Turbulent combustion of polydisperse evaporating sprays with droplet crossing: Eulerian modeling of collisions at finite Knudsen and validation

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The accurate simulation of the dynamics of polydisperse 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. In a companion paper, we have shown the capability of the Eulerian multi-fluid model to capture the dynamics and evaporation of such sprays and extended it in order to handle finite Stokes number crossing droplet trajectories, by using quadrature method of moments in velocity phase space conditioned on droplet size. Such a study was conducted in the limit of infinite Knudsen numbers. In this paper, we investigate a potential extension of such an approach in order to capture the dynamics of polydisperse spray collisions modeled by a Boltzmann operator at the mesoscopic level of description for finite Knudsen numbers. After deriving the model and presenting the dedicated numerical methods needed to preserve the moment space, we validate this approach and its capability of describing collisional crossing jets by comparing the results for both monodisperse and polydisperse clouds of particles with Lagrangian discrete particle simulations.

1. Introduction

The modeling and simulation of polydisperse multiphase flows has become a crucial issue in applications involving turbulent combustion and its optimization. Indeed, in many industrial devices, fuel is stocked in condensed form and burned as a dispersed liquid phase carried by a turbulent gaseous flow. Besides, for mixing improvement purposes, multi-point injection can be used leading to potential interactions between the liquid phase originated from separate injectors. We then want to describe the triple interaction spray/turbulence/combustion, but also its coupling with spray/spray interactions.

At the scale of a combustion chamber or in a free jet, a direct numerical simulation (DNS) of the full set of processes with a model for the dynamics of the interface between gas and liquid (modeling exchanges of mass, momentum and heat as well as the coalescence and rebound of liquid droplets) is beyond the present computational capabilities. Instead, a "mesoscopic" point of view has to be adopted, where the droplets are

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described as a cloud of point particles, the geometry of which is presumed spherical, and for which the exchanges of mass, momentum and heat are described globally and the droplet/droplet interactions are modeled. In this framework, there exists considerable interest in the development of numerical methods for simulating sprays. The physical processes that must be accounted for are (1) transport in real space, (2) droplet evaporation, (3) acceleration of droplets due to drag, and (4) rebound and coalescence of droplets leading to polydispersity. The major challenge in numerical simulations is to account for the strong coupling between these processes at a reasonable computational cost.

A first approach to simulate sprays at this mesoscopic level is to describe, in a Lagrangian way, the evolution of the point-particle cloud, solving the evolution of physical properties, such as position, velocity and temperature. This approach is called a Discrete Particles Simulation (DPS) and can be considered as a DNS for the liquid phase within the proposed model and framework. However, in the presence of droplet-droplet interactions, such an approach can only be envisioned in simplified situations because of its very high computational cost : first it is dependent on the choice of initial and injection conditions, which can not be known exactly; moreover, detecting collision leads to costly algorithms. We then have to rely directly on a statistical point of view of the collision process. Such a model is based on kinetic theory and leads to Williams (1958) transport equation. The Lagrangian approach called the Direct Simulation Monte-Carlo method (DSMC) by Bird (1994) is generally considered to be more accurate and more general than Eulerian moment methods for solving Williams equation with a collision operator. Once again, because of its high cost and the difficulty to couple it accurately with Eulerian descriptions of the gas phase, there is considerable impetus to develop Eulerian methods for the liquid dispersed phase. In the present context, we aim at describing various ranges of Knudsen numbers from the free flight regime down to the transition regime such as in rarefied flows (Struchtrup (2005)), that is we want to be able to capture out of equilibrium velocity distribution for large enough Knudsen numbers.

In a companion study (de Chaisemartin *et al.* (2009)), a new Eulerian model and its associated numerical schemes have been introduced in the infinite Knudsen limit. It is able to deal with two shortcomings of the current Eulerian two-fluid models : describing polydispersion as well as non-equilibrium velocity distributions for evaporating sprays. The first phenomenon appears to be important since droplets of different sizes have different dynamics thus depositing their fuel mass fraction through evaporation at different locations. The second one leads to a major drawback, which is the inability of the model to capture bi-modal droplet velocity distributions and thus spray crossing at finite Stokes numbers. This new model uses an improved mix of multi-fluid models for the polydispersion (Laurent and Massot (2001), Laurent *et al.* (2004), Massot (2007)) and the quadrature method of moments in velocity phase space developed for monodisperse particles by Fox (2008). The dedicated numerical schemes satisfy a crucial property, i.e. the preservation of the moment space. The validations are then done in a free jet configuration by detailed comparisons with an Euler-Lagrange direct numerical simulation solver provided by Reveillon *et al.* (2004) in the non-colliding case.

In the present study, the model developed in de Chaisemartin *et al.* (2009) is then extended to colliding sprays for finite Knudsen numbers down to the transition regime. We then investigate the capability of such Eulerian models to capture the dynamics and polydispersity of colliding sprays modeled at the kinetic level through the Boltzmann operator. Using an Euler-Lagrange DPS with hard-sphere elastic binary interactions in two dimensions and in the configuration of two colliding jets laden with droplets, we

conduct a detailed comparative analysis of the Eulerian multi-fluid model and show the ability of the proposed model to capture the physics of colliding spray jets.

