



HAL
open science

Eulerian models and three-dimensional numerical simulation of polydisperse sprays

Lucie Fréret, Stephane de Chaisemartin, Julien Reveillon, Frédérique Laurent,
Marc Massot

► **To cite this version:**

Lucie Fréret, Stephane de Chaisemartin, Julien Reveillon, Frédérique Laurent, Marc Massot. Eulerian models and three-dimensional numerical simulation of polydisperse sprays. Internation Conference on Mutiphase Flows, May 2010, Tampa - Florida USA, United States. pp.1-15. hal-00498207

HAL Id: hal-00498207

<https://hal.science/hal-00498207>

Submitted on 7 Jul 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Eulerian models and three-dimensional numerical simulation of polydisperse sprays

L. Fréret^{*}, S. de Chaisemartin[†], J. Reveillon[‡], F. Laurent[§] and M. Massot[§]

^{*} Laboratoire d'Imagerie Paramétrique, Université Paris VI, France

[†] IFP, Reuil Malmaison, France

[‡] CORIA, Saint Etienne du Rouvray, France

[§] Laboratoire EM2C, Ecole Centrale Paris, Châtenay-Malabry, France

lucie.freret@upmc.fr, stephane.de-chaisemartin@ifp.fr, julien.reveillon@coria.fr, frederique.laurent@em2c.ecp.fr,

marc.massot@em2c.ecp.fr

Keywords: Liquid Sprays, multi-fluid models, numerical analysis, scientific and parallel computing, Euler-Euler/Euler-Lagrange comparisons.

Abstract

Providing accurate simulations of polydisperse evaporating sprays dynamics in unsteady gaseous flows with large scale vortical structures is both a crucial issue for industrial applications and a challenge for modeling and scientific computing. The usual Lagrangian approaches developed in polydisperse unsteady configurations require tremendous computational costs and may lead to a low level of resolution if not enough numerical parcels are used. Besides, they induce coupling issues due to the different kind of description of the two phases that are involved. A large range of Eulerian models have been recently developed to describe the dispersed liquid phase with a lower cost and an easier coupling with a carrier gaseous phase. Among these models, the multi-fluid model allows a detailed description of polydispersity and size/velocity correlations of droplets of various sizes. It has been studied in depth from a mathematical and numerical point of view (see Laurent & al (2004); Laurent (2006); Massot & al (2009)) and validated through comparisons versus Lagrangian simulations in de Chaisemartin (2009) and experimental measurements in Fréret & al (2008) in 2D and 2D-axisymmetrical configurations. However, the validation in three-dimensional unsteady configurations still remains to be done. In this work, we study the non-evaporating droplet segregation in three-dimensional Homogeneous Isotropic Turbulence (HIT) using a reference Lagrangian spray model versus the Eulerian multi-fluid model. A spectral Direct Numerical Simulation solver is used to describe the evolution of the turbulent carrier phase, whose characteristic properties remain statistically stationary due to a semi-deterministic forcing scheme. We focus on the optimization via a parallel implementation of the multi-fluid model and dedicated numerical methods which demonstrates the ability of the Eulerian DNS model to be used in high performance computing for academic three-dimensional configurations. We provide qualitative comparisons between the Euler-Lagrange and the Euler-Euler descriptions for two different values of the Stokes number based on the initial fluid Kolmogorov time scale, $St = 0.17$ and 1.05 . A very good agreement is found between the mesoscopic Eulerian and Lagrangian predictions. We go further with first quantitative comparisons of the segregation effect of the vortices on the spray mass density distribution showing the accuracy and ability of the multi-fluid model to be used in 3D configurations from the tracer limit ($St \rightarrow 0$) to unity.

Introduction

In many industrial combustion applications such as Diesel engines, fuel is stocked in condensed form and burnt as a dispersed liquid phase carried by a gaseous flow. Two phase effects as well as the polydisperse

character of the droplet size distribution can significantly affect flame structures. Size distribution effects are also encountered in a crucial way in solid propellant rocket boosters, where the cloud of alumina particles experiences coalescence and becomes polydisperse in size, thus determining their global dynamical behav-

ior, see Doisneau & al (2010). Consequently, it is of interest to have reliable models and numerical methods able to describe precisely the two-phase flows physics where the dispersed phase is constituted of a cloud of particles of various sizes that can evaporate, coalesce or aggregate, break-up and also have their own inertia and size-conditioned dynamics. In a “mesoscopic” description of the liquid phase, droplets are considered as a cloud of point particles for which the exchanges of mass, momentum and heat are described using a statistical point of view, with eventual correlations, and the details of the interface behavior, angular momentum of droplets, detailed internal temperature distribution inside the droplet, etc., are not predicted. Instead, a finite set of global properties such as size of spherical droplets, velocity of the center of mass, temperature are modeled. Since it is the only one which provides numerical simulations at the scale of a combustion chamber or in a free jet, this mesoscopic point of view will be adopted in the present paper.

The main physical processes that must be accounted for are (1) transport in real space, (2) acceleration of droplets due to drag, (3) droplet heating and evaporation, and (4) coalescence and break-up of droplets leading to polydispersivity. Spray models have a common basis at the mesoscopic level under the form of a number density function (NDF) satisfying a Boltzmann type equation, the so-called Williams equation (Williams (1958)). The internal variables characterizing one droplet are the size, the velocity and the temperature, so that the total phase space is usually high-dimensional. Such a transport equation describes the evolution of the NDF of the spray due to evaporation, to the drag force of the gaseous phase, to the heating of the droplets by the gas and finally to the droplet-droplet interactions, such as coalescence and break-up phenomena. There are several strategies in order to solve the liquid phase and the major challenge in numerical simulations is to account for the strong coupling between all the involved processes. A first choice is to approximate the NDF by a sample of discrete numerical parcels of particles of various sizes through a Lagrangian–Monte-Carlo approach (see O’Rourke (1981)). It is called Direct Simulation Monte-Carlo method (DSMC) by Bird (1994) and generally considered to be the most accurate for solving Williams equation; it is especially suited for DNS since it does not introduce any numerical diffusion, the particle trajectories being exactly solved. This approach has been widely used and has been shown to be efficient in numerous cases. Its main drawback is the coupling of an Eulerian description for the gaseous phase to a Lagrangian description of the dispersed phase, thus encountering difficulties of vectorization/parallelization and implicitation. Besides, it brings another issue asso-

ciated with the repartition of the evaporated mass at the droplet location onto the Eulerian grid for the gas description. Moreover for unsteady computations of poly-disperse sprays, a large number of parcels in each cell of the computational domain is generally needed, thus yielding large memory requirement and CPU cost. This drawback makes attractive the use of a Eulerian formulation for the description of the disperse phase, at least as a complementary tool for Lagrangian solvers.

