A NUMERICAL METHOD FOR THE COMPUTATION OF THE DISPERSION OF A CLOUD OF PARTICLES BY A TURBULENT GAS FLOW FIELD

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The paper is concerned with the construction of a numerical method for the computation of the dispersion of a cloud of liquid droplets by a turbulent gas flow field. The cloud of droplets is modeled by a semi-fluid system intermediate between a fluid model and a kinetic description of the dispersed phase. The semi-fluid model is deduced from the kinetic model by integration with respect to the velocity variables and allows to describe clouds of particles such that the velocity distribution of any familly of particles with a given radius and a given temperature, found at a given location of the physical space is a gaussian function. A numerical scheme, consistent with the semi-fluid model and inspired from Perthame's or Deshpande's kinetic schemes is proposed. The interactions with the gas phase are taken into account thanks to a Particle in Cell method. Numerical experiments enlight the features of the method.

1 Introduction

This work deals with the numerical simulation of vaporizing two-phase fluid flows consisting of a spray of liquid droplets in a surrounding turbulent hot gas flow. The prediction of the turbulent induced mixing of the cloud of droplets is for instance of primary importance in the simulation of Diesel engines. In such devices, liquid fuel is injected at high pressure in the combustion chamber, which causes breakup of the liquid core and small droplets are formed. In this study we do not consider the atomization of fuel, which is still an open problem from the numerical viewpoint. On the contrary we propose a numerical method for the computation of the dispersion of a dilute spray by a turbulent gas flow field. We shall thus assume no interactions between droplets such as breakup or collisions. Nevertheless the mass of droplets in practicle devices such as Diesel engines is of the same order as the mass of gas and one should take into account the exchanges of mass, momentum and, of course energy between the two phases. However, for the sake of simplicity, we will not introduce combustion models in this work but only consider vaporization of droplets since our main interest lies in the prediction of the dispersion of the cloud of droplets. This study is thus a preliminary step towards the computation of the full piston in a Diesel engine.

In order to model two-phase fluid flows, we might either choose an eulerian model or a lagrangian one. In the eulerian approach, each phase is modeled as a single fluid, occupying the whole physical space. Exchange terms are included to account for the exchanges of mass, momentum and energy between the two phases. Such models are usually obtained by averaging the Navier-Stokes equations satisfied by the gas phase around the droplets and the liquid phase inside the droplets. Since the location of the droplets may change from one experiment to another one, this method defines mean quantities that characterize the two-phase flow, which are defined in the whole physical space. Nevertheless the derivation of such models is usually tricky and requires much assumptions on the velocity and radius distributions of the cloud of droplets. Furthermore the numerical treatment of eulerian models is usually a difficult task wich requires much work and the numerical results often poorly compare with experimental results. On the contrary, physical laws are easily included in lagrangian models. Here droplets are characterized by their position in the phase space and the modeling stage consists in writing the droplets trajectory in the phase space. Here the description of the motion of the droplets may be as complicated as necessary. The interaction with the gas phase is taken into account through correlations: the regression velocity of a droplets radius may depend for instance from the temperature and from the velocity of the gas around the droplet. In the same manner production terms are included in the gas phase equation so as to ensure the global conservation of mass, momentum and energy of the two-phase flow. Note that alternatly, by using Liouville's theorem, the lagrangian model may be written in the form of a kinetic one, that gives the evolution of the probability density function of the cloud of particles. This equation is also known as the spray equation (see [1] for more details).

Writing a lagrangian model is thus much easier than writing an eulerian one. But usual two-phase flow experiments involve typically $10^6 - 10^{10}$ particles and it is of course impossible to compute as many particles. Furthermore we are not interested in the precise location of particles but on average behaviors. The usual trick is to consider numerical particles which represent a group of particles with the same velocity and the same radius at a given location of the phase space. Provided that the velocity and droplet distribution of the cloud is smooth enough, this method is efficient and enables the computation of lagrangian models. However such computations still require much CPU time due to the grat number of numerical particles that should be computed in order to obtain meaningfull results. Furthermore, in the case of the dispersion of a cloud by a isotropic and homogeneous turbulent gas flow field, [2] prove that the velocity distribution of a class of particles of given radius and at a given location of the physical space asymptotically tends to a Gaussian distribution. Assuming that the last velocity distribution functions are Gaussian we introduce below a semi-fluid model where each class of droplets with a given radius and found at a given location of the phase space is characterized by its number density, its mean velocity and its mean quadratic velocity. The semi-fluid model is derived by taking the first three moments of the spray equation relative to the velocity variable. The semi-fluid model consists of three equations, written in a space with dimension four (the three position variables and the radius) while the spray equation is a single equation written in a phase space with dimension seven. The semi-fluid description of the two-phase flow thus requires much less degrees of freedom than the lagrangian description and we expect much more efficient computer codes based on this model than on fully lagrangian models without sacrifying for a precise description of the behavior of droplets.

We introduce in this paper a numerical method for the computation of our semi-fluid model. The method is inspired from the kinetic schemes of Harten, Desphande and Perthame (see [3, 4, 5]) and relies on the spray equation. Nevertheless the semi-fluid model is written in a space with dimension four and we resort to a particle description of the unknown functions rather than to a finite volume approach as in the work of Perthame. The organization of the paper is the following: section 2 is devoted to the derivation of the semi-fluid model from the spray equation. Section 3 deals with the discretization of the semi-fluid model. A finite volume method for the computation of the gas phase and the treatment of the interaction between the gas and the liquid phase thanks to a particle in cell method is proposed in section 4. Numerical results are shown in section 5.

2 Modeling

2.1 A kinetic model

In the kinetic approach, the particles are characterized by their position in the phase space, namely by their position $\mathbf{x}$, their velocity $\mathbf{v}$, and their radius r. We do not take into account here the temperature. The corresponding probability density function (pdf) is then a function $f = f(\mathbf{x}, \mathbf{v}, r, t)$ and the spray equation writes (see [1, 6]):

$$\partial_t f + \nabla_{\mathbf{x}} \cdot (f\mathbf{v}) + \nabla_{\mathbf{v}} \cdot (f\beta) + \partial_r (f\mathcal{R}) = Q(f, f). \tag{2.1}$$

The term $\beta = \beta(\mathbf{x}, \mathbf{v}, r, t)$ is the acceleration of a droplet with velocity $\mathbf{v}$ and radius r, at time t. The term $\mathcal{R}$ is the regression velocity of the radius of the droplets:

$$\mathcal{R} = \frac{dr}{dt}.$$

This term takes into account the vaporization of the droplets. There exist many models accounting for this phenomenon. Here, for the sake of simpliciy, we shall assume that when a droplet vaporizes its radius obeys the so called d^2-law: $r^2(t) = r_0^2 - Kt$ where K is a positive constant (see [1]). This means that $\mathcal{R} = -\frac{K}{2r}$. When using this simple model, one assumes that the temperature inside the droplet is constant and uniform and that the surrounding gas is still. These are reliable assumptions when there exists a certain equilibrium between the vaporizing droplet and the surrounding gas. These assumptions are not verified in most practical cases but we may use the d^2-law when the droplets are injected in a hot gas so that the temperature of the droplets reaches the boiling point in a short time compared to the time for the complete vaporization of the droplet. Hence, as a preliminary step towards more realistic models, we may omit the droplets temperature in the pdf by assuming that this temperature equals the boiling temperature of the liquid inside the droplets. Finally, $Q(f,f)$ is a nonlinear expression that takes into account the collisions of particles and the break-up. In the sequel, we consider dilute clouds of particles, so that we omit the term $Q(f,f)$ in (2.1). The spray equation reduces to the transport equation in the phase space:

$$\partial_t f + \nabla_{\mathbf{X}} \cdot (f\mathbf{v}) + \nabla_{\mathbf{V}} \cdot (f\beta) + \partial_r (f\mathcal{R}) = 0. \tag{2.2}$$

The acceleration β of a droplet includes the drag force, the acceleration of gravity, the added mass effect, the Basset term, ... In this study we shall only take into account the drag force and the gravity force, which are the two leading forces that act on droplets. The term β is thus the following

$$\beta = \beta_s + \mathbf{g} \tag{2.3}$$

where $\mathbf{g}$ is the acceleration of gravity and β_s is the drag acceleration. We model the latter acceleration by using the Stokes drag force:

$$\beta_s = -\frac{9}{2}\frac{\mu_g}{r^2\rho_l}(\mathbf{v} - \mathbf{u}_g) = -c(r)(\mathbf{v} - \mathbf{u}_g) = -\frac{\mathcal{C}}{r^2}(\mathbf{v} - \mathbf{u}_g). \tag{2.4}$$

Here, μ_g denotes the viscosity of the gas, ρ_l is the mass density of the liquid phase and, $\mathbf{u}_g$ is the velocity of the gas. We assume below that μ_g and ρ_l are positive constants. Hence, the action of the gas on the particles occurs through the acceleration β_s that depend on $\mathbf{u}_g$. Furthermore, when the velocities of the gas and of the droplets is large, the effects of gravity may be neglected and we set $\mathbf{g} = 0$ in the sequel. Finally, note that $\frac{1}{c(r)}$ is the characteristic relaxation time for a droplet with radius r to be captured by the gas flow, i.e., the time after which the velocity of the droplet equals that of the surrounding gas.

The gas flow field is modeled by the Navier-Stokes equations:

$$\begin{cases} \partial_t(\rho_g) + \nabla_{\mathbf{X}} \cdot (\rho_g \mathbf{u}_g) = \mathbf{M} \\ \partial_t(\rho_g \mathbf{u}_g) + \nabla_{\mathbf{X}} \cdot (\rho_g \mathbf{u}_g \otimes \mathbf{u}_g + p_g \underline{\underline{I}}) - \nabla_{\mathbf{X}} \cdot (\sigma_g^{'}) = \mathbf{I} \\ \partial_t(\rho_g e_g) + \nabla_{\mathbf{X}} \cdot (\rho_g e_g \mathbf{u}_g + p_g \mathbf{u}_g) - \nabla_{\mathbf{X}} \cdot (\sigma_g^{'} \cdot \mathbf{u}_g) - \nabla_{\mathbf{X}} \cdot (\kappa_g \nabla_{\mathbf{X}} \epsilon_g) = \mathbf{E}. \end{cases} \tag{2.5}$$

The functions p_g, ϵ_g, κ_g and $\sigma_g^{'}$ are respectively the pressure, the specific internal energy, the gas thermal conductivity, and the viscous stress tensor of the gas. Their expressions are given by the following formulae:

$$\begin{aligned} \epsilon_g &= e_g - \frac{\mathbf{u}_g^2}{2} \\ p_g &= (\gamma - 1)\rho_g \epsilon_g = (\gamma - 1)\rho_g (e_g - \frac{\mathbf{u}_g^2}{2}) \\ \sigma_g^{'} &= \mu_g(\nabla_{\mathbf{X}} \mathbf{u}_g + \nabla_{\mathbf{X}} \mathbf{u}_g^T) + \lambda(\nabla_{\mathbf{X}} \cdot \mathbf{u}_g)\underline{\underline{I}} \end{aligned} \tag{2.6}$$

where γ is the ratio of specific heats, μ_g is the gas viscosity, and λ is the bulk viscosity.