Let us underline that this model can be easily extended to more complex collision kernels in 3-D with coalescence and rebound (Fox *et al.* (2008), Vedula *et al.* (2008)). Besides, the model has the potential to tackle large-eddy simulations (LES).

2. Discrete particle simulation and statistical model for colliding particles

At a mesoscopic scale, droplets are assumed spherical and described as a cloud of point particles. The reference solution for the present study will be DPS and consists in solving the evolution of physical properties, such as position, velocity, size and temperature of each droplet and detecting potential collisions. As already mentioned, such an approach is only viable in 2-D and we will thus consider a 2-D framework in the present study. A statistical point of view can also be adopted associated to an ensemble average of the phenomenon we want to describe related to initial conditions which are not known exactly but through a probabilistic approach. The aim of this section is to present the two models in 2-D and associated discretizations as well as the relationship between them. For the sake of simplicity, a d^2 isothermal evaporation law and a Stokes drag force will be considered, as well as elastic 2-D rebounds. More complex physics can be easily added such as gravity, detailed heating and evaporation and detailed collision kernels.

2.1. *Lagrangian DPS algorithm*

The DPS describes the evolution of numerical "particles", each one representing one or several droplets. If L_0 denotes a reference length, u_0 a reference velocity, $t_0 = L_0/u_0$ the associated reference time scale, and S_0 a reference droplet surface area, then the evaporation and drag processes can be described by the non-dimensional equations :

$$\mathrm{d}_t \mathbf{x}_p = \mathbf{u}_p, \quad \mathrm{d}_t \mathbf{u}_p = \frac{\mathbf{F}(t, \mathbf{x}_p, \mathbf{u}_p, S_p)}{m_p}, \quad \mathrm{d}_t S_p = \mathcal{K}, \tag{2.1}$$

where $\mathbf{x}_p$ is the position of the p^{th} particle, $\mathbf{u}_p$ its velocity, S_p its surface area, m_p its mass, $\mathbf{F}(t, \mathbf{x}, \mathbf{u}, S) = (\mathbf{U}(t, \mathbf{x}) - \mathbf{u}_k)/\mathrm{St}(S)$ the Stokes drag force, and $\mathcal{K}$ its surface constant evolution rate due to evaporation. The Stokes number is the non-dimensional relaxation time $\mathrm{St}(S) = t_p(S)/t_0$, where $t_p(S) = \rho_{l0}\, S\, S_0/(18\pi\nu_0\rho_{g0})$ and ρ_{l0} and ρ_{g0} are references liquid and gas densities. It can be written $\mathrm{St}(S) = \mathrm{St}_0 S$,with $\mathrm{St}_0 = t_p(S_0)/t_0$.

Droplet-droplet collisions are taken into account inside each time step. They are naturally a 3-D phenomenon; however, for the purpose of conducting detailed DPS reference simulations, we have restricted the model to 2-D hard-sphere elastic binary collisions, i.e. we assume that the center of mass of the whole set of droplets live in a plane as well as their velocities. The general algorithm of the DPS contains three sub-steps embedded in a time step : (a) the detection of colliding particles, (2) the resolution of equations (2.1) with an explicit Runge-Kutta method of order 3, and (3) the modification of the positions and velocities of particles that collide. The most costly step is the detection of collisions: it reaches order N^2 if each particle pairs are considered, where N is the number of particles. To avoid this, an algorithm has been developed that first identify potentially colliding particles, i.e. pairs of closest particles in the sense of a maximal distance defined from maximal radius and velocities of particles (in each direction). Inside a set of such particle pairs, each trajectory is studied to detect collision, assuming that the gas velocity, the size and the acceleration of particles are constant inside the time step.

An optimization is done thanks to a reordering of particles by abscissas; this leads to a complexity of order $N^{3/2}$ for the algorithm. Let us note that the time step has then to be small enough so that the predicted trajectories are accurate enough. Moreover, it is also limited by the fact that particle can collide only once during a time step.

2.2. *Statistical description of the spray*

From a statistical point of view, a spray can be described by its joint surface area, velocity number density function (NDF) $f(t, \mathbf{x}, S, \mathbf{u})$ which satisfies Williams (1958) equation :

$$\partial_t f + \partial_{\mathbf{x}} \cdot (\mathbf{u}\, f) + \partial_S (\mathcal{K}\, f) + \partial_{\mathbf{u}} \cdot (\mathbf{F}\, f) = \frac{1}{\mathrm{Kn}} \Gamma, \tag{2.2}$$

where Γ is the dimensionless collision operator and, as for the DPS model, $\mathcal{K}$ is the constant of the d^2 evaporation law and $\mathbf{F}(t, \mathbf{x}, \mathbf{u}, S)$ is the Stokes drag force previously defined. The Knudsen number Kn is the ratio between the mean free path $l_0 = 1/(n_0 \sigma_0)$ and L_0, where σ_0 is the collision cross section (which is 1-D in our 2-D physical space) and $n_0 = N_0/(L_0)^2$ a reference droplet number density and N_0 a reference droplet number. In the infinite Knudsen number limit, that is for small enough particles and dilute enough sprays, the effect of the collisions is negligible as in de Chaisemartin *et al.* (2009). Conversely, the limit of zero Knudsen number corresponds to the hydrodynamic limit. Between these two limits droplet-droplet interactions have an impact on the spray without inducing a velocity equilibrium and this is precisely the case we will investigate.

