Turbulent Combustion of Polydisperse Evaporating Sprays with Droplet Crossing: Eulerian Modeling and Validation in the Infinite Knudsen Limit

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Turbulent combustion of polydisperse evaporating sprays with droplet crossing: Eulerian modeling and validation in the infinite Knudsen limit

By S. de Chaisemartin†, L. Fréret†, D. Kah‡, F. Laurent†, R. O. Fox¶, J. Reveillon∥ and M. Massot†∗

The accurate simulation of the dynamics of polydisperse evaporating sprays 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 difficulties encountered by the usual Lagrangian approaches make the use of Eulerian models attractive, aiming at a lower cost and an easier coupling with the carrier gaseous phase. Among these models, the multi-fluid model allows for a detailed description of the polydispersity and size/velocity correlations for droplets of various sizes. The purpose of the present study is twofold. First, we extend the multi-fluid model in order to cope with crossing droplet trajectories by using the quadrature method of moments in velocity phase space conditioned by size. We identify the numerical difficulties and provide dedicated numerical schemes in order to preserve the velocity moment space. Second, we conduct a comparison study and demonstrate the capability of such an approach to capture the dynamics of an evaporating polydisperse spray in a 2-D free jet configuration. We evaluate the accuracy and computational cost of Eulerian models and related discretization schemes vs. Lagrangian solvers and show that, even for finite Stokes number, the standard Eulerian multi-fluid model can be accurate at reasonable cost.

1. Introduction

Many industrial devices involve turbulent combustion of a liquid fuel. The transportation sector, rocket, aircraft or car engines are almost exclusively based on storage and injection of a liquid phase, which is sprayed into a chamber where turbulent combustion takes place. It is of primary importance to understand and control the physical process as a whole, from the injection into the chamber up to the combustion phenomena.

Numerical simulation is now a standard tool to optimize turbulent combustion processes in such devices. If purely gaseous problems are well-known with a wide range of suggested closures, it is not the case for two-phase flows where detailed information is needed about the physics of the triple interactions: spray/turbulence/combustion.

In general, two approaches for treating liquid sprays, corresponding to two levels of description, can be distinguished. The first one, associated with a full direct numerical simulation (DNS) of the process, provides a model for the dynamics of the interface
between the gas and liquid, as well as the details of the exchanges of heat and mass between the two phases. The second one, based on a more global point of view, describes the droplets as a cloud of point particles, the geometry of which are presumed spherical, and for which the exchange of mass, momentum and heat are described globally. It is the only one for which numerical simulations at the scale of a combustion chamber can be conducted. Thus, this “mesoscopic” point of view will be adopted in the present study.

In this framework, there exists considerable interest in the development of numerical methods for simulating sprays relying on a transport equation given by Williams (1958), based on kinetic theory. The principal physical processes that must be accounted for are (1) transport in physical space, (2) evaporation, (3) acceleration of droplets due to drag, and (4) breakup, rebound and coalescence leading to polydispersity. The major challenge in numerical simulations is to account for the strong coupling between these processes. In the context of one-way coupling, the Lagrangian Monte-Carlo approach, called Direct Simulation Monte-Carlo method (DSMC) by Bird (1994), is generally considered to be more accurate than Eulerian methods for solving Williams equation. However, its computational cost is high, especially in unsteady configurations. Moreover, in applications with two-way coupling, Lagrangian methods are difficult to couple accurately with Eulerian descriptions of the gas phase. There is thus considerable impetus to develop Eulerian methods, keeping in mind that such models still need validation.

Actually, there exists two shortcomings of the actual Eulerian models. First, they fail to describe polydispersity; however, in many industrial configurations, evaporating droplets of different sizes follow different pathways, thus depositing their fuel mass fraction at different places. One way to solve the problem is to use multi-fluid models (Massot (2007)). Second, Eulerian models are derived from Williams equations through an equilibrium assumption leading to closure at the level of velocity moment equations conditioned by droplet size. The model is not able to capture multi-modal droplet velocity distribution and thus droplet crossing, but is essentially monokinetic. Even if the multi-fluid model can afford droplet crossing for droplets of different sizes, the equilibrium assumption is too limiting and leads to the creation of singularities which have been studied analytically in Massot (2007), with a physical interpretation in de Chaisemartin (2007). Recently, the use of the quadrature method of moments in the velocity phase space has provided a closure for non-equilibrium velocity distributions for monodisperse particles allowing to capture droplet crossing at finite Stokes number (Fox (2008)).