The terms $\mathbf{M}$, $\mathbf{I}$ and, $\mathbf{E}$ in (2.5) account for the exchanges of mass, momentum and energy between the two phases. Their expressions are given by the following lemma:

Lemma 2.1 (Exchange terms) *The exchange terms* $(\mathbf{M},\mathbf{I},\mathbf{E})(\mathbf{x},t)$ *write*

$$\begin{cases} \mathbf{M}(\mathbf{x},t) = \displaystyle\int_r 2K\pi\rho_l r dr \int_{\mathbf{V}} f d\mathbf{v} \\ \mathbf{I}(\mathbf{x},t) = \displaystyle\int_r 2K\pi\rho_l r dr \int_{\mathbf{V}} f\mathbf{v} d\mathbf{v} - \int_r c(r)\frac{4}{3}\pi\rho_l r^3 dr \int_{\mathbf{V}} f(\mathbf{u}_g - \mathbf{v}) d\mathbf{v} \\ \mathbf{E}(\mathbf{x},t) = \displaystyle\int_r 2K\pi\rho_l r dr \int_{\mathbf{V}} f\frac{\mathbf{v}^2}{2} d\mathbf{v} - 2\int_r c(r)\frac{4}{3}\pi\rho_l r^3 dr \int_{\mathbf{V}} f(\mathbf{u}_g - \mathbf{v})\cdot\frac{\mathbf{v}}{2} d\mathbf{v}. \end{cases} \tag{2.7}$$

Proof: The expressions of $\mathbf{M}$, $\mathbf{I}$ and, $\mathbf{E}$ are computed so as to ensure the global conservation of mass, momentum and energy between the two phases: it suffices thus to define them as the opposite of the quantities obtained by integrating the spray equation (2.12) over the variables $\mathbf{v}$ and r against $\frac{4\pi r^3\rho_l}{3}$, $\frac{4\pi r^3\rho_l}{3}\mathbf{v}$ and, $\frac{4\pi r^3\rho_l}{3}\frac{\mathbf{v}^2}{2}$ respectively:

$$\partial_t \int_{\mathbf{V}}\int_r f\phi(\mathbf{v},r) d\mathbf{v} dr + \nabla_{\mathbf{X}}\cdot\left(\int_{\mathbf{V}}\int_r f\mathbf{v}\phi(\mathbf{v},r) d\mathbf{v} dr\right) \stackrel{def}{=} -(\mathbf{M},\mathbf{I},\mathbf{E})(x,t) \tag{2.8}$$

where the function ϕ is given by

$$\phi(\mathbf{v},r) = \frac{4}{3}\pi r^3\rho_l \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{\mathbf{v}^2}{2} \end{pmatrix}. \tag{2.9}$$

A straightforward computation gives

$$\begin{aligned} &\partial_t \int_{\mathbf{V}}\int_r f\phi(\mathbf{v},r) d\mathbf{v} dr + \nabla_{\mathbf{X}}\cdot\left(\int_{\mathbf{V}}\int_r f\mathbf{v}\phi(\mathbf{v},r) d\mathbf{v} dr\right) \\ &\quad = \int_{\mathbf{V}}\int_r f\beta\nabla_{\mathbf{V}}\cdot\phi(\mathbf{v},r) d\mathbf{v} dr + \int_{\mathbf{V}}\int_r f\mathcal{R}\partial_r\phi(\mathbf{v},r) d\mathbf{v} dr. \end{aligned} \tag{2.10}$$

Integrating by parts the expressions in the right hand side of the last equation gives the expressions (2.7) and the proof is complete. □

2.2 Turbulence modeling

Let us consider now the modeling of the turbulence in the two-phase flow. The equations written above indeed allow direct simulation of the a turbulent two-phase flow. Nevertheless direct simulation requires that the mesh size is much smaller than the size of the smallest eddies. But since eddies are expected in the wake of droplets, the mesh size should be chosen much smaller than droplets radius in order to perform direct simulation of the two-phase flow. Hence, practical computations using direct simulation would only allow very few droplets and we need turbulence modeling.

The modeling of turbulence in two-phase flows is still an open problem and we expect that the presence of droplets perturbates Kolmogorov's energy cascade. Here, we will distinguish two scales for the turbulent eddies. On the one hand, in the "macroscopic scale", we consider that the eddies are big enough so that the turbulence phenomenon may be included in the description of the mean velocity of the gas. Hence, we may write here the velocity of the gas as the sum (see [7, 8]):

$$\mathbf{u}_g = \overline{\mathbf{u}_g} + \tilde{\mathbf{u}} \tag{2.11}$$

where $\overline{\mathbf{u}_g}$ is a mean velocity in the statistical sense, and $\tilde{\mathbf{u}}$ is modeled by a centered random fluctuation. The value of $\tilde{\mathbf{u}}$ depends on the "macroscopic" turbulent kinetic energy of the gas, and acts on the droplets during the turbulence correlation time τ. When $\tilde{\mathbf{u}}$ is modeled by using random values, the total impulse of the gas flow is *a priori* not preserved. Hence, here, more realistic modelings of the turbulent coupled two-phase fluid flow would be necessary. However, this is beyond the scope of this paper.

Here, and in the following, we want to concentrate on the modeling of the effect of the small eddies. At a "microscopic" scale, where we shall assume small values of the turbulent correlation time of the eddies, the effect of the small eddies on the droplets is comparable to grazing collisions. Here, following [2], we assume homogeneous isotropic turbulence in the gas phase, characterized by the microscopic specific turbulent energy $\mathcal{K}$ and the correlation time t_d. Assuming that t_d is small in comparison with the characteristic time scales of the flow, it is proved in [9, 10, 2] that the spray equation (2.2) may be replaced by the following one:

$$\partial_t f + \nabla_{\mathbf{x}} \cdot (f\mathbf{v}) + \nabla_{\mathbf{v}} \cdot (f\beta) + \partial_r (f\mathcal{R}) - \nabla_{\mathbf{v}} \cdot (D\nabla_{\mathbf{v}} f) = 0. \tag{2.12}$$

The diffusion coefficient is given by

$$D \equiv D(r, \mathcal{K}, t_d) = \frac{2}{d}\frac{\mathcal{K}}{t_d}\left[e^{-c(r)t_d} - 1 + c(r)t_d\right]. \tag{2.13}$$

where d is the dimension of the physical space. Note that when $c(r)t_d \gg 1$ (i.e. r tends to 0), we have $D \simeq 2c(r)\mathcal{K}$, whereas when $c(r)t_d \ll 1$ we have $D \simeq c^2(r)\mathcal{K}t_d$.

The gas phase equations should also be modified: first, we have to include a turbulence model that allows to estimate the macroscopic and microscopic specific turbulent energies and correlation times. Obviously the effect of the droplets should also be taken into account and much effort should be geared to the derivation of two-phase turbulence models in the future. However, this is beyond the scope of this study. For the numerical experiment we will use ad-hoc laws.

Next the production terms in the right hand side of the Navier-Stokes equations should be modified since the spray equation itself was modified: straightforward computation show that the right hand side of Eq. (2.5) are now the following:

$$\begin{cases} \mathbf{M}(\mathbf{x},t) = \displaystyle\int_r 2K\pi\rho_l r dr \int_{\mathbf{V}} f d\mathbf{v} \\ \mathbf{I}(\mathbf{x},t) = \displaystyle\int_r 2K\pi\rho_l r dr \int_{\mathbf{V}} f\mathbf{v} d\mathbf{v} - \int_r c(r)\frac{4}{3}\pi\rho_l r^3 dr \int_{\mathbf{V}} f(\mathbf{u}_g - \mathbf{v}) d\mathbf{v} \\ \mathbf{E}(\mathbf{x},t) = \displaystyle\int_r 2K\pi\rho_l r dr \int_{\mathbf{V}} f\frac{\mathbf{v}^2}{2} d\mathbf{v} - 2\int_r c(r)\frac{4}{3}\pi\rho_l r^3 dr \int_{\mathbf{V}} f(\mathbf{u}_g - \mathbf{v})\cdot\frac{\mathbf{v}}{2} d\mathbf{v} \\ \qquad\qquad\qquad - d\displaystyle\int_r D(r)\frac{4}{3}\pi\rho_l r^3 dr \int_{\mathbf{V}} f d\mathbf{v}. \end{cases} \tag{2.14}$$

Remark 2.2 The equation (2.14) gives explicitly the expression of the exchange terms between the two phases so that a complete description of the two-phase fluid flow model is available. However, we only need for the numerical implementation of the model, the Eq. (2.8) that defines the exchange terms.

2.3 The semi-fluid model

This subsection is devoted to the derivation of the semi-fluid model. As we noticed it above, for a given radius r and a given $\mathbf{x}$, the function $f : \mathbf{v} \to f(\mathbf{x},\mathbf{v},r,t)$ asymptotically tends to a Gaussian function as time t tends to $+\infty$. More precisely we prove the following

Proposition 2.3 *Let $f^0 : (\mathbf{x},\mathbf{v},r) \to f^0(\mathbf{x},\mathbf{v},r)$ be such that for any fixed $\mathbf{x}$ and r, the function $\mathbf{v} \to f^0(\mathbf{x},\mathbf{v},r)$ is gaussian. Let f denote the solution of the* uncoupled *spray equation (2.12) with initial data f_0, where we consider that the datas of the gas flow are constant and uniform. Then, for any fixed $t \geq 0$ and for any fixed $\mathbf{x}$ and r, the function $\mathbf{v} \to f(\mathbf{x},\mathbf{v},r,t)$ is a gaussian function.*

Proof of Proposition 2.3:
We first prove the following preliminary result.

Proposition 2.4
Let f_0 be given. Then, the solution f of the Fokker-Planck equation (2.12), with initial data f_0 writes:

$$f(\mathbf{x},\mathbf{v},r,t) = S_t f_0 = \frac{1}{J_r(t)}\int_{\mathbf{X}'}\int_{\mathbf{V}'} G_{R^-}(\mathbf{X}^- - \mathbf{x}', \mathbf{V}^- - \mathbf{v}', t) f_0(\mathbf{x}',\mathbf{v}',R^-) d\mathbf{x}' d\mathbf{v}' \tag{2.15}$$

where $(\mathbf{X}^-,\mathbf{V}^-,R^-)$ are the characteristics of Definition **3.5** *and Lemma* **3.6** *below. The factor $1/J_r(t)$ is the Jacobian $\dfrac{\partial(\mathbf{X}^-,\mathbf{V}^-,R^-)(t)}{\partial(\mathbf{x},\mathbf{v},r)}$ and we have*

$$G_r(\mathbf{x},\mathbf{v},t) = \frac{1}{(2\pi)^d \Delta_r^{\frac{d}{2}}(t)} exp(-(a_r(t)\mathbf{x}^2 + 2h_r(t)\mathbf{x}\cdot\mathbf{v} + b_r(t)\mathbf{v}^2)/2\Delta_r(t)).$$

where the expressions of $a_r(t)$, $b_r(t)$, $h_r(t)$ and $\Delta_r(t)$ are given in Eq. (A.2) of Appendix **A**.