Let us describe, in its dimensionless form, the size-dependent Boltzmann collision operator corresponding to 2-D elastic binary rebounds :

$$\Gamma = \int_0^\infty \beta(S, S^*) \int_{R^2} \int_{D^+} [f'' f^{*\prime\prime} - f\, f^*]\, |\mathbf{g} \cdot \mathbf{n}|\, \mathrm{d}\mathbf{n}\, \mathrm{d}\mathbf{u}^*\, \mathrm{d}S^* \tag{2.3}$$

with the pre-collision terms $f = f(S, \mathbf{u})$, $f^* = f(S^*, \mathbf{u}^*)$ and the post-collision terms $f'' = f(S, \mathbf{u}'')$, $f^{*\prime\prime} = f(S^*, \mathbf{u}^{*\prime\prime})$, all of them also depending on t and $\mathbf{x}$, and where $\mathbf{g} = \mathbf{u} - \mathbf{u}^*$ is the velocity difference before collision. The curve D^+ is the unit half circle on which $\mathbf{g} \cdot \mathbf{n} > 0$ (i.e., velocity differences that result in collisions). The collision cross section is $\beta(S, S^*) = \sqrt{S} + \sqrt{S^*}$. Double-prime variables denote values before inverse collision, which are defined in terms of the pre-collision values by Vedula *et al.* (2008)

$$\mathbf{u}'' = \mathbf{u} - \frac{2(S^*)^{3/2}}{(S)^{3/2} + (S^*)^{3/2}} (\mathbf{g} \cdot \mathbf{n})\mathbf{n}, \quad \mathbf{u}^{*\prime\prime} = \mathbf{u}^* + \frac{2(S)^{3/2}}{(S)^{3/2} + (S^*)^{3/2}} (\mathbf{g} \cdot \mathbf{n})\mathbf{n}. \tag{2.4}$$

DSMC are usually used to solve equation (2.2). Eulerian fields for the liquid-phase mass density and velocity are then recovered by averaging over cells in physical space. However, in this paper, our aim is to develop an Eulerian model for the statistical resolution of the spray which will be compared to an ensemble average of the DPS results.

3. Crossing jet configuration and reference solutions

A simple 2-D configuration where collisions take place is a case with two crossing jets. The background gas flow is assumed time-independent and uniform in the domain, with a non-zero velocity component in the x-direction. This implies that we restrict ourselves to a one-way coupling, which is adequate for our aim of validating the Eulerian models through comparisons to Lagrangian simulations. The Reynolds number based on U_0, ν_0 and L_0 is 1000, where U_0 is the gas velocity and L_0 is the global jet width. We will eventually provide dimensional quantities for illustration purposes. These will be based on a velocity

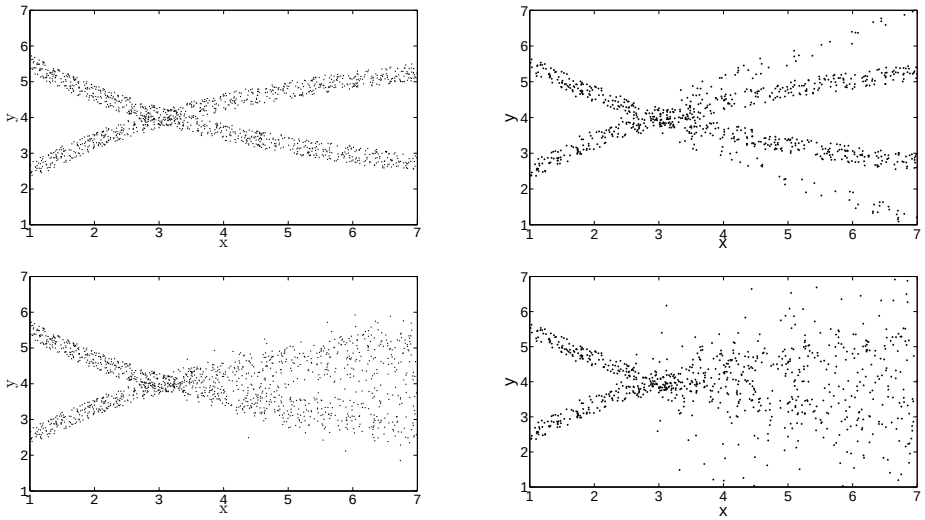
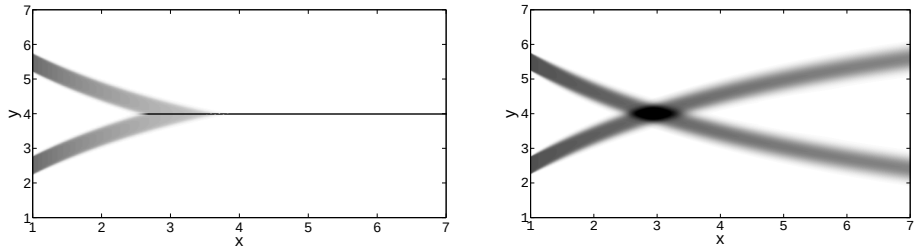


