

LAGRANGIAN/EULERIAN ANALYSIS OF THE DISPERSION OF VAPORIZING POLYDISPERSED SPRAYS IN TURBULENT FLOWS

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ABSTRACT

Direct Numerical Simulations (DNS) of turbulent two-phase flows have been carried out to study the polydispersion of a vaporizing spray in a statistically stationary grid turbulence. The evolution of various droplet size classes has been studied. It exhibits different dynamical behaviors for droplets of different sizes. The results have been used to evaluate successfully a new Eulerian model which proves its capability to capture the polydisperse spray dynamics and vaporization.

INTRODUCTION

In industrial combustion configurations, the fuel is most of the time injected as a dispersed phase of liquid droplets. In gas turbines, diesel engines, industrial furnaces and combustion chambers, the behavior of the gaseous fuel mixture fraction plays a crucial role in determining the combustion characteristics and efficiency of the process. Consequently, the description of the motion of the spray, its vaporization and its coupling with the gaseous turbulent flow field are important for the prediction of two-phase turbulent combustion. Even if the process has to be understood as a whole from injection up to combustion, one of the key issues will be the turbulent mixing and vaporization of the cloud of fuel droplets, a phenomenon strongly influenced by the polydisperse character of the spray. In this paper, we therefore focus our attention on the turbulent dispersion of a vaporizing liquid spray and on its polydispersion.

The purpose of the present study is two-fold : first, we investigate the physics of this phenomenon using a DNS Euler/Lagrange approach in the configuration of a statistically stationary spatially decaying turbulence, with a monodisperse injection. We analyze the DNS results for the dispersed phase with a Eulerian point of view and demonstrate the strong coupling of the dynamics and vaporization which generates droplets of various sizes. Second, we provide a Eulerian model and description of this phenomenon extending the recently introduced Eulerian multi-fluid models which are well suited to the presence of a polydisperse spray. Both approaches will then be compared, thus proving the ability of the Eulerian model to capture the physics and the complementarity of Lagrangian and Eulerian tools for the description of two-phase flows.

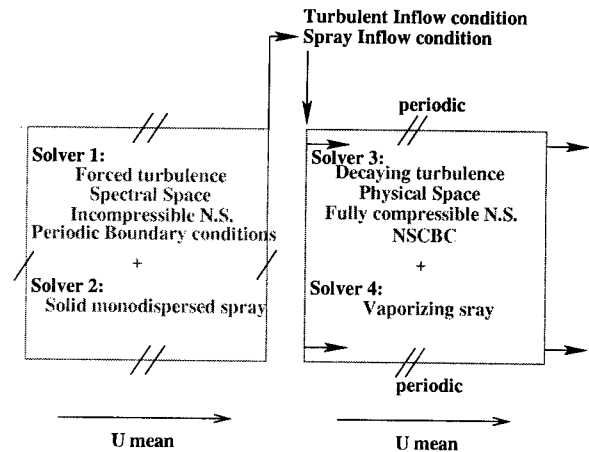


Figure 1: Sketch of the coupling between the four solvers

Two types of models may be actually considered for the description of the polydisperse liquid phase. The first one is of Lagrangian and particular type as it is described originally by Dukowicz (1980). The distribution of droplets is approximated using a finite number of computational parcels; each parcel represent a number of droplets of identical size, velocity and temperature. This kind of method is currently used in many codes and especially suited for DNS calculations since it does not introduce any numerical diffusion, the particle trajectories in the phase space being exactly resolved. It is then particularly accurate as long as the sampling of the phase space is high enough, a constraint that becomes expensive for instationary configurations.

In the context of RANS and LES numerical simulations, where some scales are not resolved but modeled, the perspective of an Eulerian model for polydisperse sprays becomes very attractive. Indeed, it is interesting to study the Eulerian form of the spray equations and to deduce the structure of physical phenomena such as waves, diffusion, etc. On the other hand, modeling of coalescence and break-up phenomena as well as the coupling with the combustion process are more straightforward by using an Eulerian formulation. Besides, a coherent way of treating the two phases yields a better ability for parallel computations and optimization.