Proof of 2.4: The proof is given in Appendix **A**. $\square$

Let us return to the proof of Proposition **2.3**. As stated in Property **3.7** below, the characteristics $(\mathbf{X}^-, \mathbf{V}^-)$ are linear functions of $(\mathbf{x}, \mathbf{v})$. Hence, if f^0 satisfies the assumptions of Proposition **2.3**, then, according to Eq. (2.15), for any fixed $t \geq 0$ and for any fixed $\mathbf{x}$ and r the function $\mathbf{v} \to f(\mathbf{x}, \mathbf{v}, r, t)$ writes in term of the convolution with respect to $\mathbf{v}$ of two gaussian functions of the variable $\mathbf{v}$ and is thus a gaussian function of the variable $\mathbf{v}$. This concludes the proof of Proposition **2.3**. $\square$

Now, in view of Proposition **2.3**, we make the following assumption for the *coupled* two-phase fluid flow system:

Hypothesis 2.5 (Modeling hypothesis) *Consider the solution f of Eq.(2.12) coupled to the gas flow Eqs.(2.5) with initial data f^0. We assume that at any point $(\mathbf{x}, r)$ and time t, the velocity distribution $\mathbf{v} \longrightarrow f(\mathbf{x}, \mathbf{v}, r, t)$ is gaussian.*

This hypothesis is essential from the mathematical viewpoint since it allows the derivation of the semi-fluid model below. The assumption is justified on mathematical grounds when the mean quantities that describe the gas are constant (or at least smooth) and when the small scale turbulence in the gas flow field is isotropic. In applications where the gas turbulent flow field is far from isotropy, more sophisticated semi-fluid models should be considered.

Coming back to the modeling hypothesis, one observes that a gaussian function is uniquely determined by its first three moments: indeed if $\mathbf{v} \to \Xi(\mathbf{v})$ denotes a gaussian function, Ξ is uniquely determined by the following three quantities:

$$\rho = \int_{\mathbf{V}} \Xi(\mathbf{v})\, d\mathbf{v}, \quad \rho \mathbf{u} = \int_{\mathbf{V}} \Xi(\mathbf{v}) \mathbf{v}\, d\mathbf{v}, \quad \rho e = \int_{\mathbf{V}} \Xi(\mathbf{v}) \frac{\mathbf{v}^2}{2}\, d\mathbf{v}.$$

Then, if $d = 1, 2, 3$ is the dimension of the physical space, Ξ writes in term of ρ, $\mathbf{u}$ and, e as follows:

$$\Xi(\mathbf{v}) \equiv \Xi(\mathbf{v}; \rho, \mathbf{u}, e) = \frac{\rho}{\left[\frac{4}{d}\pi\left(e - \frac{\mathbf{u}^2}{2}\right)\right]^{\frac{d}{2}}} exp\left(-\frac{(\mathbf{v}-\mathbf{u})^2}{\frac{4}{d}\left(e - \frac{\mathbf{u}^2}{2}\right)}\right). \tag{2.16}$$

Under Hypothesis **2.5**, the funtion f is thus characterized by the following three moments:

$$\begin{bmatrix} g \\ g\mathbf{u} \\ ge \end{bmatrix} (\mathbf{x}, r, t) = \begin{bmatrix} \frac{4}{3}\pi\rho_l r^3 \int_{\mathbf{V}} f(\mathbf{x}, \mathbf{v}, r, t) d\mathbf{v} \\ \frac{4}{3}\pi\rho_l r^3 \int_{\mathbf{V}} f(\mathbf{x}, \mathbf{v}, r, t) \mathbf{v} d\mathbf{v} \\ \frac{4}{3}\pi\rho_l r^3 \int_{\mathbf{V}} f(\mathbf{x}, \mathbf{v}, r, t) \frac{\mathbf{v}^2}{2} d\mathbf{v} \end{bmatrix}. \tag{2.17}$$

Here, since we introduced the factor $\frac{4}{3}\pi\rho_l r^3$ in the above expression, the quantities $(g, g\mathbf{u}, ge)$ may be interpreted as the mass, impulsion, and energy densities of the spray at the point $(\mathbf{x}, r, t)$. Note that e accounts for the kinetic energy and for the turbulent kinetic energy of the spray but is independent of the temperature of the liquid phase. To take into account the droplets temperature would require to introduce another dimension in the phase space.

We may now derive the semi-fluid model that characterizes the evolution of the quantities g, $g\mathbf{u}$ and, ge by integrating with respect to $\mathbf{v}$ the spray equation (2.12) against the three quantities $\frac{4}{3}\pi\rho_l r^3$, $\frac{4}{3}\pi\rho_l r^3\mathbf{v}$ and, $\frac{4}{3}\pi\rho_l r^3\frac{\mathbf{v}^2}{2}$. A straightforward computation gives the following result:

Lemma 2.6 (Semi-fluid model) *Consider the unknowns $(\rho_g, \rho_g\mathbf{u}_g, \rho_g e_g)$ for the gas and the unknown f for the spray solutions of the coupled equations (2.5)-(2.12). Assume moreover that Hypothesis* **2.5** *holds. Then the new unknowns for the spray $(g, \mathbf{u}, e)(\mathbf{x}, r, t)$, defined by (2.17), satisfy the following system of equations:*

$$\begin{cases} \partial_t g + \nabla_{\mathbf{x}} \cdot (g\mathbf{u}) - \partial_r \left(\frac{K}{2r}g\right) = -\frac{3K}{2r^2}g \\ \\ \partial_t(g\mathbf{u}) + \nabla_{\mathbf{x}} \cdot (g\mathbf{u}\otimes\mathbf{u}) + \nabla_{\mathbf{x}} q - \partial_r\left(\frac{K}{2r}g\mathbf{u}\right) \\ \qquad\qquad = -\frac{3K}{2r^2}g\mathbf{u} - cg(\mathbf{u}-\mathbf{u}_g) \\ \\ \partial_t(ge) + \nabla_{\mathbf{x}} \cdot (ge\mathbf{u} + q\mathbf{u}) - \partial_r\left(\frac{K}{2r}ge\right) \\ \qquad = -\frac{3K}{2r^2}ge - 2cg(e - \frac{\mathbf{u}_p\cdot\mathbf{u}_g}{2} - d\frac{D}{2c}). \end{cases} \tag{2.18}$$

Here, d is the dimension of the physical space and q is the pression-like term defined by

$$q(\mathbf{x}, r, t) = \frac{d}{2}g(e - \frac{\mathbf{u}^2}{2}). \tag{2.19}$$

Note that if we integrate the right hand side of (2.18) with respect to the variable r, we find the opposite of the exchange terms $(\mathbf{M}, \mathbf{I}, \mathbf{E})$ defined in Eq. (2.7). That is the exchange terms may be written explicitely in terms of the semi-fluid unknowns defined in (2.17). System (2.18) may thus be viewed as a description of the dispersed phase intermediate between a fluid model, where the unknowns would depend only on $(\mathbf{x}, t)$ and the kinetic representation by the pdf f. This is the reason why we call it a *semi-fluid* model.

Consider now a general spray whose density function is f. *A priori*, the function f does not satisfy Hypothesis **2.5** and we may not use directly the semi-fluid model derived above. However we shall use the following procedure which allows the use of the semi-fluid model together with the discretization of the spray unknowns: given an initial probability density function f^0, we shall approximate f^0 by a sum of functions f_k, $1 \leq k \leq N$ such that for each k, each $\mathbf{x}$ and each r, the function $\mathbf{v} \longrightarrow f_k^0(\mathbf{x}, \mathbf{v}, r)$ is gaussian. The probability density function f, solution of the spray equation (2.12) with initial data f^0 is then approximated by the sum $f \simeq \sum_{k=1}^N f_k$ where, for $1 \leq k \leq N$, the function f_k is the solution of (2.12), with initial data f_k^0. For each function f_k we may define the quantities g_k, $\mathbf{u}_k$ and, e_k which each satisfy the semi-fluid model equation (2.18).

Finally, the problem consists in computing the unknowns $(\rho_g, \mathbf{u}_g, e_g)(\mathbf{x}, t)$ solutions of Eqs. (2.5),(2.6) and $(g_p, \mathbf{u}_p, e_p)(\mathbf{x}, r, t) = \sum_{k=1}^N (g_k, \mathbf{u}_k, e_k)(\mathbf{x}, r, t)$, where each unknown $(g_k, \mathbf{u}_k, e_k)$ is solution of the *semi-fluid* system (2.18),(2.19). Moreover, the exchange terms (2.7) are rewritten in terms of $(g_k, \mathbf{u}_k, e_k)$. The initial data are $(\rho_g^0, \mathbf{u}_g^0, e_g^0)(\mathbf{x})$ and $(g_k^0, \mathbf{u}_k^0, e_k^0)(\mathbf{x}, r)$.

In the following two Sections, we write the numerical scheme for solving Eq. (2.18) for the spray then Eq. (2.5) for the gas.

3 A kinetic scheme for the spray

Let Δt denote the time-step and let $t^n = n\Delta t$ denote the time levels. During this section we assume that the gas flow is given and constant in each cell on the interval of time $[t^n, t^{n+1}[$. The mass density field, velocity field and specific total energy field of the gas phase are respestively denoted by ρ_g^n, $\mathbf{u}_g^n$ and, e_g^n.