The Eulerian Multi-Fluid model, extended by Laurent & Massot (2001) from the ideas of Greenberg & al (1993), allows to describe polydispersivity of a spray in size and the associated size-conditioned dynamics. This approach relies on the derivation of a semi-kinetic model from the Williams equation using a moment method for velocity conditioned by droplet size while keeping the continuous size distribution function. This distribution function is then discretized using a finite volume approach in the size phase space that yields conservation equations for mass, momentum (and eventually other properties such as temperature) of droplets in fixed size intervals. This Multi-Fluid model is developed in the framework of a DNS for laminar flows. However, it is specific of the difficulties one will encounter in the development of Large Eddy Simulation (LES) tools for turbulent flows (see Boileau & al (2010)).

In the present work, we consider monodisperse non-evaporating sprays in large scale vortical structures of an unsteady forced HIT gaseous field. As we do not want to cope with the difficulties of the two-way coupling but solely compare two descriptions of the dispersed liquid phase, we restrict the simulation to one-way coupling and thus isolate the behavior of each method. The extension to polydisperse evaporating droplets has already been discussed in Laurent & al (2004); de Chaisemartin & al (2008); Reveillon & Demoulin (2007), crossing phenomena in Kah & al (2010) and was not taken into account here since we tend to validate the multi-fluid model in 3D unsteady flows. Simulations were carried out thanks to the coupling of a solver dedicated to the Eulerian spray description (Muses3D) with an other one which solves the Lagrangian liquid phase and the gas phase on a Eulerian grid (Asphodele). Muses3D solver has been developed by S. de Chaisemartin during his thesis (de Chaisemartin (2009)) and L. Fréret at EM2C laboratory and Asphodele by J. Réveillon and co-workers at CORIA laboratory. The coupling of these two solvers allows the simultaneous numerical simulation with the use of two models Eulerian and Lagrangian for the liquid phase coupled to an unique gas carrier-phase.

The paper is organized as follows. We first recall briefly the modelling of the liquid phase, both from a La-

grangian and Eulerian descriptions, as detailed in de Chaisemartin (2009). We also discuss the numerical methods for the two different descriptions as well as for the gaseous phase. Next, we detail the optimization via MPI parallel implementation done in Muses3D connecting with numerical methods and the way we achieved the coupling between parallel Muses3D and sequential Asphodele. This allows to carry out simultaneous simulations of two descriptions of a spray dispersion in an unsteady three-dimensional HIT configuration with two different Stokes, from the tracer limit $St = 0.17$ to $St = 1.05$ which leads to maximal segregation effects. Qualitative comparisons are performed considering the Eulerian liquid density, the Lagrangian droplet positions and particle number density. Moreover, statistical properties of the dispersed phase such as particle-fluid velocity correlation and Eulerian droplet segregation are computed from both Lagrangian and Eulerian simulations. Presented results account for our first quantitative outcome on droplet segregation in an unsteady 3D configuration.

Governing equations and modelling

In this study, we restrict ourselves to physical processes such as (1) transport in real space and (2) acceleration of droplets due to drag.

In order to introduce the non-dimensional equations, we define the reference velocity U_0 and length x_0 based on the macroscopic characteristics of the computational domain allowing to define a reference time scale for the gas: $\tau_g = x_0/U_0$. These quantities, along with the physical constants for a reference physical mixture, ρ_∞ , μ_∞ are taken to define the dimensionless system. To derive the dimensionless equations, we define a normalization Reynolds number based on the reference quantities

$$Re_0 = \frac{\rho_\infty x_0 U_0}{\mu_\infty}. \quad (1)$$

The Stokes number is given by $St = \tau_p/\tau_\kappa$ where the drag relaxation time is defined by $\tau_p = \rho_l S/(18\pi\mu_g)$, the liquid density is ρ_l and μ_g is the gas viscosity and τ_κ is the Kolmogorov time scale.

Dimensionless variables are given such as:

$$\mathbf{u}^* = \mathbf{u}/U_0, \quad \mathbf{x}^* = \mathbf{x}/x_0, \quad t^* = t/\tau_g, \quad S^* = S/S_0.$$

A number density function (NDF) of the spray f^Φ is introduced, the quantity $f^\Phi(t, \mathbf{x}, S, \mathbf{u})d\mathbf{x}dSd\mathbf{u}$ being the probable number of droplets with a position in $[\mathbf{x}, \mathbf{x} + d\mathbf{x}]$, a surface in $[S, S + dS]$, a velocity in $[\mathbf{u}, \mathbf{u} + d\mathbf{u}]$ and at time t . The NDF satisfies a simplified Williams-Boltzmann equation:

$$\partial_t f + \partial_{\mathbf{x}} \cdot (\mathbf{u}f) + \partial_{\mathbf{u}} \cdot (\mathbf{F}f) = 0, \quad (2)$$

where \mathbf{F} is the dimensionless Stokes law drag force given by $\mathbf{F} = (\mathbf{u}_g - \mathbf{u})/St$ with \mathbf{u}_g the gas velocity.

Lagrangian liquid phase. To solve the kinetic equation (2) of the spray, we can use Lagrangian Monte-Carlo methods. This leads to Euler-Lagrange numerical methods, commonly used for the calculation of poly-disperse sprays in various application fields (generally, the gas phase is computed using a deterministic Eulerian solver, while the disperse phase is treated in a Lagrangian way). In our study, the Lagrangian reference is not taken as a converged DSMC method, in order to be closer to industrial concern. For the given gas DNS configuration, we perform a Discrete Particle Simulation (DPS). Indeed there is no need to use Stochastic Parcel method, since all the droplets contained in the computational domain can be tracked. One can note that in the infinite Knudsen limit meaning that there is no droplet interaction, the DSMC computation is equivalent to an ensemble of DPS, each numerical particle representing one droplet with a weight equal to one.

The physical processes are then described by the classical following non-dimensional equations:

$$\begin{cases} \frac{d\mathbf{v}_k}{dt} = \frac{1}{St(S_k)} (\mathbf{u}_g(\mathbf{x}_k, t) - \mathbf{v}_k), \\ \frac{d\mathbf{x}_k}{dt} = \mathbf{v}_k, \end{cases} \quad (3)$$

where \mathbf{v}_k and \mathbf{x}_k denote the dimensionless velocity and position vectors of each droplet k . The vector \mathbf{u}_g represents the gas velocity at the droplet position \mathbf{x}_k . The right hand-side term of the first equation in (3) stands for a drag force applied to the droplet of size S_k .

The Lagrangian numerical particles ODE systems (3) are solved with an explicit third order Runge Kutta solver.

Eulerian liquid phase. The alternative to Lagrangian particle tracking is the resolution of spray Eulerian global quantities, as number or mass density and momentum. These Eulerian methods can be seen as moment methods derived from the kinetic equation (2). The formalism and the associated assumptions needed to derive the Eulerian multi-fluid model are introduced in Laurent & Massot (2001). Two steps are to be realized in order to obtain the Eulerian multi-fluid model's equations. In a first step, the size of the phase space is reduced by considering zero and one order moments with respect to the velocity variable at a given time t , position \mathbf{x} and droplet size S : $n = \int f d\mathbf{u}$ and $\bar{\mathbf{u}} = \int \mathbf{u} f d\mathbf{u}/n$ which depend on (t, \mathbf{x}, S) . The closure of the system is obtained through the following assumptions:

[H1] For a given droplet size, at a given point (t, \mathbf{x}) , there is only one characteristic averaged velocity $\bar{\mathbf{u}}(t, \mathbf{x}, S)$.