However, actual Eulerian models present two major

Table 1: Data concerning the injected droplets. $x=0$ indicates solid particles ($s = cste$), whereas $x=1$ represents vaporizing droplets $s/s_0 = 1 - t/\tau_v$

Name	τ_p/τ_v	τ_p/τ_t
T0Vx	195	0.06
T2Vx	3.5	3.3

drawbacks : the inability to capture the polydispersion in size of the spray (only through a couple of moments such as in Vallet et al. (2001)) and the lack of direct link with the kinetic level of description for sprays. Thus, in the context of laminar flows, Laurent and Massot (2001) have introduced a multi-fluid approach, rigorously derived from the kinetic level of description, which has the capability to include coalescence and break-up as shown in Laurent et al. (2001) and to describe the vaporization, dynamics and heating of droplets of various sizes as studied in Laurent et al. (2002).

The paper is organized as follows : in a second section, the physical configuration and numerical methods are presented. We then focus on the analysis of the DNS results where we emphasize a surface conditioned Eulerian analysis of the polydisperse spray. We then conduct, in a fourth section, the derivation of the Eulerian model and present the numerical method used in the particular configuration under consideration. The DNS results and the simulations obtained from the Eulerian solver are then compared in the last section.

GEOMETRY AND NUMERICAL CONSIDERATIONS

In this paper, 2D and 3D spatially decaying turbulent (SDT) flows are considered. It simulates a grid-turbulence with a high kinetic energy at the inlet that decays along the streamwise direction. A monodisperse spray is injected through the inlet boundary and follows the main flow while being locally dispersed by the turbulent fluctuations. It is particularly interesting to notice that the coupling of vaporization and turbulent mixing generates a polydisperse spray, even if the liquid phase is injected monodisperse. This configuration is also a good candidate since the number of dimensions of the phase space remains reasonable. Moreover, the results are statistically stationary.

To ensure a statistically coherent behavior of the injected droplets with local turbulence, four solvers (fig. 1) are running simultaneously. An independent spectral code is solving the incompressible Navier-Stokes (NS) equations coupled with a one-way Lagrangian solver for the computation of the dispersion of solid particles. These two solvers are used to generate accurate turbulent boundary conditions for a physical space DNS solver (sixth order in space and third order in time) running along with another one-way Lagrangian solver. The fully compressible NS equations are then solved with periodic boundary conditions along the spanwise direction and NS characteristic boundary conditions (Poinsot and Lele, 1992) for the inlet and the outlet along the streamwise direction.

A forced turbulence, such as in Overholt and Pope (1998), is simulated in the spectral space so that the prescribed main properties of the turbulence (kinetic energy, dissipation, integral scale) are statistically stationary in time. The dispersion of particles in the phase space has been checked to be in dynamical equilibrium before the coupling with the physical space solvers took place.

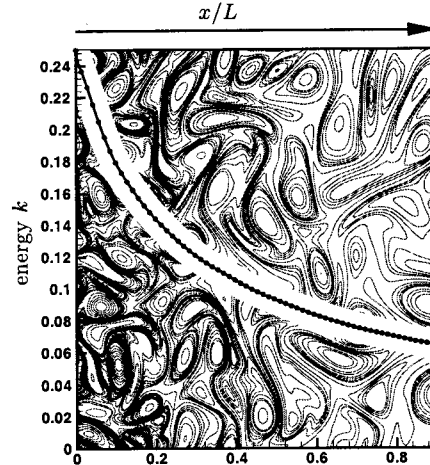


Figure 2: Vorticity isocontours of the decaying turbulence.

This coupling is done through the inlet boundary of the physical space solver where the turbulent fluctuations as well as the incoming particles are inserted. Because of the presence of the spectral solver, the vortices are really able to rotate at the boundary and therefore, local negative velocities may be considered. The technical details of the injection procedure may be found in Vervisch-Guichard et al. (2001). Once injected in the physical space DNS, the previously solid particles are considered as droplets of liquid and they are vaporizing following a *d-square* law and undergoing the drag force effects. Again, a one-way interaction with the turbulent flow is used to describe the dispersion of the droplets. It allows us to keep identical turbulence parameters while the spray properties are modified.

Before presenting the various test cases and results of this work, normalization parameters should be introduced. They are based on the properties of the flow and the spray. The droplets geometry is expressed in term of surface and it is normalized by their unique (monodisperse) injection value s_0 . The motion of the droplets in the gaseous flow and their evaporation rate lead to the characteristic times τ_p and τ_v (table 1); τ_p is the velocity response time (or kinetic time) of the droplets, quantifying their ability to follow or not the fluctuations of the flow, and $\tau_v = -s_0/\mathcal{R}$ is the vaporization time based on the initial size. They have to be compared with τ_t , the turbulent eddy turn over time. It leads to the following normalized *d-square* law : $s/s_0 = 1 - t/\tau_v$. The other parameters are the career phase mean velocity \bar{U} and consequently, the characteristic distance $L = \bar{U} * \tau_v$ covered by a droplet before its total vaporization.