Let us now consider the spray. We denote the initial probability density function by f^0 and, for computational purposes, we wish to approximate f^0 by gaussian velocity distribution functions. We may use different methods to perform this approximation. First, the finite volume method consists in defining a gridding of the reduced phase space $\Omega \times (\mathbb{R}_r)_+$ and, for each cell of the gridding, to approximate the restriction of f_0 to the cell by a gaussian velocity distribution function. The parameters that characterize the gaussian function are constant in each cell. This method allows for the velocity distribution to vary in function of the position $\mathbf{x}$ in the physical space or of the radius of the particles. Nevertheless the reduced phase space $\Omega \times (\mathbb{R}_r)_+$ has dimension four and the finite volume approach is very expensive and requires much degrees of freedom. (Note that if we take into account the temperature of the droplets in the kinetic model, the dimension of the reduced phase space becomes five so that this dimension is always at least equal to four.) A more efficient method to approximate real valued functions defined on space with dimension greater or equal to four is the particle approximation. Here the initial data f_0 is decomposed into the sum of a finite number of functions with a simple shape, the so called numerical particles. Many numerical particles may be considered. It turns however that, in the case of our model, the most convenient numerical particles have the following form:

$$f_k(\mathbf{x}, \mathbf{v}, r) = \frac{1}{\frac{4}{3}\pi\rho_l (r_k^n)^3} \xi(\mathbf{x}; \mathbf{x}_k, m_k) \Xi(\mathbf{v}; G_k, \mathbf{U}_k, E_k) \otimes \delta(r - r_k) \tag{3.1}$$

where we omitted the time-dependence and where $\mathbf{v} \rightarrow \Xi(\mathbf{v}; G_k, \mathbf{U}_k, E_k)$ is the gaussian function whose first three moments with respect to $\mathbf{v}$ are respectively G_k, $G_k \mathbf{U}_k$ and, $G_k 2E_k$ and where $\mathbf{x} \rightarrow \xi(\mathbf{x}; \mathbf{x}_k, m_k)$ is a gaussian function, centered in $\mathbf{x}_k$, such that $m_k = \int_{\mathbf{X}} \xi(\mathbf{x};\mathbf{x}_k, m_k)\mathbf{x}^2\, d\mathbf{x}$, and with mass unity. The numerical particles thus occupy positions around $\mathbf{x}_k$ within a range of typical size $S_k = \sqrt{m_k - (\mathbf{x}_k)^2}$. Finally δ denotes Dirac's delta function. Note that the use of a gaussian velocity distribution function is guided by the asymptotic behavior of the solutions of the spray equation (2.12) while the choice of a gaussian function for the $\mathbf{x}$ distribution of the numerical particle is important for computational purposes.

Here $f = \sum_k^N f_k$ thus represents the state of the spray. However, thanks to the Modeling Hypothesis **2.5**, the spray is equivalently defined by the moments:

$$(\rho_k, \rho_k \mathbf{u}_k, \rho_k e_k)(\mathbf{x}, r) = (G_k, G_k \mathbf{U}_k, G_k E_k)\xi(\mathbf{x};\mathbf{x}_k, m_k) \otimes \delta(r - r_k) \tag{3.2}$$

of each function f_k with respect to $\mathbf{v}$. Hence the state of the spray is then represented by the function

$$\begin{aligned}(\rho_p, \rho_p \mathbf{u}_p, \rho_p e_p)(\mathbf{x}, r) &= \sum_{k=1}^{N} (\rho_k, \rho_k \mathbf{u}_k, \rho_k e_k)(\mathbf{x}, r) \\ &= \sum_{k=1}^{N} (G_k, G_k \mathbf{U}_k, G_k E_k)\xi(\mathbf{x};\mathbf{x}_k, m_k) \otimes \delta(r - r_k)\end{aligned} \tag{3.3}$$

However, the numerical particle (3.1) or equivalently (3.2) is characterized by the six quantities:

$$(G_k, \mathbf{U}_k, E_k, \mathbf{x}_k, m_k, r_k) \tag{3.4}$$

and we shall denote a numerical particle by this vector in the sequel. The numerical particles are indexed by $1 \leq k \leq N$.

Now our problem is the following: given the state of the dispersed phase at time t_n in the form of the sum of numerical particles each represented by the vector (3.4), and given the gas flow, how to define the new state of the dispersed phase, at time t^{n+1}.

Recalling that the semi-fluid system (2.18) is linear we may treat the different numerical particles separately. Next, the semi-fluid model is derived from the kinetic equation (2.12) so that, inspiring ourselves from the ideas of Harten, Deshpande and Perthame (see [3, 4, 5]), we introduce the following kinetic scheme for *each* numerical particle $(G_k, \mathbf{U}_k, E_k, \mathbf{x}_k, m_k, r_k)(t)$:

Definition 3.1 (A kinetic scheme for the spray)
Let the datas of the gas flow at time t^n be given. Let $(G_k^n, \mathbf{U}_k^n, E_k^n, \mathbf{x}_k^n, m_k^n, r_k^n)$ denote a numerical particle at time t^n. Then we define the numerical particle $(G_k^{n+1}, \mathbf{U}_k^{n+1}, E_k^{n+1}, \mathbf{x}_k^{n+1}, m_k^{n+1}, r_k^{n+1})$ thanks to the following algorithm consisting of the following three steps:

(a) Set:

$$f_k^n(\mathbf{x}, \mathbf{v}, r) = \frac{1}{\frac{4}{3}\pi\rho_l (r_k^n)^3}\xi(\mathbf{x};\mathbf{x}_k^n, m_k^n)\Xi(\mathbf{v}; G_k^n, \mathbf{U}_k^n, E_k^n) \otimes \delta(r - r_k^n)$$

where Ξ is defined in Eq. (2.16).

(b) *Calculate the solution f_k of the Fokker-Planck equation (2.12) for $t \geq t^n$ with initial data as f_k^n:*

$$\begin{cases} \partial_t f_k + \nabla_{\mathbf{x}} \cdot (f_k \mathbf{v}) + \nabla_{\mathbf{v}} \cdot (f_k \beta) + \partial_r (f_k \mathcal{R}) - \nabla_{\mathbf{v}} \cdot (D \nabla_{\mathbf{v}} f_k) = 0 \\ f_k(\mathbf{x}, \mathbf{v}, r, t^n) = f_k^n(\mathbf{x}, \mathbf{v}, r). \end{cases}$$

where $\beta = (v - \mathbf{u}_g(\mathbf{x}_k^n, t^n))$ and $D = D(r, \mathcal{K}(\mathbf{x}_k^n, t^n), t_d(\mathbf{x}_k^n, t^n))$.

(c) *Set $(G_k^{n+1}, \mathbf{U}_k^{n+1}, 2E_k^{n+1}, \mathbf{x}_k^{n+1}, m_k^{n+1}, r_k^{n+1}) = \mathcal{P}(f_k(\Delta t))$ where $\mathcal{P}$ is a projector that preserves the first three moments as well as the center of mass, the inertial momentum, and the Sauter radius*[1]*, that is:*

$$\begin{pmatrix} G_k^{n+1} \\ G_k^{n+1} \mathbf{U}_k^{n+1} \\ G_k^{n+1} E_k^{n+1} \\ G_k^{n+1} \mathbf{x}_k^{n+1} \\ G_k^{n+1} m_k^{n+1} \\ G_k^{n+1} r_k^{n+1} \end{pmatrix} = \int_{\mathbf{X}} \int_{\mathbf{V}} \int_r \frac{4}{3} \pi \rho_l r^3 \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{\mathbf{v}^2}{2} \\ \mathbf{x} \\ \mathbf{x}^2 \\ r \end{pmatrix} f_k(\Delta t) d\mathbf{x} d\mathbf{v} dr$$

Remark 3.2 The discretization (3.3) of $(g_p, g_p \mathbf{u}_p, g_p e_p)(\mathbf{x}, r, t)$ is similar to that used in the SPH method ([11, 12]). But here, we omitted the collision term in the spray equation which is thus linear and, we may compute the numerical particles independently from one another. In other words, the spray has no inner pressure and interacts only with the gas flow field.

Remark 3.3 Note that the pdf obtained in step (b) is projected onto a gaussian velocity distribution function, mimmicking what is done in usual kinetic schemes applied to the Euler system of gas dynamics. In the gas dynamics case, relaxation to a gaussian velocity distribution function is caused by collisions between molecules and the characteristic time of this relaxation process depends from the Knudsen number: the relaxation time is very small in the case of gases at atmospheric pressure and much smaller than the time step used for numerical calculations. The projection step is thus justified on physical grounds. In the case of a spray the relaxation to a gaussian velocity distribution function is caused by the diffusion term $\nabla_{\mathbf{v}} \cdot (D \nabla_{\mathbf{v}} f)$ in the spray equation (2.12) and the characteristic time of this

[1] The Sauter radius r_S of the distribution $\phi(r)$ is the mean radius calculated with respect to the mass of the particles, that is:

$$r_S(\phi) = \frac{\displaystyle\int_r \frac{4}{3} \pi r^3 \phi(r) r dr}{\displaystyle\int_r \frac{4}{3} \pi r^3 \phi(r) dr} = \frac{\displaystyle\int_r r^4 \phi(r) dr}{\displaystyle\int_r r^3 \phi(r) dr}.$$

relaxation is quite large and may even by much larger than the time step of the numerical method. The use of the semi fluid model defined in Lemma **2.6** and of our numerical scheme is thus only justified for sprays close to "equilibrium", *i.e.*, when the velocity distribution function is close to a gaussian function.

We can now write the main result of this section:

Theorem 3.4 (Solution of the kinetic scheme)
Let $\mathcal{G}(\mathbf{x},\mathbf{v},r,t)$ be the elementary solution of Eq. (2.12) for the spray and let:

$$[\sigma_x^2, -\sigma_{xv}^2, \sigma_v^2](t;r) = \int_{\mathbf{X}}\int_{\mathbf{V}} [\mathbf{x}^2, \mathbf{x}\cdot\mathbf{v}, \mathbf{v}^2]\mathcal{G}(\mathbf{x},\mathbf{v},r,t)d\mathbf{x}d\mathbf{v}$$

be the second order moments of $\mathcal{G}$. Then, applying the kinetic scheme to the numerical particle $(G_k^n, G_k^n\mathbf{U}_k^n, G_k^nE_k^n, \mathbf{x}_k^n, m_k^n, r_k^n)$ at time t^n, we have the expression of the numerical particle at time $t > t^n$:

$$\left\{\begin{aligned}
&G_k(t) = G_k^n\gamma^3(t-t^n;r_k^n)\\
&(G_k\mathbf{U}_k)(t) = G_k^n\gamma^3(t-t^n;r_k^n)\mathbf{V}(t;\mathbf{U}_k^n,r_k^n,t^n)\\
&(G_kE_k) = G_k^n\gamma^3(t-t^n;r_k^n)\times\\
&\qquad\qquad\times\left[\frac{\mathbf{V}^2(t;\mathbf{U}_k^n,r_k^n,t^n)}{2} + \eta_1^2(t-t^n;r_k^n)\left(\epsilon_k^n + \frac{\sigma_v^2(t-t^n;r_k^n)}{2}\right)\right]\\
&\mathbf{x}_k(t) = \mathbf{X}(t;\mathbf{x}_k^n,\mathbf{U}_k^n,r_k^n,t^n)\\
&m_k(t) = \mathbf{X}^2(t;\mathbf{x}_k^n,\mathbf{U}_k^n,r_k^n,t^n) + (S_k^n)^2 + \alpha_1^2(t-t^n;r_k^n)2\epsilon_k^n +\\
&\; + \sigma_x^2(t-t^n;r_k^n) - 2\alpha_1(t-t^n;r_k^n)\sigma_{xv}^2(t-t^n;r_k^n) + \alpha_1^2(t-t^n;r_k^n)\sigma_v^2(t-t^n,r_k^n)\\
&r_k(t) = R(t;r_k^n,t^n) = \gamma(t-t^n;r_k^n)r_k^n.
\end{aligned}\right. \tag{3.5}$$

Here, $(\mathbf{X},\mathbf{V},R)$ are the characteristics introduced in Definition **3.5** *below with $\mathbf{u}_g = \mathbf{u}_g(\mathbf{x}_k^n,t^n)$. The functions $t\to\gamma(t-t^n;r_k^n)$, $t\to\alpha_1(t-t^n;r_k^n)$ and, $t\to\eta_1(t-t^n;r_k^n)$ are the coefficients of the characteristics defined in Eq. (3.9), and we have set:*

$$\begin{aligned}
\epsilon_k^n &= E_k^n - \frac{(\mathbf{U}_k^n)^2}{2}\\
(S_k^n)^2 &= m_k^n - (\mathbf{x}_k^n)^2
\end{aligned} \tag{3.6}$$

where d is the dimension of the physical space. Finally, the second order moments of $\mathcal{G}$ are explicitly written in terms of the coefficients of $\mathcal{G}$ (see Eq. (A.2) of Appendix **A***):*

$$\left\{\begin{aligned}
&\sigma_v^2(t-t^n;r_k^n) = da_{r_k^n}(t-t^n)\\
&-\sigma_{xv}^2(t-t^n;r_k^n) = -dh_{r_k^n}(t-t^n)\\
&\sigma_x^2(t-t^n;r_k^n) = db_{r_k^n}(t-t^n)
\end{aligned}\right. \tag{3.7}$$

where d is the dimension of the physical space.