FIGURE 1. Droplet positions in the Lagrangian simulation without collision (top) and with collisions (bottom) for the monodisperse case (left) and the bi-disperse case (right).

of $U_0 = 1$ m/s, a length $L_0 = 1.5$ cm, and kinematic viscosity $\nu_0 = 1.6 \times 10^{-5}$ m^2/s. In addition, we will let $d_0 = L_0/100$, where d_0 is the diameter corresponding to the droplet surface area S_0, and use a typical droplet number of $N_0 = 1000$. The computational domain has a size 6×6, which then corresponds to 9 cm$\times$9 cm in dimensional values.

Two spray jets with a width of 0.5 are injected into the domain at a unit dimensionless velocity in two directions forming angles $\pi/4$ and $-\pi/4$, respectively, relative to the gas velocity. The distance between the two jet centers is 3. Droplets are inertial enough so that the jets cross inside the domain (see Fig. 1). These sprays can be monodisperse, with droplets of Stokes St = 5.29, corresponding to a diameter of 195 μm or bi-disperse with droplets of Stokes St = 5.29 and St = 15.86, corresponding to diameters 195 μm and 338 μm, respectively. In the latter case, the dynamics of the two sizes are very different as seen for non-colliding case in Fig. 1(a)-right : the most inertial droplets in each jet move apart faster than the smallest ones. Moreover, in the two cases, the mass density of the spray is equal to 350 at the injection point, with an equi-repartition between the two sizes for the bi-disperse case. The reference Knudsen number is then $\mathrm{Kn} = 2L_0/(N_0 d_0) = 0.2$. The liquid phase density ρ_l is 563 times larger than the gas one.

The reference simulations are conducted with the CORIA code Asphodele where the DPS method described in Sec. 2.1 has been implemented. A random injection of the droplets is done in such a way that it is statistically time-independent and spatially uniform over the width of the jets. The computations are done with approximately 1300 droplets in the domain for the mono-disperse case and 850 for the bi-disperse one. An instantaneous snapshot of the DPS simulations, with droplet positions, is shown in Fig. 1. The chosen configurations are statistically stationary, hence the time average of the DPS converges, after a transitory regime, to the ensemble averages which are taken as the reference solution projected on a grid associated to the Eulerian solutions.



(a) Multi-fluid (b) Multi-velocity

FIGURE 2. Mass density for simulation of two crossing jets using the standard multi-fluid approach (left) and the multi-fluid/multi-velocity model (right) for droplets with St = 5.29.

4. Eulerian multi-fluid multi-velocity model with collisions

Eulerian multi-fluid models for sprays undergoing coalescence were developed in Laurent *et al.* (2004) and compared with the DQMOM method in Fox *et al.* (2008). It is an extension of the standard Eulerian multi-fluid model presented in Laurent and Massot (2001), Massot (2007) and briefly in de Chaisemartin *et al.* (2009). This model consists in a discretization $0 = S_0 < S_1 < ... < S_{N_{sec}}$ of the size phase space and in writing fluid equation on each size interval $[S_{k-1}, S_k[$, called section. However, it is based on an equilibrium assumption on the velocity for droplets of the same size without dispersion, so that only collisions of droplets of different sizes can then be described with this model. This makes it useless for the simulation of our configuration, since it can not even describe crossing of non-colliding jets, that is the infinite Knudsen limit as shown in Fig. 2(a) for the monodisperse case. Let us underline that the proposed configuration is much more challenging than the one usually used for simple jet crossing configurations, briefly recalled in de Chaisemartin *et al.* (2009) (for which injection directions are following the two axis and no drag is taken into account, so that the CFL number can be maintained at 1 in order to eliminate numerical diffusion before the jets collide). It can be seen in Fig. 2(b) that the multi-fluid multi-velocity method developed in de Chaisemartin *et al.* (2009) works well in this case. Let us note that the present case is more difficult and thus interesting because numerical diffusion starts having an effect right at injection and we can really study the capability of the method to handle its impact on the various phenomenon we aim at describing. Thus, the multi-fluid multi-velocity method is a good candidate to be extended to finite Knudsen configurations.