The present study provides a new Eulerian model, as well as dedicated numerical schemes, able to deal with polydispersity as well as non-equilibrium velocity distributions for evaporating sprays. The proposed method satisfies a crucial property: the preservation of the moment space. The model is validated in a free jet configuration by detailed comparison with a Euler-Lagrange solver provided by Reveillon (2004). After showing the accuracy of the model at capturing the dynamics of droplets of various sizes, we investigate its ability to properly evaluate the gaseous fuel mass fraction field issuing from evaporation. It is the starting point for a companion study where we investigate the capability of such Eulerian multi-fluid models to capture the dynamics and polydispersity of colliding sprays (Fréret (2009b)). The objective is the evaluation of the relative accuracy and computational cost between the Eulerian and Lagrangian approaches. The framework of the study is DNS. However, in the context of Large Eddy Simulation, Eulerian models will encounter the same issues from both a modeling and computational point of view. In this study, we evaluate the numerical methods in a 2D framework; nevertheless it can be extended to 3D configurations. This work is in progress.
2. Statistical description at the mesoscopic scale and Lagrangian discretization

At the mesoscopic scale, droplets are described as a cloud of point particles for which the exchange of mass, momentum and heat are described globally for a droplet supposed to be spherical of surface $S$, with velocity $\mathbf{u}$ and a uniform temperature $T_0$ (Laurent (2001)). For the gaseous phase, $L_0$ denotes a reference length, $U_0$ a reference velocity, and $t_0 = L_0/U_0$, the associated time scale, and a typical kinematic viscosity $\nu_0$ allows to define a Reynolds number. For the spray, $S_0$ denotes a reference droplet surface, and the droplet dynamical time, $t_p = \rho_0 S_0/(\rho g_0 18\pi \nu_0)$, defines the reference Stokes number $St_0 = t_p/\nu_0$, where $\rho_0$ and $\rho g_0$ are reference liquid and gas densities. In the following, even if heating can easily be included in the models, we will restrict the framework of the study to evaporation and drag and assume that these quantities only depend on the local gaseous phase as well as on the state of the droplet. In addition, we suppose that all the scales of the gaseous phase are resolved in the context of DNS. We adopt a statistical description of Boltzmann type and the spray can be described by its joint surface-velocity number density function (NDF) $f(t, \mathbf{x}, S, \mathbf{u})$, which satisfies the transport equation of Williams (1958):

$$\partial_t f + \partial_\mathbf{x} \cdot (\mathbf{u} f) + \partial_S (K f) + \partial_\mathbf{u} \cdot (\mathbf{F} f) = \Gamma/Kn,$$

where, for the sake of simplicity, $K$ is the constant of a $d^2$ law and $\mathbf{F} = (U_g(t, \mathbf{x}) - \mathbf{u})/St(S)$ is a linear drag force, $St(S) = St_0 S$, $U_g$ is the gas velocity and all the involved quantities are non-dimensional. The collision operator, $\Gamma$, will be the subject of a companion paper (Fréret (2009b)). The Knudsen number, $Kn = l_0/L_0$, is the ratio between the mean free path $l_0 = 1/(n_0 \sigma_0)$ and $L_0$, where $\sigma_0$ is a typical collision cross-section and $n_0$ a typical droplet number density. In this contribution, we work in the infinite Knudsen limit, i.e. in the limit of small particles and dilute sprays, the Knudsen number is large enough and the effect of the collision operator becomes negligible.

In this context, the Williams equation can be discretized through a Particle Discretization (PD), where the NDF is represented by a sum of Dirac delta functions:

$$f(t, \mathbf{x}, \mathbf{u}, S) = \sum_p w_p \delta(\mathbf{x} - \mathbf{x}_p(t)) \delta(\mathbf{u} - \mathbf{u}_p(t)) \delta(S - S_p(t)),$$

where $w_p$ is a constant weight of the $p^{th}$ numerical particle and $\mathbf{x}_p$, $\mathbf{u}_p$, $S_p$ are its position, velocity and surface, respectively. They evolve through standard differential equations involving drag acceleration $\mathbf{F}$ and evaporation $K$. This method provides, if enough numerical particles are used, an ensemble average of the droplet repartition and then yield Eulerian fields. Under the chosen set of assumptions, it is equivalent to an ensemble of discrete particle simulations (DPS), where each individual numerical particle represents one droplet and the weights are equal to one, such as in Reveillon (2004). The number density of particles for DPS corresponds to one realization of an ensemble average governed by the Williams equation and is defined by a given equivalence ratio for evaporation and combustion purposes.