[H2] The velocity dispersion around the averaged velocity $\bar{\mathbf{u}}(t, \mathbf{x}, S)$ is zero in each direction, whatever the point (t, \mathbf{x}, S) is.

It is equivalent to presume the following NDF conditioned by droplet size:

$$f(t, \mathbf{x}, S, \mathbf{u}) = n(t, \mathbf{x}, S)\delta(\mathbf{u} - \bar{\mathbf{u}}(t, \mathbf{x}, S)), \quad (4)$$

that is to reduce the support of the NDF to a one dimensional submanifold parametrized by droplet size.

Such an assumption leads to a closed system of conservation equations called the semi-kinetic model on the moments of order zero and one in velocity. It is given by two partial differential equations in the variables $n(t, \mathbf{x}, S)$ and $\bar{\mathbf{u}}(t, \mathbf{x}, S)$ which express the conservation of the number density of droplets and their momentum, respectively, at a given location \mathbf{x} and for a given size S :

$$\begin{cases} \partial_t n + \partial_{\mathbf{x}} \cdot (n\bar{\mathbf{u}}) = 0, \\ \partial_t (n\bar{\mathbf{u}}) + \partial_{\mathbf{x}} \cdot (n\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) - n\bar{\mathbf{F}} = 0, \end{cases} \quad (5)$$

where $\bar{\mathbf{F}}(t, \mathbf{x}, S)$ is the Stokes's drag force taken at $\mathbf{u} = \bar{\mathbf{u}}$.

The second step consists in choosing a discretization $0 = S(1) < S(2) < \dots < S(p) < \dots < S(N_S + 1)$ for the droplet size phase space and to average the obtained system of conservation laws over each fixed size intervals $[S_p, S_{p+1}[$, called section. The set of droplets in one section can be seen as a "fluid" for which conservation equations are written. The sections exchange mass and momentum. To close the system, the following assumptions are introduced:

[H3] In one section, the characteristic averaged velocity does not depend on the size of the droplets.

[H4] The form of n as a function of S is supposed to be independent of t and \mathbf{x} in a given section, thus decoupling the evolution of the mass concentration of droplets in a section from the repartition in terms of sizes.

The conservation equations for the k^{th} section then read, in our simplified case:

$$\begin{cases} \partial_t m^k + \partial_{\mathbf{x}} \cdot (m^k \bar{\mathbf{u}}^k) = 0, \\ \partial_t (m^k \bar{\mathbf{u}}^k) + \partial_{\mathbf{x}} \cdot (m^k \bar{\mathbf{u}}^k \otimes \bar{\mathbf{u}}^k) = m^k \bar{\mathbf{F}}^k, \end{cases} \quad (6)$$

where m^k is the mass concentration of droplets in the k^{th} section.

Eulerian multi-fluid numerical methods

Phenomena involved in our problem are of two different types: transport induces an evolution in the physical space without any interaction between the sections, and by contrast, the transport in internal coordinate space (velocity) are encountered through drag. This induces an evolution without any coupling with the spatial coordinates. It is then interesting to separate these two transport types using an operator-splitting method and to treat efficiently the different difficulties of the multi-fluid system: a complex transport term (for the physical space) and stiff source terms (for the phase space). The multi-fluid system (6) is then split into two systems that we solve alternatively. We choose a Strang splitting which is second order in time provided that all the steps are second order in time, see (Descombes and Massot 2004). The scheme then takes the form:

$$H_S^{\Delta t} \circ G_{\mathbf{x}}^{\Delta t} \circ G_{\mathbf{x}}^{\Delta t} \circ H_S^{\Delta t} = H_S^{\Delta t} \circ G_{\mathbf{x}}^{2\Delta t} \circ H_S^{\Delta t}, \quad (7)$$

where $G_{\mathbf{x}}^{\alpha}$ (respectively H_S^{α}) denotes the physical transport (respectively the phase space transport) during time α . This Strang splitting is composed of two Lie splitting step ($H_S^{\alpha} \circ G_{\mathbf{x}}^{\alpha}$) of length $\alpha = \Delta t$ and it alternates the order in which they are performed (left part of equation (7)). It is equivalent to one Strang splitting step of length $2\Delta t$ (right part of equation (7)). The splitting approach has the great advantage to preserve the properties of the schemes we use for the different contributions such as maximum principle on the velocity or positivity of density.

In physical space, the system that we get from the operator splitting is weakly hyperbolic and can generate δ -shock and vacuum zones. As precised in de Chaisemartin (2009), we use second order kinetic schemes which are finite volume schemes based on the equivalence between a macroscopic and a microscopic level of description for the pressureless gas equations (see Bouchut & al (2003)). These schemes preserve the positivity of mass density and reproduce a discrete maximum principle on the velocity. In addition, we use a dimensional Strang type splitting. This allows to use schemes in 1D configuration and it preserves the second order of the method (see LeVeque (2002)). In the 3D case, the scheme then takes the form:

$$G_x^{\Delta t} \circ G_y^{\Delta t} \circ G_z^{\Delta t} \circ G_z^{\Delta t} \circ G_y^{\Delta t} \circ G_x^{\Delta t}, \quad (8)$$

where G_d^{α} denotes the physical transport in the direction d (which can be x , y , or z) during time α . This form of splitting does not lead to CFL reduction in a direction as a classical Strang splitting algorithm would. Indeed all the transport sub-steps are computed for a timestep Δt . This splitting allows the same numerical diffusion

in each direction. The global scheme we solve is then obtained by replacing $G_x^{2\Delta t}$ by the expression (8) in (7). The system obtained in the phase space from the splitting of system (6) is solved using an efficient ODE solver based on an implicit Runge-Kutta 5th order method RadauIIA (see Hairer & Wanner (1996)).

Eulerian multi-fluid optimization. As for standard Eulerian computational fluid dynamics, domain decomposition appears, for multi-fluid computation, as a very interesting way to achieve parallel computation. Indeed it offers the ability to use an arbitrary high number of points, the number of processes used allowing to have a sub-domain on each process with a reasonable number of points, leading to reasonable computational time and memory requirement. The difficulty of such parallelization lies in the data communications due both to multi-fluid peculiarities and dedicated numerical methods.

The main issue of the multi-fluid, when dealing with domain decomposition, is the size discretization leading to an extra dimension of the problem. As this dimension typically contains five to twenty sections for “classical” multi-fluid model, a 3-D computational domain leads to a 4-D computation. Furthermore, the operator splitting used for the numerical scheme makes two blocks appear with different properties, as far as domain decomposition is concerned. On the one hand the physical space transport is local in size and would naturally lead to a domain decomposition in size, each process realizing the transport for one size section. In this case no communication would be necessary in the physical space. On the other hand, the phase space transport is local in physical space and would then lead to a decomposition in space, a process treating a space sub-domain with all the size sections on it. Here, no communication needs to take place on the phase space. The different decomposition strategies available in this context have been evaluated (see de Chaisemartin (2009)). The first strategy is limited by the number of sections used and will have to be coupled with a partially spatial decomposition, in order to use an important number of parallel processes ($\simeq 100$). A hybrid method, with size decomposition in the physical transport, and space decomposition in the size phase space transport lead to an array reorganization and consequently to a high amount of communications. Finally, the domain decomposition in space is a good compromise between data calculations and MPI communications. For this strategy, an efficacy close to one has been obtained up to 128 cores that was the limit of our cluster. The extensibility to a thousand core is eventually foreseen and is the subject of our current investigations.