To prove theorem **3.4** we first define the characteristics associated with the spray equation (2.12), without the diffusion terms modeling the effects of the gas turbulence:

Definition 3.5 (Characteristics)
The characteristics $(\mathbf{X},\mathbf{V},R)(t;\mathbf{x},\mathbf{v},r,s)$ *are defined as the solution of the following system of ordinary differential equations:*

$$\begin{cases} \dfrac{d\mathbf{X}}{dt} = \mathbf{V} \\ \dfrac{d\mathbf{V}}{dt} = -c(t)(\mathbf{V}-\mathbf{u}_g) = -\dfrac{\mathcal{C}}{R^2}(\mathbf{V}-\mathbf{u}_g) \\ \dfrac{dR}{dt} = -\dfrac{K}{2R} \end{cases} \qquad \begin{cases} \mathbf{X}(s;\mathbf{x},\mathbf{v},r,s) = \mathbf{x} \\ \mathbf{V}(s;\mathbf{x},\mathbf{v},r,s) = \mathbf{v} \\ R(s;\mathbf{x},\mathbf{v},r,s) = r \end{cases} \tag{3.8}$$

Note that when $t > s$, the characteristics are the solution of a Cauchy problem with initial data, whereas when $t < s$, the characteristics are the solution of a Cauchy problem with final data. Furthermore the function $t \longrightarrow (\mathbf{X},\mathbf{V},R)(t;\mathbf{x},\mathbf{v},r,0)$ is the trajectory of a single particule, initially located at the position $(\mathbf{x},\mathbf{v},r)$ in the phase space. For the sake of simplicity, we denote in the sequel $(\mathbf{X}^+,\mathbf{V}^+,R^+)(t) = (\mathbf{X},\mathbf{V},R)(t;\mathbf{x},\mathbf{v},r,0)$ the *direct* characteristics, and $(\mathbf{X}^-,\mathbf{V}^-,R^-)(t) = (\mathbf{X},\mathbf{V},R)(0;\mathbf{x},\mathbf{v},r,t)$ the *reverse* characteristics. These functions may be computed explicitly:

Lemma 3.6 (Expression of the characteristics)
Let be given $\mathbf{u}_g$*, a constant velocity field. The characteristics, solution of the system of ODEs (3.8) write:*

$$\begin{cases} \mathbf{X}(t;\mathbf{x},\mathbf{v},r,s) = \mathbf{x} + \dfrac{r^2}{\mathcal{C}+K}(1-\gamma^{2+\frac{2\mathcal{C}}{K}}(t-s;r))\mathbf{v} \\ \qquad\qquad + \dfrac{\mathcal{C}}{\mathcal{C}+K}\left[t - \dfrac{r^2}{\mathcal{C}+K}(1-\gamma^{2+\frac{2\mathcal{C}}{K}}(t-s;r))\right]\mathbf{u}_g \\ \mathbf{V}(t;\mathbf{x},\mathbf{v},r,s) \equiv \mathbf{V}(t;\mathbf{v},r,s) = \gamma^{\frac{2\mathcal{C}}{K}}(t-s;r)\mathbf{v} + \dfrac{\mathcal{C}}{\mathcal{C}+K}\left[1-\gamma^{\frac{2\mathcal{C}}{K}}(t-s;r)\right]\mathbf{u}_g \\ R(t;\mathbf{x},\mathbf{v},r,s) \equiv R(t;r,s) = \sqrt{(r^2-K(t-s))^+} = \gamma(t-s;r)r \end{cases}$$

where we have set $x^+ = max(x,0)$ *and* $\gamma(t-s;r) = R(t;r,s)/r$.

Proof: It suffices to integrate successively R, $\mathbf{V}$ and $\mathbf{X}$ in the ODEs (3.8). Each integration involves only one unknown. □

We shall write in the sequel the following expressions of the three functions $\mathbf{X}$, $\mathbf{V}$ and, R:

$$\begin{cases} \mathbf{X}(t;\mathbf{x},\mathbf{v},r,s) = \mathbf{x} + \alpha_1(t-s;r)\mathbf{v} + \alpha_2(t-s;r) \\ \mathbf{V}(t;\mathbf{v},r,s) = \eta_1(t-s;r)\mathbf{v} + \eta_2(t-s;r) \\ R(t;r,s) = \gamma(t-s;r)r. \end{cases} \tag{3.9}$$

with obvious notations for α_i, η_i and γ. One must remark here:

Property 3.7 *The characteristics* $(\mathbf{X}, \mathbf{V})(t; \mathbf{x}, \mathbf{v}, r, s)$ *are linear functions of the initial position* $(\mathbf{x}, \mathbf{v})$.

Let now $\mathbf{M}(\mathbf{x}, \mathbf{v}, r)$ and $f(\mathbf{x}, \mathbf{v}, r, t)$ be any functions and define the moments of f against $\mathbf{M}$ at time t as $\mathcal{M}f(t) = \int_{\mathbf{X}} \int_{\mathbf{V}} \int_r \mathbf{M} f d\mathbf{x} d\mathbf{v} dr$. When $f = S_t f_0$ is the solution of the kinetic equation (2.12) with initial data f_0, a simple corollary of Proposition **2.4** is the following:

Corollary 3.8 (Moments) *Given a function* $(\mathbf{x}, \mathbf{v}, r) \longrightarrow \mathbf{M}(\mathbf{x}, \mathbf{v}, r)$, *the moments at time* t *of* $S_t f_0$ *against* $\mathbf{M}$ *write as follows:*

$$
\begin{aligned}
(\mathcal{M} S_t f_0)(t) = \int_{\mathbf{X}'} \int_{\mathbf{V}'} d\mathbf{x}' d\mathbf{v}' \int_{\mathbf{X}} \int_{\mathbf{V}} \int_r f_0(\mathbf{x}', \mathbf{v}', r) G_r(\mathbf{x}, \mathbf{v}, t) \times \\
\times \mathbf{M}(\mathbf{X}(t; \mathbf{x}+\mathbf{x}', \mathbf{v}+\mathbf{v}', r, 0), \mathbf{V}(t; \mathbf{v}+\mathbf{v}', r, 0), R(t; r, 0)) d\mathbf{x} d\mathbf{v} dr.
\end{aligned}
\tag{3.10}
$$

We are now ready to prove Theorem **3.4**:

Proof of Theorem 3.4 (Solution of the kinetic scheme):
Consider the following numerical particle:

$$
f_k^n(\mathbf{x}, \mathbf{v}, r) = \frac{1}{\frac{4}{3}\pi \rho_l (r_k^n)^3} \xi(\mathbf{x}; \mathbf{x}_k^n, m_k^n) \Xi(\mathbf{v}; G_k^n, \mathbf{U}_k^n, E_k^n) \otimes \delta(r - r_k^n) \tag{3.11}
$$

Then, define $\mathbf{M} = (M_j)_{j=1,5} \in \mathbb{R}^5$ as the vector $\mathbf{M} = \frac{4}{3}\pi\rho_l r^3 (1, \mathbf{v}, \frac{\mathbf{v}^2}{2}, \mathbf{x}, \mathbf{x}^2, r)$ and let $\mathcal{M}$ denote the operator defined in Eq. (3.10). From the Definition **3.1** of the kinetic scheme, it is now clear that the kinetic scheme for the spray writes in terms of S_t and $\mathcal{M}$ as follows:

$$
(G_k^{n+1}, G_k^{n+1}\mathbf{U}_k^{n+1}, G_k^{n+1}E_k^{n+1}, G_k^{n+1}\mathbf{x}_k^{n+1}, G_k^{n+1}m_k^{n+1}, G_k^{n+1}r_k^{n+1}) = \mathcal{M} S_{\Delta t} f_k^n
$$

and we know, thanks to Corollary **3.8** and the expression (3.11) of f_k^n, that we have

$$
\begin{aligned}
\mathcal{M} S_{\Delta t} f_k^n = &\frac{1}{\frac{4}{3}\pi\rho_l (r_k^n)^3} \times \\
&\times \int_{\mathbf{V}'} \int_{\mathbf{X}'} \xi(\mathbf{x}'; \mathbf{x}_k^n, m_k^n) \Xi(\mathbf{v}'; G_k^n, \mathbf{U}_k^n, E_k^n) d\mathbf{x}' d\mathbf{v}' \int_{\mathbf{X}} \int_{\mathbf{V}} \mathcal{G}_{r_k^n}(\mathbf{x}, \mathbf{v}, \Delta t) \times \\
\times \mathbf{M}(\mathbf{X}(t^{n+1}; \mathbf{x}+\mathbf{x}', \mathbf{v}+\mathbf{v}', r_k^n, t^n), &\mathbf{V}(t^{n+1}; \mathbf{v}+\mathbf{v}', r_k^n, t^n), R(t^{n+1}; r_k^n, t^n)) d\mathbf{x} d\mathbf{v}.
\end{aligned}
$$

We have thus to compute five moments to get the expressions in Theorem **3.4**. We only compute the expression of the fifth moment $(G_k^{n+1} m_k^{n+1})$, corresponding to $M_5(\mathbf{x}, \mathbf{v}, r) = \frac{4}{3}\pi\rho_l r^3 \mathbf{x}^2$, the computation of the four other moments being analogous:

$$(G_k^{n+1}m_k^{n+1}) = \left(\frac{R(t^{n+1};r_k^n,t^n)}{r_k^n}\right)^3 \int_{\mathbf{X}'}\int_{\mathbf{V}'} \xi(\mathbf{x}';\mathbf{x}_k^n,m_k^n)\Xi(\mathbf{v}';G_k^n,\mathbf{U}_k^n,E_k^n)d\mathbf{x}'d\mathbf{v}'$$
$$\times \int_{\mathbf{X}}\int_{\mathbf{V}} \mathcal{G}_{r_k^n}(\mathbf{x},\mathbf{v},\Delta t)\mathbf{X}^2(t^{n+1};\mathbf{x}+\mathbf{x}',\mathbf{v}+\mathbf{v}',r_k^n,t^n)d\mathbf{x}d\mathbf{v}. \tag{3.12}$$