3. Development of the Eulerian multi-fluid multi-velocity approach

3.1. Standard Eulerian multi-fluid model and its limitations

The formalism needed to derive the Eulerian multi-fluid model was introduced in Laurent (2001), extending the ideas of Greenberg (1993). We recall briefly the main features.

[H1] We presume the form of the NDF $f(t, \mathbf{x}, S, \mathbf{u}) = n(t, \mathbf{x}, S) \delta(\mathbf{u} - \bar{\mathbf{u}}(t, \mathbf{x}, S))$ through an equilibrium distribution around the average velocity conditioned on size $\bar{\mathbf{u}}(t, \mathbf{x}, S)$.†

† This corresponds to a generalized Maxwell-Boltzmann distribution at zero temperature, an
The droplet size phase space is divided into intervals $[S_{k-1}, S_k], k \in [1, N]$, called sections. In one section, $\bar{u}^{(k)}$ does not depend on size, and we assume $n^{(k)}(t, x, S) = m^{(k)}(t, x) \kappa^{(k)}(S)$, where $\kappa^{(k)}(S)$ is assumed independent of $(t, x)$ in each section.

We write conservation equations on $m^{(k)}$, the non-dimensional mass density, and $m^{(k)} \bar{u}^{(k)}$ the momentum in section $k$. These equations describe the set of droplets in one section as well as the exchanges of mass and momentum between the coupled sections or "fluids". Droplets in different sections can have different dynamics, with an a priori control of the precision in the size phase space. Such an approach focuses on one moment in the size variable within a section; the mass moment is chosen because of its relevance in the evaporation and combustion process. Higher order approximations exist (Massot (2008)).

The conservation equations for the $k^{th}$ section then read:

$$
\begin{align*}
\partial_t m^{(k)} + \partial_x \cdot (m^{(k)} \bar{u}^{(k)}) &= (E_1^{(k)} + E_2^{(k)}) m^{(k)} - E_1^{(k+1)} m^{(k+1)} \\
\partial_t (m^{(k)} \bar{u}^{(k)}) + \partial_x \cdot (m^{(k)} \bar{u}^{(k)} \otimes \bar{u}^{(k)}) &= (E_1^{(k)} + E_2^{(k)}) m^{(k)} \bar{u}^{(k)} - E_1^{(k+1)} m^{(k+1)} \bar{u}^{(k+1)} + m^{(k)} \bar{F}^{(k)}
\end{align*}
$$

(3.1)

where $E_1^{(k)}$ and $E_2^{(k)}$ are the evaporation coefficients and $\bar{F}^{(k)}$ is the averaged drag force, function of a mean surface of the section $S_{\text{mean}}^{(k)}$. The $E_1^{(k)}$ and $E_2^{(k)}$ terms, respectively, represent the exchange between successive sections and exchange with the gaseous phase through evaporation. These conservation equations have the same mathematical structure as the pressure-less gas dynamic equation. They potentially lead to singular behavior and require well-suited numerical methods (see Massot (2007); de Chaisemartin (2007)).

One typical configuration for which the Eulerian multi-fluid model predicts an artificial averaging is the one presented in Fig. 1 when two droplet jets are crossing without drag nor evaporation, and for a monodisperse spray. Indeed, at the collision location, there are at the same space and time location two velocities leading to a bi-modal velocity distribution that is out of equilibrium. The Eulerian multi-fluid multi-velocity model, presented in the next subsection, predicts in Fig. 1 (right) the exact solution (CFL number is always one) for this simple configuration for which the two jets do not interact in the chosen “infinite Knudsen limit”. The classical method, because of the equilibrium assumption [H1], cannot handle this case and rather predicts an artificial collisional “zero Knudsen limit” presented in Fig. 1 (center) and a $\delta$-shock is created.

“equilibrium” distribution, even if there is no collision operator in the model. It can also be seen as a single node quadrature method of moments in velocity phase space conditioned by size
Assumption [H1] corresponds to an equilibrium assumption and can be too restrictive. Within the \( k \)th section, we then extend [H1] and assume the following form for the NDF:

\[
f(t, \mathbf{x}, S, \mathbf{u}) = n^{(k)}(t, \mathbf{x}, S) g^{(k)}(t, \mathbf{x}, \mathbf{u}),
\]

where \( n \) is a size number density function that still satisfies [H2], and \( g \), the velocity probability density function, is assumed independent of size inside the \( k \)th section.