Gas solver and turbulence forcing. The gaseous carrier-phase is solved using a solver for Low Mach or incompressible flows. This solver is based on finite-difference (FD) prediction correction method for the velocity evolution, as introduced in Chorin (1968). As far as numerical methods are concerned, the time resolution is provided by a third order explicit Runge Kutta scheme. Spatial evolution is done with a FD scheme, the derivatives being computed with a Pade 6th order scheme (see Lele (1992)).

At each time step, we perform a turbulence forcing method to generate an isotropic homogeneous turbulence. To maintain the major properties (energy, dissipation rate, integral scale) of the spectral turbulence close to constant values, a controlled amount of energy must be transferred into the spectral simulation through a forcing procedure. There are various ways to achieve the forcing of isotropic homogeneous turbulence in a spectral DNS. In this work, we use the fully controlled deterministic forcing scheme (FC-DFS) developed by Guichard & al (2004). Inspired from Overholt & Pope (1998)’s deterministic scheme, FC-DFS scheme has an efficient convergence rate and reduces drastically the fluctuations of the prescribed properties. Turbulence is forced by adding a linear source term to the balance equation for the velocity field \hat{u} in wavenumber space:

$$\frac{\partial \hat{u}}{\partial t} = \hat{a} + \frac{f_\kappa}{\tau_f} \hat{u},$$

where \hat{a} represents the classical Navier-Stokes contributions for an incompressible flow. The forcing function f_κ is real and depends on both time t and wavenumber magnitude κ . The value τ_f is the characteristic relaxation delay of the simulated spectrum E_s towards a model spectrum E_m . The principle of FC-DFS model is to relax the simulated spectrum E_s towards a model one E_m only for a given range of low wavenumbers ($\kappa < \kappa_F$). The interested reader is referred to Guichard & al (2004) for further information. The vorticity of the field extracted at dimensionless time $t = 20$ from this computation is plotted in Fig 1(a).

3D DNS configuration

A uniformly monodispersed non-evaporating spray with a zero initial velocity is distributed initially in the gaseous field in order to study droplet ejection from the core of the vortices. The drag force sets particles in motion. Owing to the multi-fluid size distribution description, the evaporating case is easy to carry out and will be addressed in a near future, the non-evaporating case was a necessary first step.

Droplet dispersion and preferential segregation have

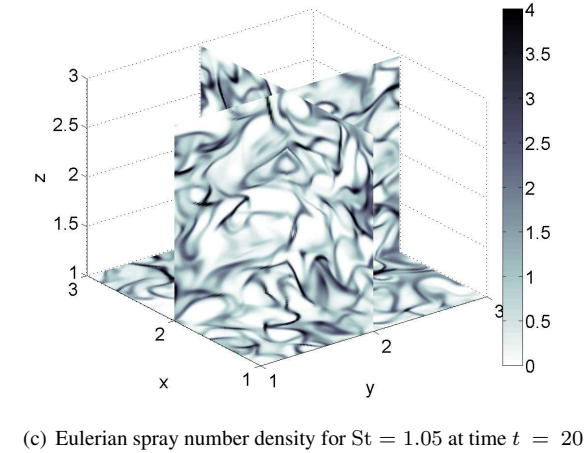
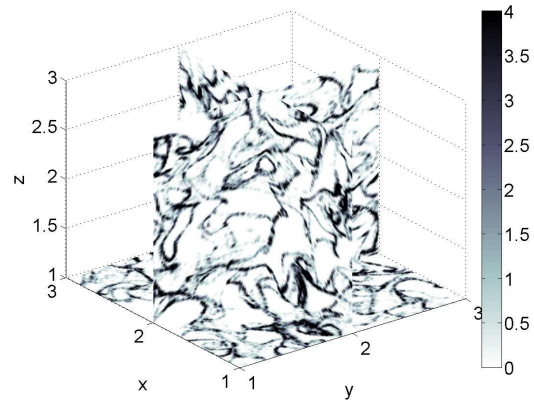
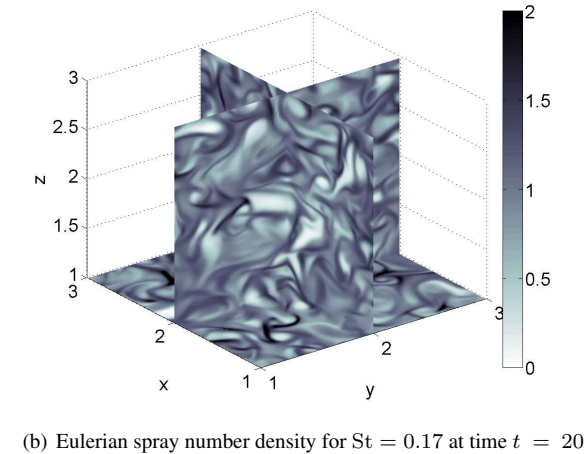
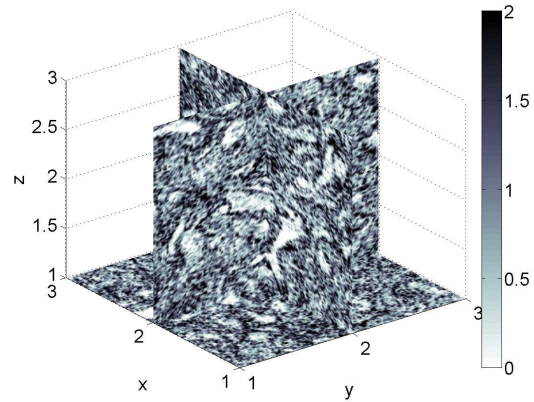
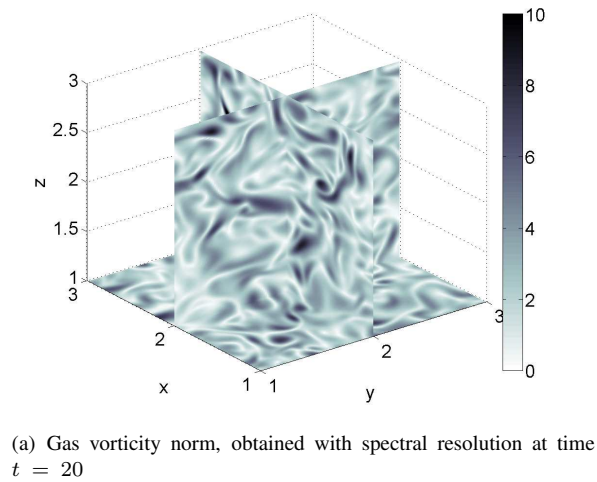


Figure 2: Eulerian spray number density $\bar{\xi}/\bar{\xi}_0$ obtained from a Lagrangian simulation of 128^3 particles by considering the droplets accumulated around each numerical grid node, at time $t = 20$. Slice planes at $x = 2$, $y = 2$, $z = 1$ for two Stokes number: (a) $St = 0.17$, (b) $St = 1.05$.

