic energy (not shown but equal to 0.08 by forcing) his very close to the gas kinetic energy. From this simulation it appears than the liquid kinetic energy experience bigger fluctuations than the gas liquid kinetic energy. This happens because the liquid phase is the minor phase ( $\phi_l = 5\%$ ). Thus even with a special averaging there is no sufficient statistical convergence.

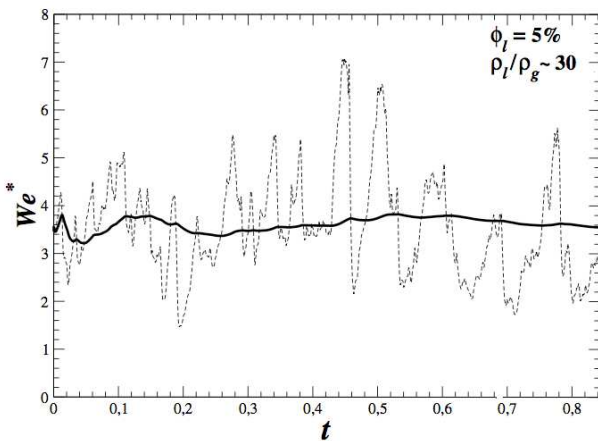
Additionally, the velocity of a liquid parcel can be very different than the surrounding gas because of their inertia. Due to linear forcing a liquid parcel velocity can increase rapidly. The redistribution happen suddenly when collisions occurs with another liquid parcels. This phenomenon explains the important fluctuations of liquid kinetic energy. It is confirmed by the figure 3 that shows the surface density fluctuations. They are clearly correlated to the sudden decrease of liquid kinetic energy. Liquid collisions ensure the redistribution of the liquid velocity in all direction and at smaller length scale. This increases the velocity fluctuation dissipation that reduces the liquid kinetic energy. Additionally liquid kinetic energy is transferred to the surface energy by increasing the liquid surface.

Figure 2 and 3 show also that the liquid kinetic energy is not equal to the gas kinetic energy. There is a little bit more kinetic energy in the liquid than in the gas. This may be due to the linear forcing and collision phenomena as described above but also to a difference of kinematic viscosity between both phases.



**Figure 3:** In black: spatial average of surface density; in red ratio of liquid kinetic energy over the gas kinetic energy.

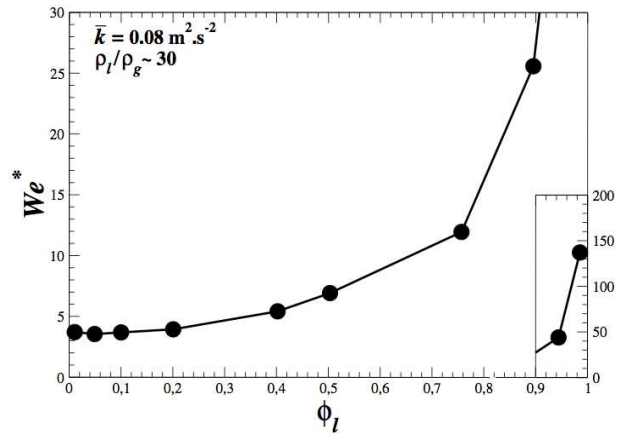
From this analysis it is possible to compute the equilibrium Weber number  $We^*$  defined according to equation (11). Figure 4 presents the evolution of the Weber number as a function of time.



**Figure 4:** Temporal variation of the Weber number; dashed line: spatial average; solid line: spatial and temporal average.

Not surprisingly this Weber number show strong oscillations that correspond to liquid surface oscillations. The result value is about 3.6 for this. This is below the values proposed on the previous models (equation 11). It is important to recall that previous model consider only collision between spherical droplets. Figure 1 shows that most of the droplets are not spherical. Due to their internal agitation before a collision they are more affected by the collision than spherical droplet. Consequently the equilibrium is achieved for a certain level of turbulence with a surface density. This trend induces a decrease of the equilibrium Weber number.

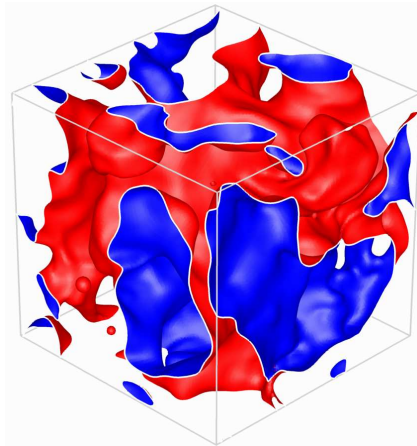
For really diluted mixture, it is expected that droplets may recover their spherical shapes between two successive collisions.



**Figure 5:** Equilibrium Weber number  $We^*$  for different liquid volume fractions.

Figure 5 shows the effect of the volume fraction on the equilibrium Weber number. The range of variation for extends from  $\phi_l = 0.01$  to  $\phi_l = 0.99$  due to the size of the computational domain. More diluted cases would suffer of bias due to periodic boundaries.

For flows with a major quantity of gas (sprays), the equilibrium Weber number does not take the values proposed in previous modelling approaches, though it is in the same range. For flows with a major quantity of liquid the definition of the Weber number  $We^*$  is not suitable because it diverges toward the infinity.



**Figure 6:** Liquid-gas interface for  $\phi_l = 0.50$ ; Blue: surface seen from the gas; Red: surface seen from the liquid.

Notice that small values of the liquid volume fraction correspond to a liquid discrete phase (droplets), while values close to the unity referred to a gaseous discrete phase (bubbles). Intermediate cases, where no discrete phase can be defined, are also covered by this study. For this later case a snapshot of the liquid-gas interface is presented in figure 6.



The two-phase flow in this case is continuous for both phases, though one bubble can be seen in the down left corner. This kind of turbulent flows should be difficult to explore with classical measurement techniques. The DNS in this case appears as a powerful tool.

## CONCLUSIONS

In the context of the collision/coalescence modelling the importance of the dense zone of a spray has been outlined. To characterise interactions between turbulence motion and the state of the liquid-gas interface an equilibrium Weber number has been used. To find its value a well defined DNS configuration has been set up. It has been demonstrated that present numerical techniques allow such a Weber number to be determined for a wide range of liquid volume fractions. From this study it was possible to follow continuously with the same numerical tools a situation ranging from bubble flows to droplets flows. However the current definition of the Weber number is not valid for the whole range of liquid volume fractions. A more general definition should be proposed. Cases with about the same level of liquid and gas can be studied. Contrary to bubble and droplet flows no discrete phase can be defined. This equally dense two-phase flow will be studied in further works.

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