We consider the same mass-velocity moments of the NDF defined by:

\[
m_{j,l}^{(k)} = \int_{V} \rho dV \int_{\mathbb{R}^d} \mathbf{u}_{j,l}^{(k)} g^{(k)}(t, \mathbf{x}, \mathbf{u}) d\mathbf{u}, \quad k \in [1, N], \quad m_{00}^{(k)} = 1,
\]

and the resulting system of conservation laws on moments reads, from Eq. (3.1):

\[
\partial_t m_{j,l}^{(k)} + \partial_x (m_{j,l}^{(k)} M_{j+1,l}) = -(E_1^{(k)} + E_2^{(k)}) m_{j,l}^{(k)} M_{j+1,l} + E_1^{(k+1)} m_{j,l}^{(k+1)}
\]

\[
+ j m^{(k)} U_{g,x} M_{j-1,l} - M_{j,l}^{(k)} + l m^{(k)} U_{g,y} M_{j+1,l-1} - M_{j,l}^{(k)}.
\]

where the closure of the convective fluxes will define the index set for \( j \) and \( l \).

In order to close the transport in physical space and to be able to extend this method to more complex models, we will use a quadrature method of moments in the spirit of Fox (2008). Let \( d = 2 \) denote the number of velocity-phase space dimensions and \( \alpha \in \{1, \ldots, N^d \} \) denote the set of weights and abscissas with a \( \mathcal{N} \) quadrature level in one direction. In the present contribution, we take \( \mathcal{N} = 2 \) and will then investigate a \( 2^d = 4 \)-node quadrature approximation of \( g \) and thus, we will work with moments up to order 3 in velocity, i.e. \( j + l \leq 3 \). Higher \( \mathcal{N} \) can be considered at the price of much more complex algebra and combinatorics, and for the sake of simplicity and efficiency, we will limit ourselves to the case \( \mathcal{N} = 2 \). The velocity moments are then easily related to the quadrature weights \( \omega \) and abscissas \( \{(u_{\alpha,x}, u_{\alpha,y})\} \) by \( M_{j,l}^{(k)} = \sum_{\alpha=1}^{2^d} \omega_\alpha (u_{\alpha,x}^{(k)})^j (u_{\alpha,y}^{(k)})^l \), where \( j + l \leq 3 \), whereas the issue is to evaluate the abscissas and weights from the data of the velocity moment vector of size 10. The correspondence is one-to-one in one space dimension. However, in dimension greater or equal to two, we will transport the whole set of moments but effectively restrict the moment subspace recursively structured from the set of second-order velocity moments for which the correspondence is one-to-one, and insure that the velocity moment vector lives in this subspace.

We introduce a linear transformation \( L^{(k)} \) as well as a rotation matrix, such that \((R^{(k)} L^{(k)})^T R^{(k)} L^{(k)} = (\sigma_{ij})_{i,j \in \{x,y\}, j \in \{x,y\}} = \sigma\), with \( \sigma_{ij}^{(k)} = \int \mathbf{u}_i u_j g^{(k)}(\mathbf{u}) d\mathbf{u} \), where \( \sigma^{(k)} \) is the related covariance matrix. Up to a rotation, the linear transformation \( L \), which is chosen as a Cholesky decomposition of \( \sigma \) in the rotated set of axes, allows for a natural change of variable. With this choice, we take \( A = (R^{(k)} L)^T \) and introduce the vector \( \mathbf{X} = [X_1, X_2] \), defined by \( \mathbf{X} = \mathbf{A}^{-1}(\mathbf{u} - \bar{\mathbf{u}}) \), so that \( \mathbf{u} = \mathbf{A} \mathbf{X} + \bar{\mathbf{u}} \). This variable is a good candidate in order to perform tensorial 1-D quadrature based on the set of reconstructed centered third-order moments in the two new basis directions. There are fundamental grounds for using the Cholesky decomposition rather than the other methods. Defining matrix \( A \) in terms of the eigenvectors of the covariance matrix is a good choice for the passive transport of a distribution function. However, because the velocity is a dynamic variable, the fundamental difficulty comes from the fact that the eigenvectors of \( \sigma \) do
not vary smoothly with its components]. As a consequence, the fluxes computed from the abscissas are then discontinuous, leading to “random” fluctuations in the moments. In contrast, the Cholesky matrix $L$ with $R = I$ defines $A_x$, which varies smoothly with the components of $\sigma$ and, hence, the fluxes are well-behaved (Fox (2008)).