Figure 1: (a) Gas vorticity norm, obtained on a 129^3 grid with spectral resolution at time $t = 20$, slice planes inside the domain ($x = 2$, $y = 2$, $z = 1$). Eulerian spray number density obtained with the multi-fluid method on a 129^3 Cartesian grid at time $t = 20$. Slice planes at $x = 2$, $y = 2$, $z = 1$, for two Stokes number: (a) $St = 0.17$, (b) $St = 1.05$.

been analyzed from a Eulerian point of view. Instantaneous fields of density are plotted for $St = 0.17$ in Fig 1(b) and for $St = 1.05$ in Fig 1(c). This latter case is a case of a Stokes number close to unity leading to maximal segregation effects. The corresponding vorticity field is presented in Fig 1(a). These three fields have been captured at exactly the same dimensionless time $t = 20$. Even without any quantitative analysis, it is possible to see the dramatic impact on the particles' inertia on their dispersion properties. Particles tend to leave the vortex cores and segregate in weak vorticity areas. For $St = 1.05$, the normalized liquid density varies between 0 (no droplets) and 4 (four times the mean density).

Numerical setup. We use a cubic computational domain with periodic boundary conditions. As far as spatial discretization is concerned, the same grid of 129^3 points is used for the gas solver and the Eulerian spray solver. One has to note that the space domain decomposition for the multi-fluid method, implemented using the MPI library, allows to use for the spray computation a refined Eulerian grid at a low computational time cost. This refinement is already available through a trilinear interpolation procedure but was not used in this study since our objectives were the validation of the Eulerian model in a 3D unsteady and realistic context. As the gas field is solved sequentially, it is globally known on each processor and this allows to distribute uniformly Lagrangian particles on each core. This reduces significantly the number N_l of Lagrangian particles on each core keeping the total particles number N very high. We have $N_l = N/n_p$ where n_p is the core number. As the evaporation phenomena is not taken into account and there is no interaction between Lagrangian droplets, numerical particles are independent from one to each other and no information goes from droplets to the gas. Hence, there is no need to consider MPI communications between nodes. No particles have to be moved from one core to another as it has to be done when the gas field is divided into distinct sub-domains, see Garcia (2009). An other point of view is to consider that we are doing n_p DPS simulations with few numerical particles. The parallel efficiency of such method is thus optimal and equal to one. The simulations corresponding to the results that are presented were performed on a cluster made of 8 nodes with 2 processors AMD Opteron 64 bits dual core with speed 2.4 GHz, the 32 cores being connected by an infiniband gigabit network. A computational time of twenty hours was necessary to obtain the Eulerian and the Lagrangian simulation up to a dimensionless time $t = 20$.

In our simulations, $N = 128^3$ mono-dispersed

non-evaporating particles are randomly embedded throughout the computational domain with a zero initial velocity. Hence, thanks to the use of 32 cores, $N_l \simeq 65530$ droplets are tracked through the unsteady gas field on each core. Droplet dispersion is usually characterized by the Stokes number $St = \tau_p/\tau_k$, τ_k being the Kolmogorov length scale, which indicates the ability of droplets to capture local variations of the carrier-phase velocity. Turbulence properties being fixed, simulations were carried out by varying the τ_p parameter. Two Stokes numbers have been considered, 0.17 and 1.05, corresponding to droplet diameters of 15 and 45 μm . The Reynolds number defined in (1) is equal to 1000. We eventually provide dimensional quantities for illustration purposes, based on an estimated velocity of $U_0 = 1.5m/s$ and $x_0 = 0.01m$, as well as a typical value of $1.5 \times 10^{-5} m^2 / s$ for μ_∞ . In addition, we will let $d_0 = 0.001x_0$ (for $St = 0.17$) and $d_0 = 0.003x_0$ (for $St = 1.05$), where d_0 is the diameter corresponding to the droplet surface area S_0 . The computational domain has a size L^3 with $L = 2$, which corresponds to 8 cm^3 in dimensional values. We take as a reference solution for the liquid phase the Lagrangian Discrete Particle Simulation with N particles in the computational domain. We provide comparisons between this Lagrangian reference and the Eulerian multi-fluid monokinetic computations by plotting the Lagrangian particle positions and the particle number density measured from the Lagrangian simulation versus the Eulerian number density.

Eulerian-Lagrangian comparisons

Qualitative liquid dispersion comparisons. The Eulerian multi-fluid description of the spray dynamics are presented in this section for two Stokes number, based on the Kolmogorov length scale:

- $St = 0.17$, corresponding to droplet with diameter $d = 15\mu m$, see Fig 1(b).
- $St = 1.05$, corresponding to droplet with diameter $d = 45\mu m$, see Fig 1(c).

These two different inertia allow to study a spray ejected from the center core and segregated in weak vorticity areas. They are thus well suited for robustness evaluation of the multi-fluid method. Indeed high density regions, as well as vacuum, are created, that represent a challenging issue for a Eulerian method. Higher Stokes number are not tackled here since it was shown in Reveillon & Demoulin (2007) that, for Stokes number greater than unity, effects of maximal segregation in turbulent flow occur. The droplets are inertial enough to be ejected from a vortex and not follow the fluid

particle like a tracer. Their velocities become decorrelated from the gaseous carrier phase velocity. In this case droplet trajectory crossings have a strong impact on the spray repartition and the mono-kinetic assumption of the multi-fluid method might not allow to describe it. Recently, Kah & al (2010) extended the multi-fluid method to higher order moment method to take into account these droplet crossings and it would be interesting to enrich the presented comparisons with Eulerian results provided by the extended multi-fluid multi-velocity model.

To assess the multi-fluid description of the size-conditioned dynamics, Eulerian density fields are compared to Lagrangian droplet positions computed for the same Stokes numbers at the same time $t = 20$, see Fig 2(a) and Fig 2(b). Qualitative comparisons are applied in the planes $x = 2$ and $y = 2$. In the chosen inertial range, the spray is ejected from the vortex cores and accumulated in low vorticity areas. In order to link the spray dispersion given by both methods to the gas vorticity structure, the square norm of the gas vorticity is given in Fig 3(d) and Fig 4(d), for the planes $x = 2$ and $y = 2$, respectively. Qualitative comparisons between both approach can be done focusing on the vacuum zones description. These zones correspond to the gas vortex cores, that can be identified from the vorticity representation. The repartition of these vacuum zones obtained by the classical Lagrangian method is very precisely reproduced by the multi-fluid on the different planes (see Fig 3(a) and Fig 3(e) for the plane $x = 2$ and Fig 4(a) and Fig 4(e) for the plane $y = 2$). Furthermore, the evolution of droplet repartition with inertia is very well captured by the multi-fluid. Indeed, the Eulerian density fields for higher Stokes number still a present very good agreement with the Lagrangian droplet repartitions, see Fig 3(b), Fig 3(c) and Fig 3(f) for the plane $x = 2$ and Fig 4(b), Fig 4(c) and Fig 4(f) for the plane $y = 2$.