Following Eq. (3.9), we shall write $\frac{R(t^{n+1};r_k^n,t^n)}{r_k^n} = \gamma(t^{n+1};r_k^n,t^n)$ in the sequel. Next, from Eq. (3.9), we know that the characteristic $\mathbf{X}$ writes in the form $\mathbf{X}(t;\mathbf{x}+\mathbf{x}',\mathbf{v}+\mathbf{v}',r_k^n,t^n) = \mathbf{x}+\mathbf{x}'+\alpha_1(t;r,t^n)(\mathbf{v}+\mathbf{v}')+\alpha_2(t;r,t^n)$, so that we may write in Eq. (3.12):

$$\mathbf{X}^2(t^{n+1};\mathbf{x}+\mathbf{x}',\mathbf{v}+\mathbf{v}',r_k^n,t^n) = (\mathbf{x}'+\alpha_1\mathbf{v}'+\alpha_2)^2 + (\mathbf{x}^2+2\alpha_1\mathbf{x}\cdot\mathbf{v}+\alpha_1^2\mathbf{v}^2)$$
$$+ (\mathbf{x}'+\alpha_1\mathbf{v}'+\alpha_2)(\mathbf{x}+\alpha_1\mathbf{v}). \tag{3.13}$$

where we noted $\alpha_i \equiv \alpha_i(t^{n+1}-t^n;r_k^n)$. Then, we integrate the last expression against $\int_{\mathbf{X}}\int_{\mathbf{V}} Gd\mathbf{x}d\mathbf{v}$: first, the contribution of the last term is zero since the function $(\mathbf{x},\mathbf{v}) \to \mathcal{G}_{r_k^n}(\mathbf{x},\mathbf{v})$ is centered in $\mathbf{x}$ and $\mathbf{v}$. The contribution of the second term writes exactly in terms of the second moments of $\mathcal{G}$: $\sigma_x^2 - 2\alpha_1\sigma_{xv}^2 + \alpha_1^2\sigma_v^2$. Because $\mathcal{G}$ is gaussian in $(\mathbf{x},\mathbf{v})$, straightforward calculations allow us to rewrite the second moments of $\mathcal{G}$ as stated in (3.7). Finally, the contribution of the first term of (3.13) in the second integral is the first term itself since G has mass unity. Then, rewrite the first term of (3.13) as follows:

$$(\mathbf{x}'+\alpha_1\mathbf{v}'+\alpha_2)^2 = (\mathbf{x}_k^n+\alpha_1\mathbf{U}_k^n+\alpha_2)^2 + \left[(\mathbf{x}'-\mathbf{x}_k^n)^2+\alpha_1^2(\mathbf{v}'-\mathbf{U}_k^n)^2\right]$$
$$+ 2\alpha_1(\mathbf{x}'-\mathbf{x}_k^n)(\mathbf{v}'-\mathbf{U}_k^n) + 2(\mathbf{x}_k^n+\alpha_1\mathbf{U}_k^n+\alpha_2)\left[(\mathbf{x}'-\mathbf{x}_k^n)+\alpha_1(\mathbf{v}'-\mathbf{U}_k^n)\right] \tag{3.14}$$

and calculate its contribution in Eq. (3.12). Here, we know that:

$$\begin{array}{c}\int_{\mathbf{X}'}\int_{\mathbf{V}'} \xi(\mathbf{x}';\mathbf{x}_k^n,m_k^n)\Xi(\mathbf{v}';G_k^n,\mathbf{U}_k^n,E_k^n)[1,\mathbf{v}',\frac{\mathbf{v}'^2}{2},\mathbf{x}',\mathbf{x}^{2'},\mathbf{x}'\cdot\mathbf{v}']d\mathbf{x}d\mathbf{v} \\ [G_k^n,\mathbf{U}_k^n,E_k^n,\mathbf{x}_k^n,m_k^n,\mathbf{x}_k^n\cdot\mathbf{v}_k^n]\end{array} \tag{3.15}$$

so that the contribution of the last two terms of (3.14) in Eq. (3.12) is zero. The first term is independent of $(\mathbf{x}',\mathbf{v}')$ and is exactly $\mathbf{X}^2(t^{n+1};\mathbf{x}_k^n,\mathbf{U}_k^n,r_k^n,t^n)$, so that its contribution is $G_k^n\mathbf{X}^2(t^{n+1};\mathbf{x}_k^n,\mathbf{U}_k^n,r_k^n,t^n)$. Finally, thanks to the definition of S_k^n and ϵ_k^n given in Theorem **3.4**, the contribution of the terms of Eq. (3.14) is $G_k^n(\mathbf{X}^2(t^{n+1};\mathbf{x}_k^n,\mathbf{U}_k^n,r_k^n,t^n)+(S_k^n)^2+\alpha_1^2 2\epsilon_k^n)$.

Summing the contributions of (3.13)and (3.14) in (3.12) gives finally the expression of $(G_km_k)(t)$, that is the result (3.5) stated in Theorem **3.4**. This concludes the proof of Theorem **3.4**. □

We have the corollary:

Corollary 3.9
The nonconservative unknowns $(G_k^{n+1},\mathbf{U}_k^{n+1},E_k^{n+1},\mathbf{x}_k^{n+1},r_k^{n+1})$ *are the solutions at*

time t^{n+1} of the following system of ODEs:

$$\left\{\begin{aligned} \frac{dG_k}{dt} &= -2\pi K r_k \\ \frac{d\mathbf{U}_k}{dt} &= -c_k(\mathbf{U}_k - (\mathbf{u}_g)_k^n) \\ \frac{d\epsilon_k}{dt} &= -2c_k\left(\epsilon_k - d\frac{D_k}{2c_k}\right) \\ \frac{d\mathbf{x}_k}{dt} &= \mathbf{U}_k \\ \frac{dr_k}{dt} &= -\frac{K}{2r_k} \end{aligned}\right. \qquad \left\{\begin{aligned} G_k(t^n) &= G_k^n \\ \mathbf{U}_k(t^n) &= \mathbf{U}_k^n \\ \epsilon_k(t^n) &= \epsilon_k^n \\ \mathbf{x}_k(t^n) &= \mathbf{x}_k^n \\ r_k(t^n) &= r_k^n \end{aligned}\right. \tag{3.16}$$

where we noted $\eta_1 = \eta_1(t - t^n; r_k^n)$, where $c_k = c(r_k(t))$ is the drag force coefficient defined in (2.4) and $D_k = D(r_k(t), \mathcal{K}(\mathbf{x}_k^n, t^n), t_d(\mathbf{x}_k^n, t^n))$ is the diffusion coefficient of Eq. (2.12) defined in (2.13). Finally we have written the gas velocity $(\mathbf{u}_g)_k^n = \mathbf{u}_g(\mathbf{x}_k^n, t^n)$.

Proof of Corollary 3.9: According to theorem **3.4**, the quantities G_k^{n+1}, $\mathbf{U}_k^{n+1}$, ϵ_k^{n+1}, $\mathbf{x}_k^{n+1}$ and r_k^{n+1} are respectively obtained as the values of the following functions at time $t = t^{n+1}$:

$$\left\{\begin{aligned} & G_k(t) = \frac{4}{3}\pi\rho_l r_k^3(t) \\ & \mathbf{U}_k(t) = \mathbf{V}(t; \mathbf{U}_k^n, r_k^n, t^n) \\ & \epsilon_k(t) = \eta_1^2(t; r_k^n, t^n)\left(\epsilon_k^n + \frac{\sigma_v^2(t; r_k^n, t^n)}{2}\right) \\ & \mathbf{x}_k(t) = \mathbf{X}(t; \mathbf{x}_k^n, \mathbf{U}_k^n, r_k^n, t^n) \\ & r_k(t) = R(t; r_k^n, t_n) \end{aligned}\right. \tag{3.17}$$

Derivating the above expressions with respect to t shows that the functions G_k, $\mathbf{U}_k$, $\mathbf{x}_k$ and, r_k satisfy the differential equations given in Corollary **3.9**. The initial data proposed in this lemma are of course correct and the differential equations for $G_k(t)$, $\mathbf{U}_k(t)$, $\mathbf{x}_k(t)$ and $r_k(t)$ are obtained from straightforward computations. Let us now consider the kinetic energy. We compute:

$$\frac{d\epsilon_k}{dt} = 2\frac{(d\eta_1/dt)}{\eta_1}\epsilon_k(t) + \eta_1^2\frac{d\sigma_v^2}{dt}.$$

But we know that $\sigma_v^2(t) = da_{r_k^n}(t - t^n) = d\int_{t^n}^t D_k(s)/\eta_1^2(s)ds$ so that $(d\sigma_v^2/dt) = dD_k(t)/\eta_1^2(t)$. Now, from the definition of $\eta_1 = \partial_v\mathbf{V}(t; \mathbf{v})$ and the regularity of the characteristic $\mathbf{V}$ with respect to t and $\mathbf{v}$, we may write: $\frac{d\eta_1}{dt} = \partial_t(\partial_v\mathbf{V}(t; \mathbf{v})) =$

$\partial_v(\partial_t \mathbf{V}(t;\mathbf{v}))$. This gives, thanks to the Definition **3.5** of the characteristics, $\frac{d\eta_1}{dt} = \partial_v[-c_k(t)(\mathbf{V}(t;\mathbf{v}) - (\mathbf{u}_g)_k^n)] = -c_k(t)\eta_1$ because c_k is independent of $\mathbf{v}$. This allows us to rewrite $\frac{d\epsilon_k}{dt}$ as in Corollary **3.9**. This concludes the proof of Corollary **3.9**. $\square$

Note that the expressions of the unknowns $(\mathbf{x}_k(t), \mathbf{U}_k(t), r_k(t))$ are the characteristics introduced in Definition **3.5**. This means that the position, velocity and radius of a *numerical* particle behaves like a *physical* particle. The same result would be obtained with more general numerical particles. Here, it suffices that the velocity distribution Ξ appearing in the kinetic scheme be a centered distribution in each direction of the velocity space. Hence, this study gives more insight in the commonly made assumption that the numerical particles follow the physical trajectories. Moreover, the equations (3.16) for $\mathbf{U}_k(t)$ and $\epsilon_k(t)$ show that the mean velocity and the specific internal kinetic energy of the numerical particle are equivalent to $\mathbf{u}_g$ and $d\frac{D}{2c}$ respectively when t becomes large. This result is consistent with the semi-fluid system (2.18) for the spray. Note also that when $K = 0$, the limit $d\frac{D}{2c}$ of $\epsilon_k(t)$ as t tends to infinity is a constant. This corresponds to a "thermalisation" of the cloud of particles.