SPRAY TURBULENT DISPERSION

Statistical considerations

The study of the dispersion of droplets in a spatially decaying turbulence implies to define some new parameters. An individual tracking has been introduced for every droplet in the flow whose Lagrangian time, position, velocity and surface are $(t_l, \mathbf{x}_d, V_d, s_d(t_l))$. As soon as a droplet is injected and begins to evaporate, it is associated to a 'reference particle' whose initial properties $(t_l, \mathbf{x}_r, \bar{U}, s_r = s_d)$ are the same. The reference particle travels at the mean stream-

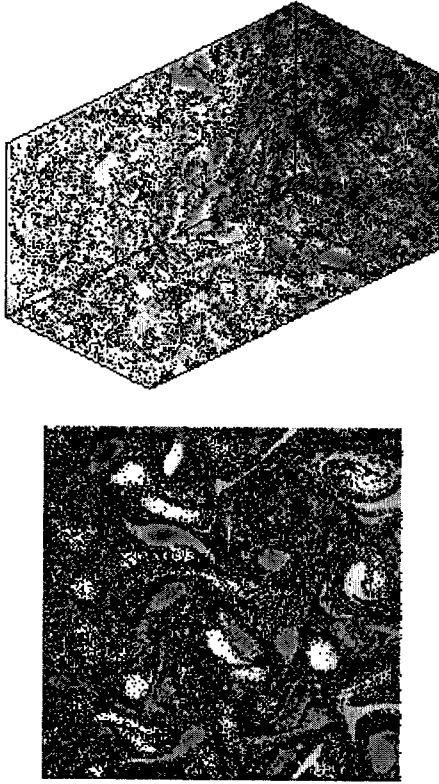


Figure 3: 3D (top) and 2D (bottom) droplets dispersion in a spatially decaying turbulence. dots : Droplets, iso-grey-colors : vorticity.

wise velocity whereas its corresponding droplet undergoes the turbulence fluctuations. By statistically studying the difference of position and velocity between the real droplet and its 'reference', we may characterize the turbulent dispersion. The dispersion statistics are then deduced from the following parameters : $\mathbf{x}^* = \mathbf{x}_d - \mathbf{x}_r$, $\mathbf{v}^* = \mathbf{V}_d - \bar{\mathbf{U}}$ and $\xi = s_d - s_0(1 - x_d/L)$. ξ is the relative surface between the tracked droplet and a droplet that would be at the same position without undergoing the turbulence.

Statistics are considered in time and along the spanwise direction.

Spray polydispersion

Examples of instantaneous 2D and 3D distributions of droplets are shown in figures 3. A qualitative comparison between 2D and 3D simulations showed a similar evolution of the spray properties. The figure 4-(a) shows an example of the evolution of the coupled PDF : $P(x, s)$ of the droplets streamwise position x and their surface s . It allows us to observe the joint effects of the evaporation and of the turbulence on the injected spray. Several positions of analysis along both x and s directions have been plotted. These positions labeled respectively x_i ($i = 1$ to 6) and s_j ($j = 1$ to 5) have been extensively used in this work. The profiles of $P(x, s)$ along the x direction for the fixed surfaces s_j show (fig. 4-(c)) a symmetrical Gaussian dispersion around a reference position $x_j^r/L = (1 - s_j/s_0)$ corresponding to the position of a droplet with the same s_j surface but which did not undergo the turbulence. Similarly, a spreading of the