Quantitative spray equilibrium comparisons. As studied in Reveillon & Demoulin (2007), the equilibrium of the spray with its carrier phase is detected through the statistics of the slip velocity

$$\omega^E(\mathbf{x}, t) = (\mathbf{u}_g - \mathbf{u})(\mathbf{x}, t),$$

where \mathbf{u}_g and \mathbf{u} are the Eulerian gas velocity field and the liquid velocity field both taken at the numerical grid point \mathbf{x} . From a Lagrangian point of view, the slip velocity of a droplet k is given by

$$\omega^L(k, t) = (\mathbf{u}_g(\mathbf{x}_k) - \mathbf{v}_k)(t),$$

where \mathbf{v}_k is its velocity and $\mathbf{u}_g(\mathbf{x}_k)$ is the gas velocity taken at the droplet position \mathbf{x}_k . The mean value of the Lagrangian slip velocity is defined by

$\tilde{\omega}(t) = 1/N \sum_{k=1}^N \omega^L(k, t)$ with N the total particle number while its Eulerian equivalent is $\bar{\omega}(t) = L^{-3} \int \omega^E(\mathbf{x}, t) d\mathbf{x}$. In the following, an overbar stands for a Eulerian quantity whereas a tilde denotes a Lagrangian one. Because of the homogeneous nature of the turbulence and the dispersion, the mean value of the slip velocity remains equal to zero. However, the slip velocity root mean square respectively defined by $\tilde{\omega}'(t) = 1/N \left(\sum_{k=1}^N (\omega^L(k, t) - \tilde{\omega}(t))^2 \right)^{1/2}$ and $\bar{\omega}'(t) = L^{-3} \left(\int (\omega^E(\mathbf{x}, t) - \bar{\omega}(t))^2 d\mathbf{x} \right)^{1/2}$ evolves towards a stationary value ω_∞ which corresponds to the equilibrium of the spray with the carrier gas phase. At initial time $t = 0$, the liquid spray is initially distributed in the computational domain with a zero velocity, so $\bar{\omega}'(0)/\bar{\mathbf{u}}'_g = \tilde{\omega}'(0)/\bar{\mathbf{u}}'_g = 1$ with $\bar{\mathbf{u}}'_g$ the initial gas velocity r.m.s. As prescribed previously, the drag force set the liquid spray in motion and, depending on the Stokes number, the mean value of the slip velocity reaches a steady state at $t = 0.2$ for a small Stokes number ($St = 0.17$) whereas a longer time is needed for the largest value of the Stokes number ($St = 1.05$). The final mean stationary value of the slip velocity standard deviation ω'_∞ is close to zero when the droplets are small enough to follow all the velocity fluctuations of the flow ($St = 0.17$) and it increases to reach 0.21 corresponding to droplets of $St = 1.05$. This result accords with those presented in Reveillon & Demoulin (2007) and are plotted in Fig 5. Values of $\bar{\omega}'_\infty$ and $\tilde{\omega}'_\infty$ show a very good agreement for $St = 0.17$, whereas $\bar{\omega}'_\infty$ is smaller than $\tilde{\omega}'_\infty$ and equal to 0.16 for $St = 1.05$.

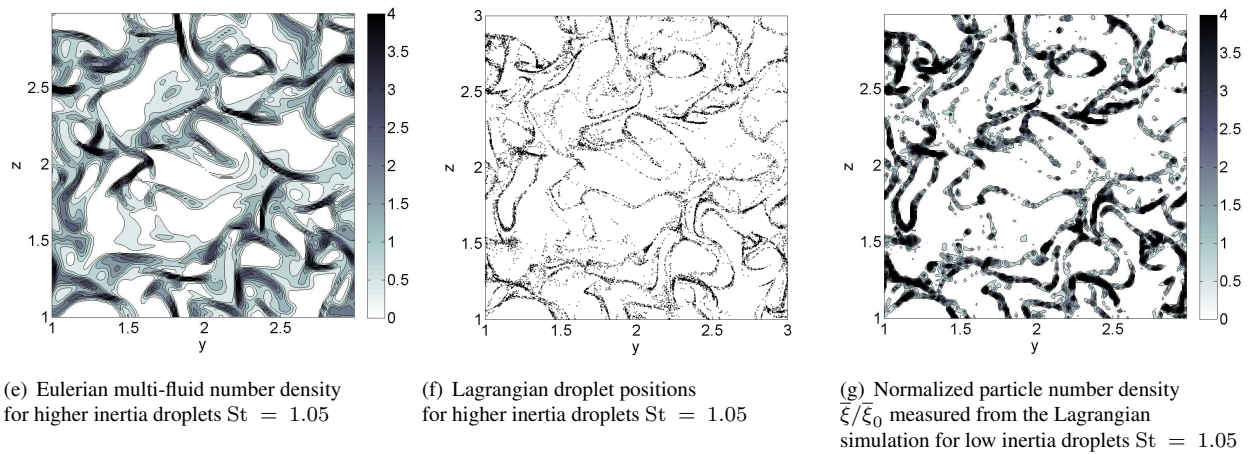
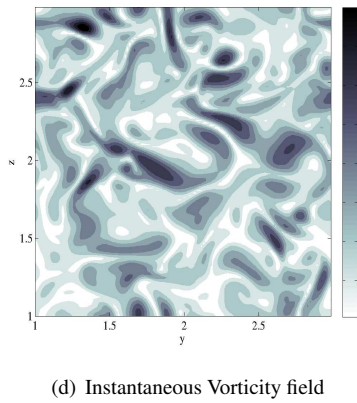
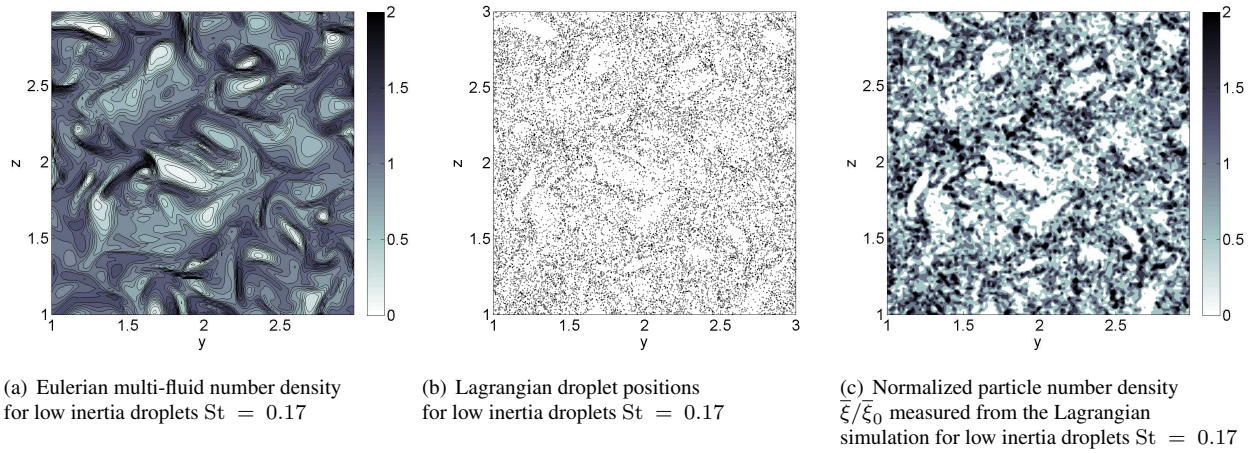


Figure 3: Eulerian Lagrangian comparisons of the liquid phase for two different Stokes $St = 0.17$ and $St = 1.05$, in the $(y - z)$ plane at $x = 2$ at time $t = 20$.