Remark 3.10 Notice that the value $d\frac{D}{2c(r)}$ is always less than the (microscopic) turbulent kinetic energy of the gas. Indeed, the diffusion term D accounts for the dispersion of particles. On the one hand, when $c(r)t_d \gg 1$, that is when the droplets may be considered as passive scalars, we find $d\frac{D}{2c(r)} = \mathcal{K}$ which is normal. On the other hand, when $c(r)t_d \ll 1$, we have $d\frac{D}{2c(r)} = \frac{c(r)t_d}{2}\mathcal{K}$, which means that only a ratio of the turbulent kinetic energy of the gas participates to the dispersion of the droplets.

Finally, when the radius r tends to 0, this constant is exactly the turbulent internal specific energy $\mathcal{K}(\mathbf{x}_k^n, t^n)$ of the small eddies of the gas. This is normal since in the limit as r tends to 0, the droplets become passive particle following the motion of the gas.

***Remark 3.11** Theorem **3.4** and Corollary **3.9** are available in both the laminar and turbulent cases, as well as in the burning and non-burning cases. In the laminar case, the expressions are simply rewritten with $D = 0$. In the case of non-burning droplets, that is in the limit where K tends to zero, we simply write $K = 0$, $\gamma(t; r_k^n, s) = 1$, $\eta_1(t; r_k^n, s) = e^{-c(t-s)}$ and $\alpha_1(t; r_k^n, s) = \frac{1-e^{-c(t-s)}}{c}$ in all the expressions. Hence, in the case of non burning droplets, that is when $K = 0$, the characteristics are simply given by the following expressions:

$$\begin{cases} \mathbf{X}(t;\mathbf{x},\mathbf{v},r,s) = \mathbf{x} + \dfrac{1-e^{-c(t-s)}}{c}\mathbf{v} + \left((t-s) - \dfrac{1-e^{-c(t-s)}}{c}\right)\mathbf{u}_g \\ \mathbf{V}(t;\mathbf{v},r,s) = e^{-c(t-s)}\mathbf{v} + (1-e^{-c(t-s)})\mathbf{u}_g \\ R(t;r,s) = r \end{cases} \tag{3.18}$$

4 A finite volume scheme for the gas unknowns.

4.1 The gas scheme

This subsection is devoted to the construction of a numerical scheme for approximating the quantities relative to the gas flow. The scheme below is written in two space dimensions but may easily be extended to the three dimensional case. We choose a finite volume method for approximating the solution of the Navier-Stokes equations (2.5) which write in the following condensed form:

$$\partial_t W + [\partial_x F(W) + \partial_y G(W)] + [\partial_x P(W, \nabla W) + \partial_y Q(W, \nabla W)] = Z. \tag{4.1}$$

Here, writing $\mathbf{u}_g = (u, v)$, we have set:

$$\begin{aligned}
&W = (\rho, \rho u, \rho v, \rho e)^T \\
&F(W) = (\rho u, \rho u^2 + p, \rho uv, (\rho e + p)u) \\
&G(W) = (\rho v, \rho uv, \rho v^2 + p, (\rho e + p)v) \\
&P(W, \nabla W) = (0, \mu_g 2\partial_x u + \lambda(\partial_x u + \partial_y v), \mu_g(\partial_x v + \partial_y u), \\
&\qquad [\mu_g 2\partial_x u + \lambda(\partial_x u + \partial_y v)]u + [\mu_g(\partial_x v + \partial_y u)]v + \kappa\partial_x \epsilon) \\
&Q(W, \nabla W) = (0, \mu_g(\partial_x v + \partial_y u), \mu_g 2\partial_x v + \lambda(\partial_x u + \partial_y v), \\
&\qquad [\mu_g(\partial_x v + \partial_y u)]u + [\mu_g 2\partial_y v + \lambda(\partial_x u + \partial_y v)]v + \kappa\partial_y \epsilon) \\
&Z = (\mathbf{M}, \mathbf{I}, \mathbf{E})
\end{aligned}$$

Note that we have omitted the subscript g in the above expressions. The quantity p is the gas pressure, given by $p = (\gamma - 1)\rho(e - \frac{1}{2}(u^2 + v^2))$ while F and G denote the convection fluxes of Eq. (2.5) and, P and Q are the viscous fluxes.
Now, let be given a mesh whose cells are denoted by $\mathcal{C}_i$, $1 \leq i \leq I$. These cells are quadrangles or triangles. In the cell-center approach, one considers the quantity $W_i(t)$, defined as the mean value of W over the cell $\mathcal{C}_i$:

$$W_i(t) = \frac{1}{|\mathcal{C}_i|} \int_{\mathcal{C}_i} W(\mathbf{x}, t) d\mathbf{x}$$

where $|\mathcal{C}_i|$ denotes the surface of the cell $\mathcal{C}_i$. The numerical scheme is aimed at defining an approximation of quantities $W_i(t^n)$, $1 \leq i \leq I$, $n \geq 0$. Of course the quantities $W_i(t^0)$ are given in function of the initial data. In order to write the numerical scheme assume first that an exact smooth solution W of (4.1) is known. Then, integrate Eq. (4.1) over $\mathcal{C}_i$:

$$\frac{d}{dt} W_i + \frac{1}{|\mathcal{C}_i|} \int_{\partial \mathcal{C}_i} \left([F(W) n_x + G(W) n_y] + [P(W, \nabla W) n_x + Q(W, \nabla W) n_y] \right) ds = \Omega_i \tag{4.2}$$

where $\partial\mathcal{C}_i$ is the boudary of $\mathcal{C}_i$, $\mathbf{n} = (n_x, n_y)^T$ is the outward unit normal to $\mathcal{C}_i$ on $\partial\mathcal{C}_i$, s is the arc-length abcissa on $\partial\mathcal{C}_i$ and where we have set

$$\Omega_i(t) = \frac{1}{|\mathcal{C}_i|}\int_{\mathcal{C}_i}\Omega(\mathbf{x},t)d\mathbf{x}$$

Considering next the cells $\mathcal{C}_j$, neighbouring $\mathcal{C}_i$, Eq. (4.2) may be rewritten as follows:

$$\frac{d}{dt}W_i + \sum_{i\neq j}\frac{1}{|\mathcal{C}_i|}\int_{\partial\mathcal{C}_i\cap\partial\mathcal{C}_j}\mathcal{F}ds + \sum_{i\neq j}\frac{1}{|\mathcal{C}_i|}\int_{\partial\mathcal{C}_i\cap\partial\mathcal{C}_j}\mathcal{P}ds = \Omega_i$$

where $\mathcal{F} = [F, G]$ and $\mathcal{P} = [P, Q]$. Finally, assume that $\mathcal{F}_{ij}$ (resp. $\mathcal{P}_{ij}$) is a numerical approximation of the flux $\mathcal{F}$ (resp. $\mathcal{P}$) on the interface $\partial\mathcal{C}_i \cap \partial\mathcal{C}_j$. Let L_{ij} and $\mathbf{n}_{ij}$ be respectively the length of the interface $\partial\mathcal{C}_i \cap \partial\mathcal{C}_j$ and the outward unit normal to $\mathcal{C}_i$ on the interface. Then, we may write the following semi-discrete numerical scheme:

$$\frac{d}{dt}W_i + \sum_{i\neq j}\mathcal{F}_{ij}\cdot\mathbf{n}_{ij}\frac{L_{ij}}{|\mathcal{C}_i|} + \sum_{i\neq j}\mathcal{P}_{ij}\cdot\mathbf{n}_{ij}\frac{L_{ij}}{|\mathcal{C}_i|} = \Omega_i$$

Now, let W_i^n (respectively $\mathcal{F}_{ij}^n$, $\mathcal{P}_{ij}^n$, and Ω_i^n) denote the approximate value of $W_i(t^n)$ (respectively $\mathcal{F}_i(t^n)$, $\mathcal{P}_i(t^n)$, and $\Omega_i(t^n)$), where $t^n = n\Delta t$. A first order numerical scheme for the unknowns $(W_i)_{i=1,I}$ is the following:

$$\frac{W_i^{n+1} - W_i^n}{\Delta t} + \sum_{i\neq j}\Phi_{ij}^n\frac{L_{ij}}{|\mathcal{C}_i|} + \sum_{i\neq j}\Psi_{ij}^{n+1}\frac{L_{ij}}{|\mathcal{C}_i|} = \Omega_i^n. \tag{4.3}$$

where we noted $\Phi_{ij}^n = \mathcal{F}_{ij}^n\cdot\mathbf{n}_{ij}$ and $\Psi_{ij}^{n+1} = \mathcal{P}_{ij}(W_i^n, \nabla W_i^{n+1})\cdot\mathbf{n}_{ij}$. We expect this scheme to be stable under the following CFL condition (note that the diffusion terms are treated implicitly so that no stability condition is associated with these terms):

$$\Delta t \leq \Delta T_{\mathrm{CFL}} \tag{4.4}$$

where ΔT_{CFL} will be defined later. The end of the section is devoted to the derivation of the approximate fluxes $\mathcal{F}_{ij}^n$ and $\mathcal{P}_{ij}^n$.

Consider first the convection fluxes $\Phi_{ij}^n = \mathcal{F}_{ij}^n\cdot\mathbf{n}_{ij}$. A convenient approximation of this flux is provided by the solution of a one-dimensional Riemann problem in the direction normal to the interface whose left and right states are respectively W_i^n and W_j^n. Further, an approximate Riemann solver may be used. In other words, if $W_{ij}(t > t^n)$ is the value of the *exact solution of the Riemann problem* on the interface, we set $\mathcal{F}_{ij}^n = \mathcal{F}(W_{ij})$ which also defines Φ_{ij}^n. We call this process a *Riemann solver* and denote it in the following condensed way: $\Phi_{ij}^n = \Phi(W_i^n, \mathbf{n}_{ij}, W_j^n)$.