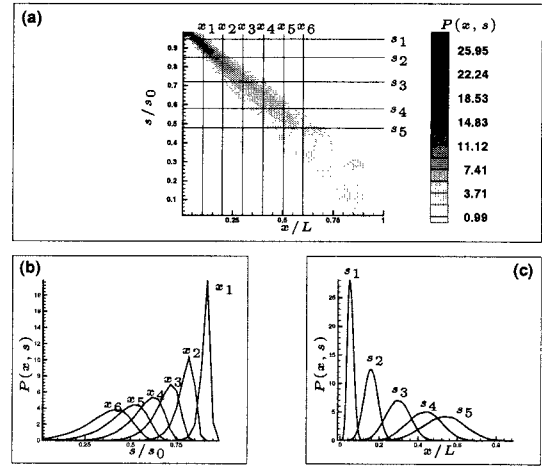


Figure 4: Isocontours (top) and profiles (bottom left and right) of the pdf $P(s, x)$. The profiles are made along x (bottom left) and s (bottom right) directions for several different positions shown on the top figure. $x_1/L = 0.092$, $x_2/L = 0.198$, $x_3/L = 0.304$, $x_4/L = 0.41$, $x_5/L = 0.516$, $x_6/L = 0.622$, and $s_1/s_0 = 0.95$, $s_2/s_0 = 0.85$, $s_3/s_0 = 0.72$, $s_4/s_0 = 0.58$, $s_5/s_0 = 0.48$

droplets surface may be observed (fig. 4-(b)) for a given x_i streamwise position. But, on the contrary to the previous profiles, the dispersion is not symmetrical around the reference surface $s_j^r/s_0 = (1 - x_i/L)$ corresponding to the surface of a vaporizing droplet moving with the reference velocity \bar{U} .

It is possible to examine the PDF : $P(u^*)$ corresponding to the droplets velocity fluctuations with regard to the gas mean flow. Indeed, as it will be shown later, a distinction has to be made between the gas phase mean velocity and the particles mean velocity. The u^* statistics have been made for every droplets without any distinction of class and a Gaussian shaped dispersion may be observed along the streamwise direction. Figure 5 depicts the fact that $P(u^*)$ develops a general Gaussian shape centered on $u^* = 0$. Three profiles of $P(u^*)$ extracted from the DNS are plotted figure 5-(a) along with the corresponding PDF presumed from the first two moments (\bar{u}^* , σ) of the velocity dispersion. A Gaussian shape function (3) has been used. σ has been determined from the values of $P(u^*)$ extracted from the DNS. The Gaussian presumed shape and the DNS data are similar. That confirms a Gaussian behavior of dispersion for the droplets considered as a whole without reference to their size. Moreover, the Gaussian curves being centered on $u^* = 0$, the mean droplets velocity is equal to the mean flow velocity (as soon as the droplets are not considered by classes).

The droplets energy σ has been determined for every streamwise position and compared to the gas decaying kinetic energy k on figure 6. For each droplet family, vaporizing and non-vaporizing cases have been plotted. As expected, it is possible to observe a mass-dependent behavior of the droplets. The light droplets (T0Vx, $x=0, 1$), with a small Stokes number ($S_t = 0.06$), follows closely the turbulent fluctuations of the gas. As soon as the droplets mass (and therefore Stokes number) increases (T2Vx), the inertia of the droplets is increasingly significant and they do not capture any more the whole fluctuations of the career phase. Thus, for a given spray, three energy levels can be differentiated according to the characteristic kinetic time of the droplets : k the real level of the gas kinetic energy, κ_p

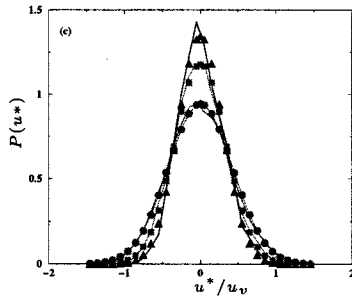


Figure 5: Profiles of $P(u)$, lines : DNS extracted, symbols : corresponding Gaussian reconstruction (circles : x_1 , squares : x_3 and triangles : x_6).

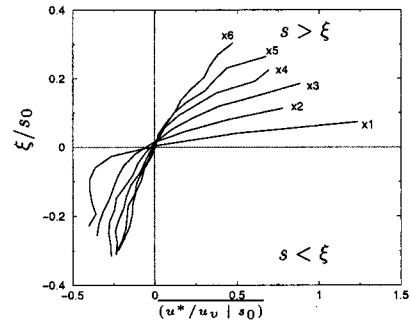


Figure 7: Mean droplet velocity conditioned by the droplet surface (T0V1, Eulerian positions : x_i , $i = 1, 6$).