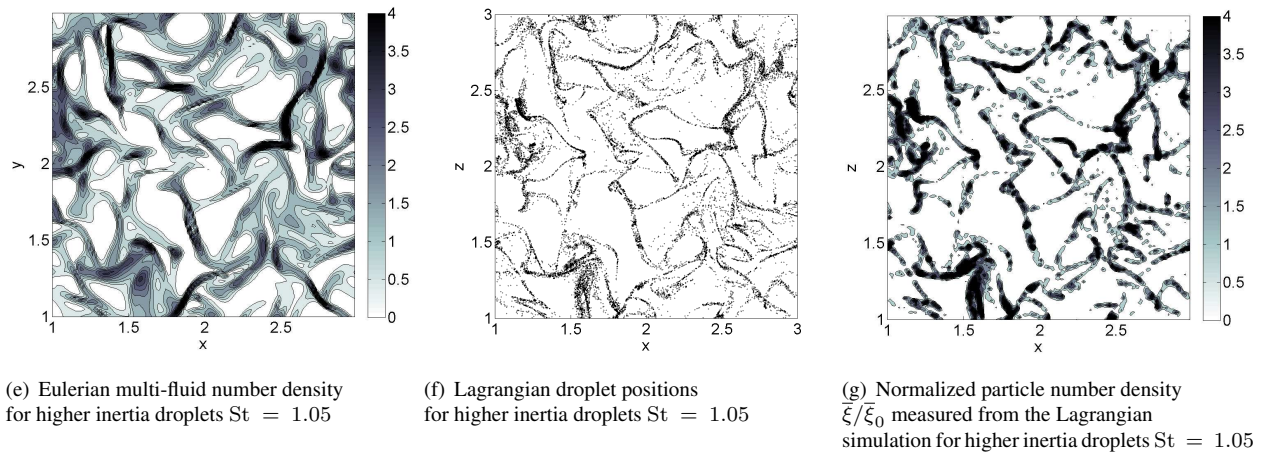
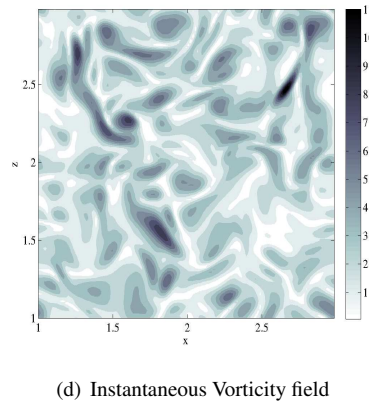
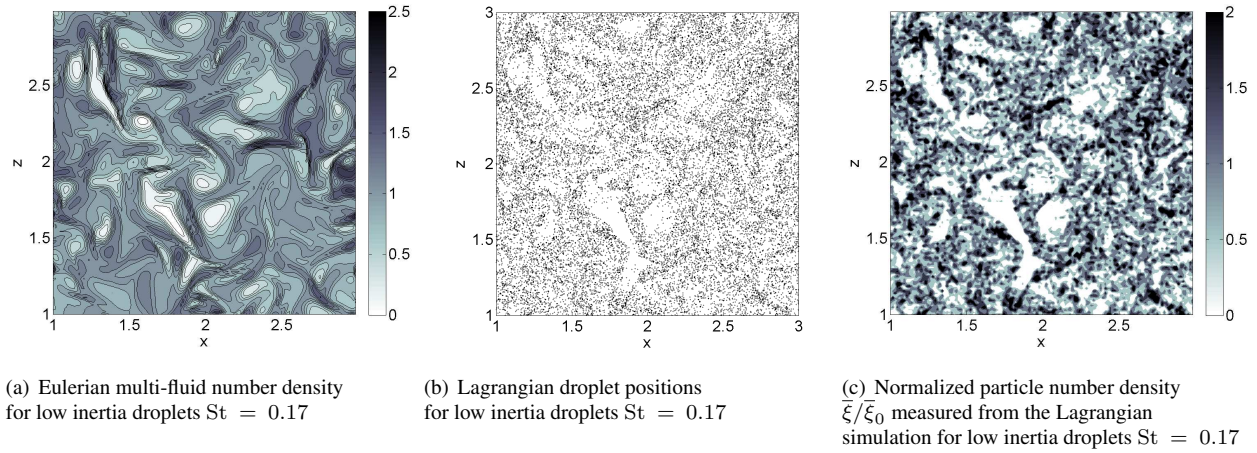


Figure 4: Eulerian Lagrangian comparisons of the liquid phase for two different Stokes $St = 0.17$ and $St = 1.05$, in the $(x - z)$ plane at $y = 2$ at time $t = 20$.

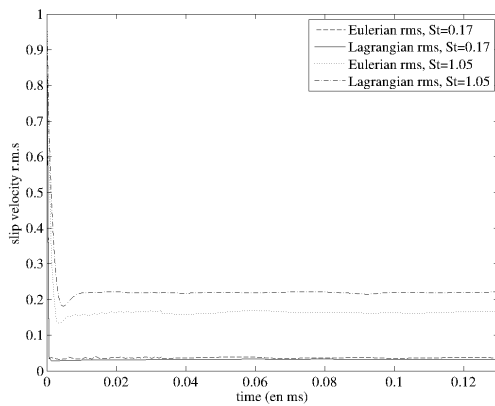


Figure 5: Time evolution of the Eulerian $(\overline{\omega}'(t)/\overline{u}'_g)$ and Lagrangian $(\tilde{\omega}'(t)/\tilde{u}'_g)$ slip velocity r.m.s. for $St = 0.17$ and $St = 1.05$.

Conclusions and perspectives

We have presented comparisons between Lagrangian and Eulerian liquid spray computations in a context of three-dimensional unsteady forced HIT carrier-phase gas. Results were presented for two different Stokes values showing the impact of inertia on droplet segregation as well as the robustness of the multi-fluid model since Stokes values from tracer limit to unity were used. Qualitative comparisons were conducted considering two slice planes and a very good agreement has been obtained up a Eulerian density prediction quantitatively close to DPS results. Preferential concentration was quantitatively studied through the comparison of the slip velocity r.m.s. These results are a first step in spray equilibrium comparisons between the Eulerian and Lagrangian approach and will be completed in a near future in both improved quantitative comparisons and an extension to evaporating case.