4.1. *Multi-fluid multi-velocity approach*

We are interested in the following velocity moments in one section $[S_{k-1}, S_k[$:

$$m^{(k)}(t,\mathbf{x})M_{j,l}^{(k)}(t,\mathbf{x}) = \rho_l \int_{S_{k-1}}^{S_k} S^{3/2} \int_{\mathcal{R}^2} (u_1)^j (u_2)^l f(t,\mathbf{x},S,\mathbf{u})\,\mathrm{d}\mathbf{u}\mathrm{d}S \tag{4.1}$$

with the convention $M_{00}^{(k)} = 1$. The assumption resulting in the multi-fluid/multi-velocity method introduced by de Chaisemartin *et al.* (2009) can be written :

$$\forall S \in [S_{k-1}, S_k[\qquad f(t,\mathbf{x},S,\mathbf{u}) = m^{(k)}(t,\mathbf{x})\kappa_k(S)\sum_{\alpha=1}^{N} w_\alpha^{(k)}(t,\mathbf{x})\delta(\mathbf{u}-\mathbf{u}_\alpha^{(k)}(t,\mathbf{x})) \tag{4.2}$$

with, for each k from 1 to the total number of sections N_{sec},

$$\sum_{\alpha=1}^{N} w_\alpha^{(k)} = 1, \qquad \rho_l \int_{S_{k-1}}^{S_k} S^{3/2} \kappa_k(S) \mathrm{d}S = 1.$$

The N weights $w_\alpha^{(k)}$ and N velocity abscissas $\mathbf{u}_\alpha^{(k)}$ are computed from the velocity moments $M_{j,l}^{(k)}$ using the quadrature method given in de Chaisemartin *et al.* (2009), with $N = 4$ in our 2-D configuration. This quadrature is the improvement of the one given by Fox (2008) in such a way that no direction is privileged. The conservation equations for the k^{th} section then read :

$$\begin{aligned}\partial_t m^{(k)} M_{j,l}^{(k)} + \partial_{\mathbf{x}}(m^{(k)} M_{j+1,l}^{(k)}) = -(E_1^{(k)} + E_2^{(k)}) m^{(k)} M_{j,l}^{(k)} + E_1^{(k+1)} m^{(k+1)} M_{j,l}^{(k+1)} \\ + j\, m^{(k)} \frac{U_{g,x} M_{j-1,l}^{(k)} - M_{j,l}^{(k)}}{\mathrm{St}(S_{\text{mean}}^{(k)})} + l\, m^{(k)} \frac{U_{g,y} M_{j,l-1}^{(k)} - M_{j,l}^{(k)}}{\mathrm{St}(S_{\text{mean}}^{(k)})} + \frac{\Gamma_{j,l}^{(k)}}{\mathrm{Kn}}, \quad (4.3)\end{aligned}$$

where $j + l \leq 3$ and $E_1^{(k)}$ and $E_2^{(k)}$ are the "classical" evaporation coefficients and $S_{\text{mean}}^{(k)}$ a mean surface for the section (Laurent and Massot (2001)).

4.2. *Quadrature-based closure of the Boltzmann collision term*

Through a classical change of variables and an assumption (4.2), the 2-D size-dependent Boltzmann collision term can be written :

$$\begin{aligned}\Gamma_{j,l}^{(k)} = \rho_l m^{(k)} \sum_{i=1}^{N_{\text{sec}}} m^{(i)} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} w_\alpha^{(k)} w_\beta^{(i)} |\mathbf{u}_\alpha^{(k)} - \mathbf{u}_\beta^{(i)}| \\ \int_{S_{k-1}}^{S_k} \int_{S_{i-1}}^{S_i} S^{3/2} \left(\sqrt{S} + \sqrt{S^*}\right) \kappa_k(S) \kappa_i(S^*) \mathcal{I}_{jl}(S, S^*, \mathbf{u}_\alpha^{(k)}, \mathbf{u}_\alpha^{(k)} - \mathbf{u}_\beta^{(i)}) \mathrm{d}S^* \mathrm{d}S \quad (4.4)\end{aligned}$$

with

$$\mathcal{I}_{jl}(S, S^*, \mathbf{u}, \mathbf{g}) = \int_{-\pi/2}^{\pi/2} \left[(u_1{}')^j (u_2{}')^l - (u_1)^j (u_2)^l \right] \cos\theta \, \mathrm{d}\theta, \quad (4.5)$$

where θ is the angle between $\mathbf{g}$ and $\mathbf{n}$, and

$$u_1{}' = u_1 - \lambda(S, S^*) \cos\theta [g_1 \cos\theta - g_2 \sin\theta], \quad (4.6)$$

$$u_2{}' = u_2 - \lambda(S, S^*) \cos\theta [g_2 \cos\theta + g_1 \sin\theta] \quad (4.7)$$

with

$$\lambda(S, S^*) = \frac{(S^*)^{3/2} \left[1 + \alpha(S, S^*)\right]}{\left[(S)^{3/2} + (S^*)^{3/2}\right]}. \quad (4.8)$$