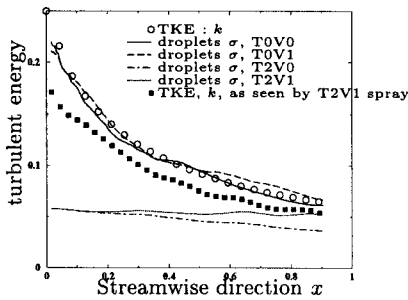


Figure 6: Comparison of the spatial evolution of the droplets energy σ with the gas turbulent kinetic energy k .

the level seen by the droplets and σ the level reached by the droplets. For light droplets with small τ_p , these levels are coinciding. As soon as τ_p increases, the three levels are differentiated with a fixed hierarchy : $k > \kappa_p > \sigma$.

Surface conditioned dispersion

The spray is initially monodisperse but it undergoes the effects of both droplets vaporization and turbulence mixing. These two phenomena lead to a polydisperse spray in both x and s directions of the phase space. In the previous section it has been shown that the spray position dispersion for a fixed droplet surface follows a Gaussian behavior. Now, It seems interesting to focus on the velocity behavior of the droplets considered class by class.

First, from an analytical point of view, it is possible to affirm that the mean velocities of the droplets depend on their surface for a given Eulerian position x . At any x position and by using the reference parameters ξ and u^* , we know that the droplets such as $\xi = 0$ and $u^* = 0$ have the same mean properties than the reference droplets which did not undergo the turbulence. If $\xi > 0$, then the droplet surface is larger than the reference one. Thus, these droplets traveled more quickly than the average flow. In the same way, the droplets such as $\xi < 0$ went more slowly. This is confirmed by figure where the mean droplet velocity conditioned by droplets surface $\overline{(u^* | \xi)}$ has been plotted. The analysis have been done for several Eulerian position previously defined (fig. 4). Close to the injection (x_1), the surface range dispersion is limited but, because of the high turbulent energy of the flow, velocity levels of the droplets are the highest. As the droplets move away in the flow, their sur-

face range increases but their mean velocity range decreases because of the weaker turbulent mixing.

The conditioned mean velocity being known, it is now particularly interesting to focus on the velocity dispersion of the droplets around this mean. Figure shows, for a given streamwise position, the PDF : $P(u, s)$ representing the velocity dispersion as a function of the droplet surface. Gaussian reconstructions around this mean value have been carried out. The presumed isocontours are shown figure (dotted contours) and are very close to the dispersion levels extracted from the DNS (plain contours). It appears that even by considering the dispersion as a function of the droplets surface, it follows a Gaussian law. But this is true only around the mean velocity of the particles and not around the local mean velocity of the gas flow, the two of them being different. Moreover, an integration of the dispersion along the s direction gives a global Gaussian dispersion around the mean flow velocity (fig. 5). But the corresponding energy σ is a global property for the whole spray and it does not allow a description of the dynamic of every class of droplets. This dynamic highly depends on the mass of the droplets, thus, to have an accurate description of their dispersion, a surface dependence should be introduced in any model developed to describe the dispersion of evaporating or polydisperse droplets.

Examples of the surface conditioned energy $\sigma(\xi)$ are shown figure 9 for both T0V1 and T2V1 cases. The statistics have been extracted for the reference Eulerian positions and correspond to the agitation energy of the droplets around their mean velocity. For the whole Eulerian positions, the light droplets have a similar $\sigma(\xi)$ whatever the droplet surface is. In fact, even the 'heaviest' ($\xi > 0$) of the light droplets (T0V1) are small and follow the turbulent fluctuations of the career phase without noticeable damping due to their inertia. Therefore, $\sigma(\xi)$ is almost constant for every value of the surface. On another hand, the vaporizing heavy droplets case (T2V1) leads to another conclusion. Indeed, because of their large Stokes number, the droplets proved to have an inertial behavior, going through turbulent structures without fully undergoing every one of them. Two main conclusions can be drawn from the figure 9-(b). First of all, for every increasing analysis Eulerian position (x_1, x_2, \dots) the general energy level $\sigma(\xi)$ increases as well because the droplet loss of mass implies a decrease of the effects of their inertia. In the same way, for a given analysis position, the dependence of $\sigma(\xi)$ with the surface of the droplets (ξ) is significant and follows a quasi-linear behavior.