On the other hand, the disadvantage of using the Cholesky matrix is that it depends on the ordering of the covariance matrix, and is thus different for each of the two permutations (six in three dimensions) of the coordinates corresponding to the two $R$ matrices identity and rotation by $\pi/2$. It is thus desirable to replace these two linear transforms $A_x$ or $A_y$ in the two preceding choices with a permutation-invariant linear transform. Here we consider the half-angle between these two transforms. This treats each direction in the same manner, and is now independent of the ordering of the covariance matrix. Besides this choice is stable and defines a subspace of the moment space in which the conservative variables live.

3.3. Numerical methods

The transport in physical space obeys a system of weakly hyperbolic conservation laws and relies on kinetic finite volume schemes as introduced by Bouchut (2003) in order to solve the pressure-less gas dynamics equation. Once a quadrature method is designed, it defines a kinetic description that is equivalent to the moment system of equations for smooth solutions and allows the proper definition of the fluxes for transport of the moments in one space dimension. The resulting scheme is second-order accurate in space and time for the multi-fluid model, and first order in space and time for the multi-fluid multi-velocity model (Fox (2008)) in order to strictly preserve the moment space during the reconstruction part of the algorithm, that is to guarantee that the eigenvalues of the covariance matrix are both non-negative. In this contribution, we aim at working also at the boundary of the moment space since we want to tackle cases where the velocity distribution is reduced to a monokinetic distribution where the proposed quadrature degenerates to the original multi-fluid model and the covariance matrix can be zero.

Because the transport in physical space and the transport in phase space through evaporation and drag have different structures, we use a Strang splitting algorithm (de Chaisemartin (2007); Massot (2007)). The interest is two fold. First, this approach preserves the properties of the schemes we use for the different contributions, for example maximum principle or positivity. If we assume that the involved phenomena evolve at roughly the same time scales, this Strang splitting algorithm guarantees second-order accuracy in time provided that each of the elementary schemes has second-order time accuracy. Furthermore, from a computational point of view, this is optimal and yields high parallelization capabilities. For the transport in physical space, we further use a dimensional Strang splitting of the 1-D scheme previously described in de Chaisemartin (2007). The corresponding scheme offers the ability to treat the delta-shocks and vacuum states, and preserves the positivity of mass density as well as the moment space.

The preservation of the moment space is also important during transport in phase space. The local dynamical system defined in Eqs. (3.1) or (3.4) can be rewritten $\partial_t Y^j = \Phi(Y^j)$, with, in case of the multi-fluid multi-velocity method,

$$Y^j = (m^j, m^j M^j_{1,0}, m^j M^j_{0,1}, m^j M^j_{0,2}, m^j M^j_{1,1}, m^j M^j_{1,2}, m^j M^j_{2,1}, m^j M^j_{2,2}, m^j M^j_{3,0}, m^j M^j_{3,1}, m^j M^j_{3,2}, m^j M^j_{3,3}).$$

This system is solved using an implicit Runge-Kutta Radau IIA method of order 5 with

† Because of intrinsic geometrical reasons, we can get around this difficulty in 2D but not in 3D so that such an approach will not be further studied.
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Figure 2. Free jet: (left) gaseous vorticity at time $t=20$, obtained on a $400 \times 200$ grid; (right) polydisperse log-normal distribution discretized with 5, dashed lines, to 10, dotted lines, sections.

adaptive time steps. Whereas this resolution in case of multi-fluid method does not yield any difficulty, for the multi-velocity case it can lead to a non-realizable set of $Y^j$. The preservation of the moment space requires working with the centered moments:

$$\tilde{M}^{(k)}_{j,l} = \int_{\mathbf{u}} (u_x - M^{(k)}_{1,0})^j (u_y - M^{(k)}_{0,1})^l g^{(k)}(t, \mathbf{x}, \mathbf{u}) \, d\mathbf{u},$$

for $j+l \geq 2$. Starting from there, even if it leads to additional non-linear terms in the ODE system, the Radau solver can be adapted and yields a robust solver on the conservative centered moments that strictly preserves the moment space and allows working up to the boundary of the moment space, i.e., the monokinetic velocity distribution.