A choice has to be made for κ_k, and the coefficients $\mathcal{I}_{jl}$ can then be computed. It is easy to see that $\mathcal{I}_{jl}(S, S^*, \mathbf{u}, \mathbf{g})$ is a polynomial function of $\lambda(S, S^*)$ with coefficients depending only on $\mathbf{g}$ and $\mathbf{u}$. Hence, a preliminary computation and storage of an integral of the form :

$$\mathcal{L}_{kip} = \int_{S_{k-1}}^{S_k} \int_{S_{i-1}}^{S_i} (\lambda(S, S^*))^p \, S^{3/2} \left(\sqrt{S} + \sqrt{S^*}\right) \kappa_k(S) \kappa_i(S^*) \mathrm{d}S^* \mathrm{d}S$$

is enough to compute the collision terms, regardless of the choice of the function κ_k. A

simpler solution is to take a Dirac delta function for κ_k inside the collision term :

$$\kappa_k(S) = \frac{1}{\rho_l (S_k^{\mathrm{m}})^{3/2}} \delta\left(S - S_k^{\mathrm{m}}\right),$$

where S_k^{m} is a mean surface, which can correspond to $S_{\mathrm{mean}}^{(k)}$. This choice is interesting due to its simplicity but also through possible extension done for evaporation, which mixes multi-fluid and QMOM-like methods for the size space phase to obtain a higher-order method (Massot *et al.* (2009)). The collision term in Eq. (4.4) can be approximated by :

$$\Gamma_{j,l}^{(k)} = \frac{1}{\rho_l} m^{(k)} \sum_{i=1}^{N_{\mathrm{sec}}} m^{(i)} \frac{\sqrt{S_k^{\mathrm{m}}} + \sqrt{S_i^{\mathrm{m}}}}{(S_i^{\mathrm{m}})^{3/2}} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} w_\alpha^{(k)} w_\beta^{(i)} |\mathbf{u}_\alpha^{(k)} - \mathbf{u}_\beta^{(i)}| \mathcal{I}_{jl}(S_k^{\mathrm{m}}, S_i^{\mathrm{m}}, \mathbf{u}_\alpha^{(k)}, \mathbf{u}_\alpha^{(k)} - \mathbf{u}_\beta^{(i)}) \quad (4.9)$$

where all terms on the right-hand side can be evaluated using the quadrature weights and velocity abscissas.

4.3. *Numerical method and preservation of velocity moment space*

As presented in de Chaisemartin *et al.* (2009), we use a splitting algorithm to separate the transport in physical space through convection and the transport in phase space through drag and collisions. The interest is to preserve the properties of the schemes that we use for different contributions; it is computationally optimal and yields high parallelization capabilities. For transport in physical space, we also use a dimensional splitting. The scheme is described in de Chaisemartin *et al.* (2009), Fox (2008) and based on kinetic finite volume schemes in order to solve weakly hyperbolic systems as the pressureless gas dynamics. It is first order accurate in space and time in order to strictly preserve the moment space. In this contribution, we aim at working also at the frontier of the moment space since we want to tackle cases where the velocity distribution is monokinetic and where the proposed quadrature degenerates to the original multi-fluid model since the covariance matrix is zero.

The transport in phase space results from the resolution, through an implicit Runge-Kutta Radau IIA method of order 5 with adaptive time stepping, of a system similar to de Chaisemartin *et al.* (2009) where we have added collision terms of the form (4.9). The preservation of the moment space is crucial and achieved using centered velocity moments. Thus we use modified coefficients $\mathcal{I}_{jl}$ depending on the velocity relative to the mean velocity of section k and on the difference of velocity abscissas.

5. Results and discussion

A solver developed at EM2C is used for Eulerian simulations with the multi-fluid/multi-velocity models. A 300×300 grid is used, with only one section for the monodisperse case and two for the bidisperse case, since both are non-evaporating and elastic collisions conserve droplet size. Let us note that the values of $S_k^{\mathrm{m}} = S_{\mathrm{mean}}^{(k)}$ corresponds to the sizes of the droplets. Lagrangian reference solutions are performed using DPS, as explained in Sec. 3. This implies only 1300 or 850 droplets in the computational domain. In order to make satisfactory comparisons with Eulerian simulations, a statistical Eulerian analysis of the Lagrangian solutions is done by averaging over the Eulerian cells and over 1325 time steps (the configurations are statistically stationary after the transitory regime).

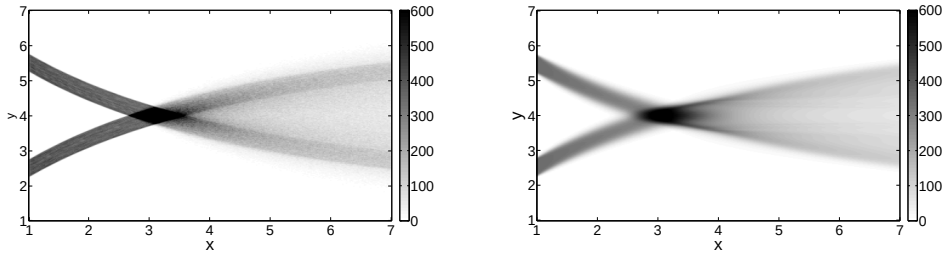


FIGURE 3. Mass density for the simulations of two crossing monodisperse jets using the DPS approach averaged and projected onto the Eulerian grid (left) and the multi-fluid/multi-velocity model (right) for droplets with $\mathrm{St} = 5.29$ undergoing collisions.