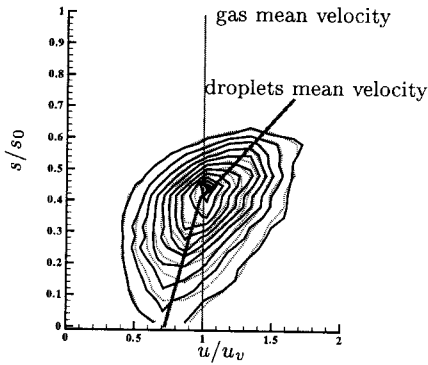


Figure 8: Comparisons of the spray velocity dispersion function $P(u, s)$ (black lines) with a presumed Gaussian shape dispersion function (dotted lines), case T0V1, Eulerian position : x_6 .

MULTI-FLUID MODELING

The fact that the turbulent dispersion of a vaporizing sprays is a surface conditioned phenomenon is very coherent with the work done on the Eulerian multi-fluid modeling of polydisperse sprays conducted in Laurent and Massot (2001). The purpose of this section is to present the derivation of such an approach in the turbulent case and the associated numerical methods.

Derivation of the model

The spray is described at the kinetic level by a distribution function $f(t, x, s, V_d)$ which satisfies a transport equation introduced by Williams (1958) :

$$\frac{\partial f}{\partial t} + V_d \cdot \nabla_x f + \frac{\partial \mathcal{R}f}{\partial s} + \nabla_{V_d}(\mathcal{F}f) = 0, \quad (1)$$

where \mathcal{F} is the Stokes drag acceleration. The vaporization rate \mathcal{R} is assumed to be independent of U , thus neglecting the convective correction term (see Laurent and Massot (2001) for detailed modeling assumptions).

For turbulent flows, the gas velocity seen by the particles can be decomposed into $U = \bar{U} + U'$, \bar{U} , its average value and U' , a fluctuation which is assumed to be a Gaussian Wiener process characterized by a Lagrangian correlation time along the trajectories τ_d as well as a turbulent kinetic energy κ_p . It is at this level that we can choose the scales which will be resolved. In this paper, for the first investigation of the Eulerian multi-fluid model, we will consider that the fluctuation describes the whole turbulence of the gas and the average value will be taken as the mean gas velocity. The LES point of view will be investigated in a subsequent study.

Once the scales have been chosen we need to derive a kinetic equation “in the mean” where the effects of the gas turbulence only appear through its characteristics quantities τ_d and κ_p . We use the framework introduced by Reeks (1991) and justified rigorously in Clouet and Domelevo (1997). We obtain an equation on the average for \bar{f} , which is the statistical expectation of f ; it reads :

$$\begin{aligned} \frac{\partial \bar{f}}{\partial t} + V_d \cdot \nabla_x \bar{f} + \frac{\partial \mathcal{R} \bar{f}}{\partial s} + \nabla_{V_d}(\bar{\mathcal{F}} \bar{f}) \\ - \nabla_{V_d} \cdot (D_x \nabla_x \bar{f} + D_{V_d} \nabla_{V_d} \bar{f}) = 0, \end{aligned} \quad (2)$$

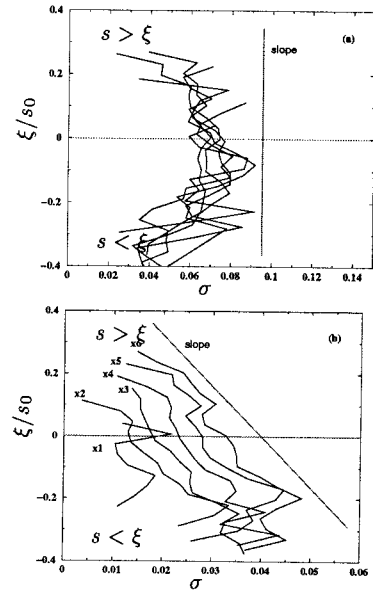


Figure 9: Droplet velocity dispersion parameter σ as a function of the droplet relative surface ξ . Left : T0V1 case, the profiles are similar, right : T2V1 case a significant effect of the droplet volume may be observed on the dispersion.

where the averaged drag force reads:

$$\bar{\mathcal{F}} = \frac{1}{\tau_p s} (\bar{U} - V_d).$$

The random fluctuations in the gas velocity then generate, on average, a diffusion process in the phase space. This approach requires the use of a simple vaporization model, which decouples the vaporization process from the velocity fluctuations; in a more general case, some additional terms should be added in (2). An exact expression of the diffusion coefficients can be obtained as functions of τ_d and κ_p along the lines given in Clouet and Domelevo (1997) and Reeks (1991).