4. Free jet configuration and reference solutions

In order to assess the Eulerian methods, we focus on a 2-D Cartesian free jet. A polydisperse spray is injected in the jet core with a log-normal size distribution (see Fig. 2, right), of which the mean diameter $d_0$ corresponds to the reference surface $S_0$. The simulations are conducted with a code coupling a gas solver to a Lagrangian solver (both developed at CORIA) and to a Eulerian solver (developed at EM2C) wherein the multi-fluid and multi-fluid multi-velocity methods are implemented.

With regard to the gas phase, we used a 2-D Cartesian low-Mach number dilatable solver. The gas jet is computed on a $400 \times 200$ grid. In order to destabilize the jet, we inject turbulence through a Klein method with 10% fluctuations. The Reynolds number based on $U_0$, $\nu_0$ and $L_0$ is 1000, where $U_0$ is the injection velocity and $L_0$ is the jet width. We will eventually provide dimensional quantities for illustration purposes. These will be based on an estimated velocity of $U_0 = 1 \text{ m/s}$ and $L_0 = 1.5 \text{ cm}$, as well as a typical value of $1.6 \times 10^{-5} \text{ m}^2/\text{s}$ for $\nu_0$. Finally, we have $d_0 = L_0/300$, where $d_0$ is the diameter corresponding to the typical droplet surface $S_0$. The gas vorticity is presented in Fig. 2 (left). Since we aim at validating the Eulerian models through comparisons to a Lagrangian simulation, we restrict ourselves to one-way coupling. We take as a reference solution for the liquid phase a Lagrangian Discrete Particle Simulation with 10000 to 70000 particles in the computational domain depending on the cases. The number of droplets is determined by stoichiometry. We provide comparisons between this Lagrangian reference and the Eulerian multi-fluid monokinetic and multi-fluid multi-velocity computations plotting the Lagrangian particle positions vs. the Eulerian number density. Thanks to the multi-
Figure 3. Non-evaporating polydisperse spray, low inertia droplets, Stokes 0.011 to 0.12 (diameters $d = 9 \mu m$ to $d = 30 \mu m$, at time $t=20$; (top) Lagrangian particle positions with 40000 particles, (bottom) Eulerian multi-fluid monokinetic number density on a $400 \times 200 \times 5$ grid.

For the non-evaporating case we use five sections for the Eulerian multi-fluid monokinetic simulation. We have 70000 Lagrangian particles in the computational domain at the considered time. We choose to present in this section a comparison for low-inertia droplets and find a very good agreement for the droplets with a Stokes range from 0.011 to 0.12 corresponding to diameters from 9 $\mu m$ to 30 $\mu m$, as shown in Fig. 3. The multi-fluid monokinetic method is thus able to simulate the dynamics of a polydisperse spray where droplet crossings are limited. Droplet dynamics is close to the gas dynamics for this range of sizes, and the model remains therefore in its validity domain (see Sec. 3.1). In fact, the same level of comparison is obtained for any of the five size ranges in the simulation, as it will be presented below for the evaporating case.

The free jet is also assessed with an evaporating spray. For the $d^2$ law, we take a constant Spalding number: $Bm = (\left[Y_f\right]_s - \left[Y_f\right]_\infty)/(1 - \left[Y_f\right]_s) = 0.1$, $Y_f$ being the fuel mass fraction. The results are presented in the way chosen for the non-evaporating case. In order to describe correctly the evaporation process, we take ten sections for the Eulerian multi-fluid simulation, whereas 30000 Lagrangian particles are present in the domain at the considered time. In this case, we focus on the size-conditioned dynamics of higher Stokes number droplets. These more inertial droplets are ejected from the vortices and crossing trajectories are likely to occur, breaking the monokinetic multi-fluid assumption described in Sec. 3.1. Nevertheless, the dynamics are still very well-reproduced for the
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higher Stokes numbers. The results are plotted in Fig. 4 for Stokes numbers from 0.48 to 1.1 corresponding to diameters from 60 µm to 90 µm. Note that the number density is concentrated in a few cells in this case and the numerical method does not encounter any problems to capture it, illustrating again the method’s robustness and accuracy.

This polydisperse evaporating free jet shows the ability of the multi-fluid method to treat more complex cases, closer to realistic configurations. From these comparisons, we demonstrate that the Eulerian method captures size-conditioned dynamics that carry droplets of different sizes to different locations. It is then essential to evaluate the ability of the Eulerian model to capture the evaporation process as a whole.