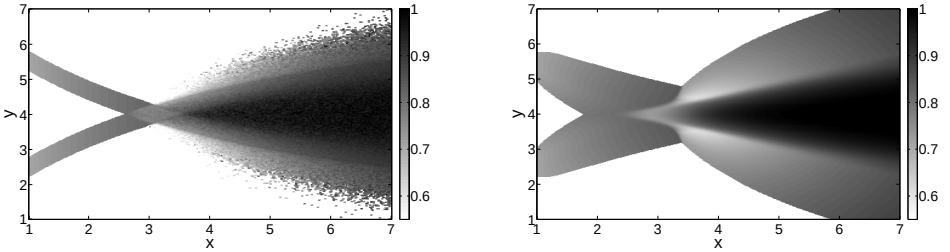


FIGURE 4. Mean particle velocity in the x-direction for the simulations of two crossing monodisperse jets using the DPS approach averaged and projected onto an Eulerian grid (left) and the multi-fluid/multi-velocity model (right) for droplets with $\mathrm{St} = 5.29$ undergoing collisions.

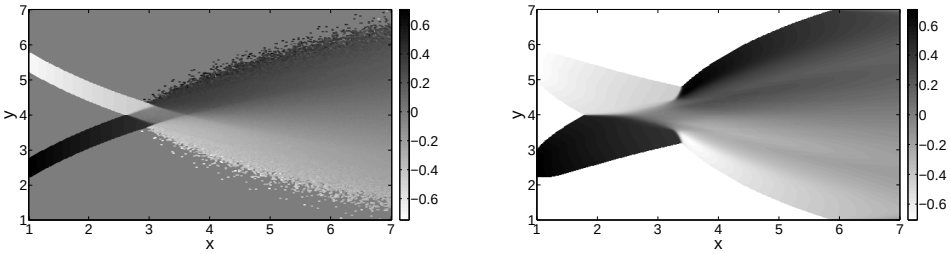


FIGURE 5. Mean particle velocity in the y-direction for the simulations of two crossing monodisperse jets using the DPS approach averaged and projected onto an Eulerian grid (left) and the multi-fluid/multi-velocity model (right) for droplets with $\mathrm{St} = 5.29$ undergoing collisions.

5.1. *Lagrangian versus multi-velocity model for a monodisperse spray*

For a monodisperse non-evaporating spray, the Eulerian model reduces to the one developed in Fox (2008) for a BGK collision operator and Vedula *et al.* (2008) for the Boltzmann operator, except for the improvement of the quadrature done in de Chaisemartin *et al.* (2009). The infinite Knudsen case has already be shown to be well captured by the method in Sec. 4. The finite Knudsen case is weakly collisional so that some droplets of the jets follow their original trajectories as if they did not see the other ones, whereas the other droplets undergo collisions and are deviated from their original trajectories. This can be seen very clearly from the Eulerian analysis of the Lagrangian simulations (see Fig. 3a). The Eulerian simulation reproduces this phenomenon, as seen in Fig. 3b, even if a limit does not appear so clearly due to the numerical diffusion induced by the numerical

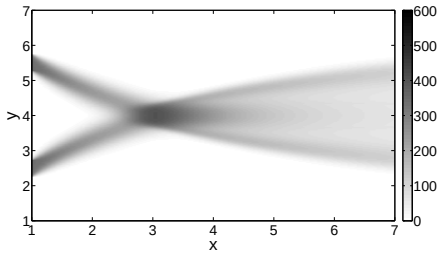


FIGURE 6. Mass density for the simulations of two crossing jets using the BGK model with multi-fluid multi-velocity model for droplets with St = 5.29 undergoing collisions.

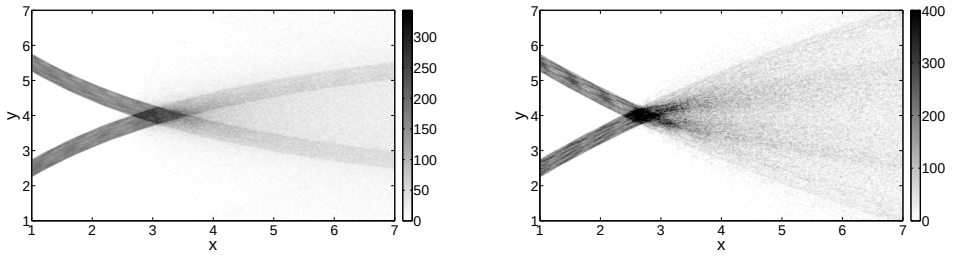
method used for the transport solver in the Eulerian model. However, the level of mass density are very similar, showing a very good description of the collisions. Moreover, there is also a very good agreement for the mean velocities of the droplets computed by the two methods, as can be seen in Figs. 4 and 5. Only the numerical diffusion explains the spreading of this fields, the mass density being however very small in locations where there are no droplets for the Lagrangian simulations.