Once the kinetic equation “in the mean” is derived, we can generalize the framework of the Eulerian multi-fluid model to the present case. As in Laurent and Massot (2001), we make an assumption on \bar{f} which appears as a closure at the kinetic level. We assume that, for a given size, there is only one characteristic velocity, with a Gaussian dispersion around it:

$$\bar{f}(t, x, s, V_d) = n(t, x, s) \varphi_{\sigma(t, x, s)}(V_d - \bar{V}_d(t, x, s)),$$

where φ_{σ} is a Gaussian of dispersion σ in the d -dimensional space :

$$\varphi_{\sigma}(v) = \frac{1}{\left(\frac{4}{d}\pi\sigma\right)^{d/2}} \exp\left(-\frac{v^2}{\frac{4}{d}\sigma}\right). \quad (3)$$

We will then obtain the semi-fluid equations on the three moments n , \bar{V}_d and σ , which can be interpreted as an internal energy of a monoatomic gas. From equations 2 and 3 it is possible to derive an Eulerian semi-fluid model that will not be detailed in this paper. Interested reader may refer to Laurent and Massot (2002). The system describes the evolution of the density of droplets, their velocity and their internal energy.

Resolution and results

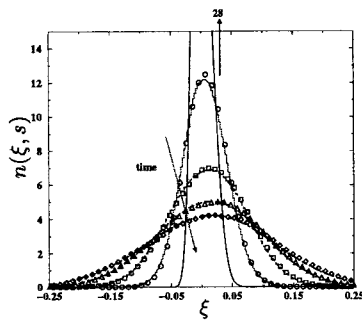


Figure 10: Droplet number density in the frame moving with the mean flow for various droplet sizes. Symbols : DNS statistics (circles : s_2 , squares : s_3 , triangles : s_4 , losanges : s_5). Lines : Eulerian multi-fluid simulations, T2V1 case.

An initial surface $s_1 = 0.95$ is selected close to the injection point. Initial fields of density, velocity and internal energy as a function of ξ are extracted from the s_1 DNS profiles. The resulting initial value problem for the system of equation is then resolved using a MUSCL second order extension of finite volume method with a minmod slope limiter and an explicit second order time discretization on a fine discretization which is reachable in this one-dimensional problem.

Comparisons between DNS statistics issued from the Lagrangian dispersion of the droplets and the Eulerian resolution of the multi-fluid model are shown in figures 10 and 11. For both heavy (T2V1) and light (T0V1) droplets, the evolution of the density of droplets is accurately captured by the multi-fluid formulation (fig. 10). Moreover, in the case T2V1 where the droplets are not strictly following the gas evolution, the Eulerian resolution of the evolution of the droplets conditioned velocity and internal energy has been captured by the model (fig. 11).

CONCLUSIONS AND ACKNOWLEDGMENTS

For the first time, comparisons between a DNS (coupled with a Lagrangian solver) of a statistically stationary turbulent two-phase flow and a Eulerian model dedicated to spray dispersion have been carried out. DNS showed its ability to capture the evolution of some complex interactions between the flow and the vaporizing droplets. Then, the Eulerian multi-fluid model, has been resolved and compared with the DNS results. The multi-fluid model proved to be able to capture the evolution of a polydisperse vaporizing spray in a turbulent environment. This is a very encouraging result for the modeling of complex configurations such as combustion chambers. Indeed, even if more tests and developments are needed, the multi-fluid formulation may be an alternative to the actual Lagrangian model which may have difficulties to capture some phenomena such as coalescence or break-up of the droplets.

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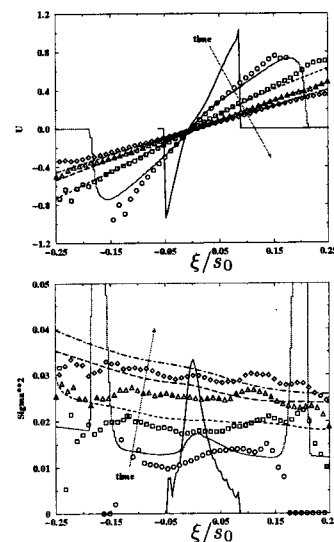


Figure 11: Droplets mean velocity **top** and droplets internal energy **bottom** in the frame moving with the mean for various droplet sizes in the T2V1 case. Symbols : DNS statistics (circles : s_2 , squares : s_3 , triangles : s_4 , losanges : s_5). Lines : Eulerian multi-fluid simulations.

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