Because our interest is in combustion applications, a key issue of evaporating spray modeling is the gaseous fuel mass fraction prediction. We thus present comparisons between this gaseous fuel mass fraction, obtained from the Lagrangian and the Eulerian multi-fluid descriptions of the spray. These results are obtained within the same coupled code run, the spray being described on one hand by the Lagrangian method and on the other hand by the Eulerian multi-fluid model. This simulation is still done in one-way coupling. Indeed, the evaporated fuel is not added as a mass source term in the gaseous equations, but is stored in two passive scalars, one for each description of the spray, that are transported by the flow. The Lagrangian gaseous fuel mass fraction is obtained through a projection of the droplet evaporation over the neighbor cells of the gaseous mesh. These two fields are plotted in Fig. 5. One can see the very good agreement of both descriptions for spray evaporation. This comparison underlines the efficiency of the Eulerian multi-fluid model in describing polydisperse evaporating sprays. Furthermore, as we can see in Fig. 5, the Eulerian description provides a smoother field than the Lagrangian
Figure 5. Comparison of the gaseous fuel mass fraction at time $t = 20$, obtained from evaporation using (top) a Lagrangian method with 30000 droplets at the considered time and (bottom) a Eulerian multi-fluid monokinetic model with a $400 \times 200 \times 10$ grid.

Figure 6. Evaporating polydisperse spray, high-inertia droplets, Stokes 0.48 to 1.1 (diameters $d = 60 \, \mu m$ to $d = 90 \, \mu m$), at time $t=15$: (left) Lagrangian particle positions with 7000 particles, (right) Eulerian multi-fluid multi-velocity number density with a $400 \times 200 \times 10$ grid.

one. It illustrates the difficulties arising when coupling the Lagrangian description of the liquid to the Eulerian description of gas and underlines the advantage of the Eulerian description of the spray for the liquid-gas coupling.

4.2. Multi-fluid multi-velocity model vs. Lagrangian method

We have plotted the results of the multi-velocity model with evaporation in the case of the polydisperse spray jet in Fig. 6. Once again, this figure demonstrates the ability of the proposed method to capture the dynamics conditioned by size as well as evaporation for a range of small to finite Stokes numbers.

For the simulations using the multi-velocity model, we focus on the level of agreement between the Eulerian and the Lagrangian simulation. Thus, Fig. 7 (left) presents a fair comparison, similar to the level obtained in previous simulations. In order to quantify the
Figure 7. Non-evaporating monodisperse spray, high-inertia droplets, Stokes 1.32 (diameters $d = 100 \mu m$), at time $t=20$: (top-left) Lagrangian particle positions with 20000 particles, (bottom-left) Eulerian multi-fluid multi-velocity number density with a $400 \times 200 \times 1$ grid. (right-top) Trace of covariance matrix and (right-bottom) Difference between eigenvalues.

ability of the method to capture droplet crossing, we have also plotted in the right part of the figure the half-trace of the covariance matrix, which amount to a “temperature” in the case of isotropic velocity distributions. However, since this is also present in areas of very small mass due to numerical diffusion, we have also plotted the absolute value of the difference of the two eigenvalues of this matrix, thus showing areas where there is strong anisotropy and corresponding to crossing “in progress”. This fits neatly with the plots in Fig. 7 (left).

5. Conclusions

In this paper, we have described a new Eulerian model that is able to capture both polydispersity and size-conditioned dynamics, and droplet crossing for evaporating sprays. Using this model, we have conducted a series of detailed comparisons with a Lagrangian solver in the configuration of a 2-D free jet, and shown the capability of the Eulerian model to reproduce very accurately the Lagrangian results, from small Stokes numbers up to finite ones, where droplet crossing becomes important. We thus claim that we have validated the proposed model. However, one important issue that has yet to be addressed is the relative computational cost. The DPS conducted here is roughly 10 times faster than the corresponding Eulerian multi-fluid model simulated sequentially. It corresponds to a single realization of the Williams equation, and can be shown to contain information much noisier than the Eulerian model with the given discretization. In a complementary study, we have investigated this issue and shown that a real DMSC resolution of the Williams equation associated to a same level of refinement of the Eulerian fields leads to a similar cost between the two approaches (de Chaisemartin (2007)). Thus, this is promising for the Eulerian model since it is expected to have a high parallelization capability and scalability and will allow 3-D calculations in the near future.
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