Acknowledgements

This research was supported by an ANR-05-JCJC-0013 Young Investigator Award (PI : M. Massot, 2005-2009) which provided a post-doctoral grant for L. Fréret at EM2C Laboratory (2007-2008) and a DGA/CNRS Ph.D. grant for S. de Chaisemartin (Mathematics and Engineering Departments of CNRS - 2005-2009). The authors also acknowledge the support from IDRIS CNRS (Institut de Développement et de Ressources en Informatique Scientifique, Centre National de la Recherche Scientifique) where some of the computations were performed.

References

- Bird, G.A., Molecular gas dynamics and the direct simulation of gas flows. Oxford science publications, vol 42, 1994.
- Boileau, M., Chalons, C., Bourgoign, J.F., Terrier, C., Laurent, F., de Chaisemartin, S., Massot, M., Robust numerical schemes for Eulerian spray DNS and LES in two-phase turbulence flows, 7th International Conference on Multiphase Flow, 2010.
- Bouchut, F., Jin, S., Li, X., Numerical approximations of pressureless and isothermal gas dynamics. SIAM J. Num. Anal, vol 41, pp 135-158, 2003.
- Chorin, A.J., Numerical solution of the Navier-Stokes equations. Math. comp. 22, vol 217, pp 745-762, 1968.
- de Chaisemartin, S., Polydisperse evaporating spray turbulent dispersion: Eulerian model and numerical simulation. PhD thesis, Ecole Centrale Paris, available in english at <http://tel.archives-ouvertes.fr/tel-00443982/en/>, 2009.
- de Chaisemartin, S. Fréret, L., Kah, D., Laurent, F., Fox, R.O., Réveillon, J., Massot, M., Eulerian models for turbulent spray combustion with polydispersity and droplet crossing. C. R. Mécanique vol 337(6-7), pp 438-448, 2009.
- Descombes, S. Massot, M. Operator splitting for non-linear reaction-diffusion systems with an entropic structure: singular perturbation and order reduction. Numer. Math. 97(4), pp 667-698, 2004.
- Doinseau, F, Laurent, F., Murrone, A., Dupays, J., Massot, M., Optimal Eulerian model for the simulation of dynamics and coalescence of alumina particles in solid propellant combustion, 7th International Conference on Multiphase Flow, 2010.
- Fréret, L., Lacour, C., de Chaisemartin, S., Laurent, F., Massot, M., Birbaud, A.L., Ducruix, S., Durox, D., Pulsated free jets with polydisperse spray injection: experiments and numerical simulations. Proceedings of the combustion institute, vol 32(2), pp 2215-2229, 2009.
- Garcia, M., Development and validation of the Euler-Lagrange formulation on a parallel and unstructured solver for large-eddy simulation. PhD thesis, Institut National Polytechnique de Toulouse, available in english at <http://tel.archives-ouvertes.fr/tel-00414067/en/>, 2009.
- Greenberg, J.B., Silverman, I. Tambour, Y., On the origin of spray sectional conservation equations. Combustion and Flame, 93: 90-96, 1993.

- Guichard, L. Réveillon, J., Hauguel, R., Direct numerical simulation of statistically stationary one- and two-phase turbulent combustion: a turbulent injection procedure, *Flow Turbulence Combustion*, Vol. 73, pp 133-167, 2004.
- Hairer, E., Wanner, G., Solving ordinary differential equations. II. Berlin: Springer-Verlag. Stiff and differential-algebraic problems, second revised edition, 1996.
- Kah, D., Laurent, F., Fréret, L., de Chaisemartin, S., Fox, R.O., Réveillon, J., Massot, M., Eulerian quadrature-based moment models for polydisperse evaporating sprays, accepted in *Flow, Turbulence and Combustion*, available at <http://hal.archives-ouvertes.fr/hal-00449866/en/>, 2010.
- Kaufmann, A., Moreau, M., Simonin, O., Helie, J., Comparison between Lagrangian and mesoscopic Eulerian modelling approaches for inertial particles suspended in decaying isotropic turbulence, *Journal of Comp. Phys.* vol 227, pp:6648-6472, 2008.
- Laurent, F. and Massot, M., Multi-fluid modeling of laminar poly-dispersed spray flames: origin, assumptions and comparison of the sectional and sampling methods, *Combustion theory and Modelling*, vol 5, issue 4, pp 537-572, 2001.
- Laurent, F., Massot, M. Villedieu, P., Eulerian multi-fluid modeling for the numerical simulation of coalescence in polydisperse dense liquid sprays. *Journal of computational physics*, vol 194, pp 505-543, 2004.
- Laurent F., Numerical analysis of Eulerian multi-fluid models in the context of kinetic formulations for dilute evaporating sprays, *M2AN Math. Model. Numer. Anal.* 40(3): 431-468, 2006.
- Lele, S.K., Compact finite difference schemes with spectral like resolution. *J. Comput. Phys.* 103, pp 16-42, 1992.
- LeVeque, R.J., Finite volume methods for hyperbolic problems. Cambridge texts in applied Mathematics. Cambridge University press, Cambridge, 2002.
- Massot, M., de Chaisemartin, S., Fréret, L., Kah, D., Laurent, F., Eulerian multi-fluid models: modeling and numerical methods. In *Modelling and Computation of Nanoparticles in Fluid Flows*, Lectures of the von Karman Institute. NATO RTO AVT 169, available at <http://hal.archives-ouvertes.fr/hal-00423031/en/>, 2009.
- O'Rourke, P.J., Collective drop effects on vaporizing liquid sprays. PhD thesis, Princeton University, 1981.
- Overholt, M.R. and Pope, S.B., A deterministic forcing scheme for direct numerical simulation of turbulence. *Computer fluids*, vol 27, pp 11-28, 1998.
- Poinsot, T. and Lele, S.K., Boundary conditions for direct simulations of compressible viscous flows. *J. Comput. Phys.* 101(1), pp 104-129, 1992.
- Reveillon, J., Péra, C., Massot, M., Knikker, R., Eulerian analysis of the dispersion of evaporating polydispersed sprays in a statistically stationary turbulent flow. *Journal of turbulence*, 5(1), pp 1-27, 2004.
- Reveillon, J. and Demoulin, F.X., Effects of the preferential segregation of droplets on evaporation and turbulent mixing. *Journal of fluids mechanics*, 583, pp 273-302, 2007.
- Reveillon, J. and Demoulin, F.X., Evaporating droplets in turbulent reacting flows, *Proceedings of the combustion institute*, vol 31, issue 2, pp 2319-2326, 2007.
- Simonin, O., Fevrier, P., Laviéville, J., on the spatial distribution of heavy-particle velocities in turbulent flow: from continuous field to particulate chaos. *J Turbulence*, vol 118, pp 97-118, 1993.
- Squires, K.D. and Eaton, K.J., Presential concentration of particles by turbulence. *Phys. Fluides*, vol 3, pp 1969-1178, 1991.
- Williams, F.A., Spray combustion and atomization. *Physics of fluids*, vol 1, pp 541-545, 1958.