Let us also compare the simulation with Boltzmann collisions to the one with BGK collisions. The numerical model can be found in Fox (2008) with the quadrature of de Chaisemartin *et al.* (2009). The great advantage of the BGK model is its cost, smaller because it is linear in the abscissas number whereas the Boltzmann one is quadratic. The characteristic dimensionless collision time is given by $\tau_{\text{col}} = L_0/(2\,d\,d_0 N_0 n\sqrt{\sigma_{eq}})$, where d is the non-dimensional droplet diameter, n is the non-dimensional number density of the spray and σ_{eq} is the dispersion of the equilibrium distribution defined in Fox (2008). The same type of simulation on a grid 200×200 is done and gives very similar results as the Eulerian model with Boltzmann collisions as seen in Fig. 6 for the mass density.

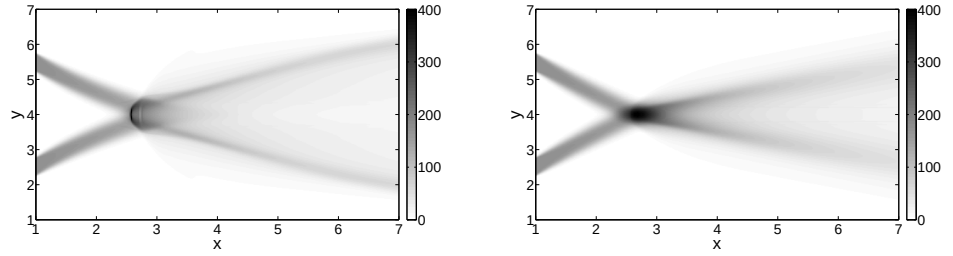
5.2. *Lagrangian versus multi-velocity model for a bi-disperse spray*

For the bidisperse case, droplets of different inertia are used. First, the non-colliding case is very well reproduced, as previously seen for the monodisperse case, which could be foreseen since this configuration can be thought of as the superposition of two monodisperse cases because droplets do not interact. The situation is different for the colliding case : droplets collide with droplets of the same size and with droplets of different size (the only effect that the classical multi-fluid method could take into account). Velocities are not presented here, but the results are nearly as good as seen for the monodiperse case. Concerning the mass density, Fig. 7 shows the results for the Lagrangian and the Eulerian simulations, separating droplets by their sizes. The behavior of both large and small droplets is similar for the two simulations as seen in Fig. 7. Note that collisions cause the droplets to spread in a fan shape, the width of which depends on the Stokes number. Compared to the monodisperse case, the bi-disperse case appears to be more collisional due to the larger velocity difference between droplets with different sizes.

The cost of Lagrangian and Eulerian simulations are of the same ordre of magnitude in this case, a litle longer for Lagrangian. But this flow configuration is favorable to a Lagrangian approach since it becomes statistically stationary. Indeed, implementing ensemble averages instead of time averages would be much more costly in order to obtain comparable statistical accuracy including the transitory regime. Because we have presented a non evaporating case, Eulerian simulations are conducted with a very limited number of sections and the cost of the Eulerian method is quadratic in the number of



(a) Lagrangian



(b) Eulerian

FIGURE 7. Mass density for the simulations of two crossing bi-disperse jets using the DPS approach averaged and projected onto the Eulerian grid (a) and the multi-fluid/multi-velocity model (b). Droplets of Stokes number $\mathrm{St} = 5.29$ are represented on the left side and droplets of Stokes number $\mathrm{St} = 15.86$ are represented on the right side

sections, as well as in the number of delta functions used for the quadrature. Let us note that no BGK type collision operator seems accurate enough for polydisperse case, so that Boltzmann operator has to be used and the cost cannot be reduced that way. Finally, we note that the computational cost is very sensitive to the local number density for the Lagrangian model (i.e. quadratic) in contrast to the Eulerian model. For all these reasons, the presented configurations, even if they allow to show the capability of the proposed approach to capture the right physical behavior, do not provide precise conclusions on computational costs. We can only estimate that in more realistic unsteady configurations the Eulerian model is going to be cheaper than the Lagrangian one, the ratio being very configuration-dependent and higher for highly collisional sprays.

6. Conclusions

In this paper, we have extended to weakly collisional sprays the Eulerian model of de Chaisemartin *et al.* (2009), which is able to capture both polydispersity and size-conditioned dynamics, and droplet crossing and collisions for polydisperse sprays. We have conducted a series of detailed comparisons with a Lagrangian solver for the configuration of 2-D crossing jets, and shown the capability of the Eulerian model to reproduce accurately the results, for mono-disperse as well as for bi-disperse sprays. We thus claim that we have proposed a first validation of the model. Finally, we note that the quadrature representation of the Boltzmann collision term can be easily extended to 3-D flows and to other physics such as coalescence.

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