We are thus left with the problem of computing $\Phi(W_i^n, \mathbf{n}_{ij}, W_j^n)$. Thanks to the Galilean invariance of Eq. (4.1), we may deduce this quantity from the solution of a Riemann problem in a fixed direction, e.g. the horizontal direction: let indeed $\mathbf{n}_{ij}$ be given, and let θ be the oriented angle $\theta = (\mathbf{n}_{ij}, \mathbf{e}_x)$ such that $\mathbf{n}_{ij}$ transforms to $\mathbf{e}_x$ in the rotation of angle θ. Now, let R_{ij}^θ denote the following transformation, that preserves the scalar quantities and rotates the velocity vectors:

$$R_{ij}^{\theta} W = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & cos(\theta) & -sin(\theta) & 0 \\ 0 & sin(\theta) & cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} W.$$

Then, since Eq. (4.1) is invariant under a Galilean transformation, we have:

$$\Phi(W_i^n, \mathbf{n}_{ij}, W_j^n) = R_{ij}^{-\theta} \Phi(R_{ij}^{\theta} W_i^n, \mathbf{e}_x, R_{ij}^{\theta} W_j^n). \tag{4.5}$$

We deduce that instead of solving the Riemann problem for system (4.1), we may consider the solution of the Riemann problem for the unknown: $\tilde{W} = R_{ij} W = (\rho, \rho U, \rho V, \rho e)$, which obeys the following hyperbolic system:

$$\partial_t \tilde{W} + \partial_x (\tilde{\mathcal{F}}(\tilde{W})) = 0,$$

where $\tilde{\mathcal{F}}(\tilde{W}) = (\rho U, \rho U^2 + p, \rho UV, (\rho e + p)U)$, and $p = (\gamma - 1)\rho(e - \frac{1}{2}(U^2 + V^2))$. Solving this equation, the original unknown W is recovered by writing $W = R_{ij}^{-\theta} \tilde{W}$ so that we have finally:

$$\Phi_{ij}^n \stackrel{def}{=} \Phi(W_i^n, \mathbf{n}_{ij}, W_j^n) = R_{ij}^{-\theta} \Phi(R_{ij}^{\theta} W_i^n, \mathbf{e}_x, R_{ij}^{\theta} W_j^n)$$

and we are left to write an approximate Riemann solver in the usual horizontal direction.

The approximate Riemann solver that we choose is Roe's solver:

$$\Phi(W_L, \mathbf{e}_x, W_R) \simeq \Phi_{Roe}(W_L, W_R),$$

where

$$\Phi_{Roe}(W_L, W_R) = \frac{\tilde{\mathcal{F}}(W_L) + \tilde{\mathcal{F}}(W_R)}{2} + \frac{1}{2} \left| \mathcal{A}_{Roe}(W_L, W_R) \right| (W_L - W_R).$$

Here, $|\mathbf{M}|$ denotes the absolute value of a diagonalisable matrix $\mathbf{M}$:
if $W = \sum_{i=1,4} \alpha_i \mathbf{r}_i$ where, for $i = 1, 4$, $\mathbf{r}_i$ denote an eigenvector of $\mathbf{M}$, associated with the eigenvalue λ_i, then we set $|\mathbf{M}| W = \sum_{i=1,4} \alpha_i |\lambda_i| \mathbf{r}_i$. Furthermore the Roe linearization of the flux function $\tilde{\mathcal{F}}$, $\mathcal{A}_{Roe}$ should satifiy:

1. $\mathcal{A}_{Roe}(W_L, W_R)$ can be diagonalized, with real eigenvalues
2. $\mathcal{A}_{Roe}(W_L, W_R) \cdot (W_L - W_R) = \tilde{\mathcal{F}}(W_L) - \tilde{\mathcal{F}}(W_R)$
3. $\mathcal{A}_{Roe}(W_L, W_L) = \mathbf{A}(W_L)$

where $\mathbf{A} = \partial_{\tilde{W}} \tilde{\mathcal{F}}$ denotes the Jacobian matrix of $\tilde{\mathcal{F}}$. Following Roe's strategy, we may take $\mathcal{A}_{Roe}(W_L, W_R) = A(\tilde{W}(W_L, W_R))$ where $\mathbf{A}$ is indeed the Jacobian of $\tilde{\mathcal{F}}$ and $\tilde{W}(W_L, W_R)$ is the following average state (see [13] for more details):

$$\sqrt{\tilde{\rho}} = \frac{\sqrt{\rho_L} + \sqrt{\rho_R}}{2}, \quad \tilde{\phi} = \frac{\sqrt{\rho_L}\phi_L + \sqrt{\rho_R}\phi_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad \text{for } \phi = U, V, e.$$

Finally, the convection terms in the scheme (4.3) are written:

$$\Phi_{ij}^{n} = R_{ij}^{-\theta} \Phi_{Roe}(R_{ij}^{\theta} W_i^n, R_{ij}^{\theta} W_j^n) \tag{4.6}$$

We expect that Roe's scheme is stable under the following CFL condition:

$$\sup_{i,j,p,n} \ \Delta T_{\text{CFL}} \frac{d_i |\lambda_{ij}^{n,p}|}{|\mathcal{C}_i|} \leq \frac{1}{2} \tag{4.7}$$

where d_i is the diameter of the greatest circle contained in $\mathcal{C}_i$ and $(\lambda_{ij}^{n,p})_{p=1,4}$ denote the eigenvalues of $\mathcal{A}_{Roe}(R_{ij}^{\theta} W_i^n, R_{ij}^{\theta} W_j^n)$. The main advantage of using Roe's numerical scheme is that it provides us with a robust and efficient scheme for the discretization of the convection terms. But Roe's method may replace some rarefaction waves by non-physical discontinuous weak solutions of the Euler system of gas dynamics. Such spurious solutions are expected when sonic points are present in rarefaction waves. In order to avoid them, an entropy correction is needed. Here, we use Roe's entropy correction (see [14] for more details).

Consider next the second order term $\Psi_{ij}^{n+1} = \mathcal{P}_{ij}(W_i^n, \nabla W_i^{n+1}) \cdot \mathbf{n}_{ij}$ in the scheme (4.3). Omiting the superscripts n and $n+1$, $\mathcal{P}_{ij}$ stands for an approximation of $\mathcal{P}(W, \nabla W)(\mathbf{a}_{ij})$ where $\mathbf{a}_{ij}$ denotes the center of the interface $\partial \mathcal{C}_i \cap \partial \mathcal{C}_i$, so that we may define:

$$\mathcal{P}_{ij} = \mathcal{P}(W_{ij}, \nabla W_{ij})$$

where, W_{ij} and ∇W_{ij} are approximate values of $W(\mathbf{a}_{ij})$ and $\nabla W(\mathbf{a}_{ij})$ respectively. But $\mathbf{a}_{ij}$ is the center of $\partial\mathcal{C}_i \cap \partial\mathcal{C}_i$: $\mathbf{a}_{ij} = \frac{1}{2}(\mathbf{a}_{ij}^- + \mathbf{a}_{ij}^+)$ where $\mathbf{a}_{ij}^{\pm}$ are the vertices of the segment $\partial\mathcal{C}_i \cap \partial\mathcal{C}_i$, and we set $W_{ij} = \frac{1}{2}(W_{ij}^- + W_{ij}^+)$ (resp. $\nabla W_{ij} = \frac{1}{2}(\nabla W_{ij}^- + \nabla W_{ij}^+)$) where $W_{ij}^{\pm}$ (resp. $\nabla W_{ij}^{\pm}$) are some approximate values of $W(\mathbf{a}_{ij}^{\pm})$ (resp. $\nabla W(\mathbf{a}_{ij}^{\pm})$). Now, it is possible to define $W_{ij}^{\pm}$ and $\nabla W_{ij}^{\pm}$ in terms of the unknowns $(W_i)_{i=1,I}$. Let indeed $\mathcal{C}_m$ denote a cell for which $\mathbf{a}_{ij}^-$ is a vertex. We define the volume control $\mathcal{V}(\mathbf{a}_{ij}^-)$ around $\mathbf{a}_{ij}^-$ as the union of the cells $\mathcal{C}_m$ that contain $\mathbf{a}_{ij}^-$: $\mathcal{V}(\mathbf{a}_{ij}^-) = \bigcup_m \mathcal{C}_m$. Then, we may define W_{ij}^- as the following average:

$$W_{ij}^- = \frac{1}{|\mathcal{V}(\mathbf{a}_{ij}^-)|} \int_{\mathcal{V}(\mathbf{a}_{ij}^-)} W(\mathbf{x}) d\mathbf{x} = \sum_m \frac{|\mathcal{C}_m|}{|\mathcal{V}(\mathbf{a}_{ij}^-)|} W_m$$

the quantity W_{ij}^+ is defined in the same manner, and finally, we succeded in writing W_{ij} in terms of the unknowns $(W_i)_{i=1,I}$.

The term ∇W_{ij} is also defined as $\nabla W_{ij} = \frac{1}{2}(\nabla W_{ij}^- + \nabla W_{ij}^+)$ and, the quantity ∇W_{ij}^- (resp. ∇W_{ij}^+) is approximated by the mean of the same quantity over a control volume around $\mathbf{a}_{ij}^-$ (resp. $\mathbf{a}_{ij}^+$). But here, using Stokes formula, we write:

$$\begin{aligned} \nabla W_{ij}^- &= \frac{1}{|\mathcal{V}(\mathbf{a}_{ij}^-)|} \int_{\mathcal{V}(\mathbf{a}_{ij}^-)} \nabla W(\mathbf{x}) d\mathbf{x} = \frac{1}{|\mathcal{V}(\mathbf{a}_{ij}^-)|} \int_{\partial\mathcal{V}(\mathbf{a}_{ij}^-)} W \cdot \mathbf{n} ds \\ &\simeq \frac{1}{|\mathcal{V}(\mathbf{a}_{ij}^-)|} \sum_j L_{mj} W_m \cdot \mathbf{n}_{mj} \end{aligned}$$

with obvious notations. Finally, the viscous terms in the numerical scheme (4.3) are written as follows:

$$\Psi_{ij}^{n+1} = \mathcal{P}(W_{ij}^n, \nabla W_{ij}^{n+1}) \cdot \mathbf{n}_{ij} \tag{4.8}$$

Hence, the scheme for the gas consists in Eqs. (4.3), (4.4), (4.6), (4.7), (4.8) plus the expression (4.13) below of $Z_i^n \Delta t$, given in the following subsection.

4.2 The coupling between the two phases

After having introduced numerical schemes that compute approximate values of the quantities relative to both phase, it remains us to explain how the source terms in the Navier-Stokes equations (2.5) and in the semi-fluid model (2.18) are treated. The method that we use is inspired from Particle in Cell approximations.
We first consider the approximation of the production terms in the system of the Navier-Stokes equations (2.18). Set $\mathbf{g}_k^n = (g_k^n, \mathbf{u}_k^n, e_k^n, \mathbf{x}_k^n, m_k^n, r_k^n)$, the vector that characterizes the k-th numerical particle at time $t = t^n$. The source terms in cell $\mathcal{C}_i$ is given by the following expression:

$$Z_i \Delta t \stackrel{def}{=} \int_{t^n}^{t^{n+1}} \int_{\mathcal{C}_i} (\mathbf{M}, \mathbf{I}, \mathbf{E})(\mathbf{x}, t) d\mathbf{x} dt \tag{4.9}$$

and we want to write the last expression in term of the vectors $\mathbf{g}_k^n$, $1 \leq k \leq K$. According to Eq. (2.8), the quantity Z_i is given by

$$Z_i \Delta t = \int_{t^n}^{t^{n+1}} \int_{\mathcal{C}_i} \left[\partial_t \int_{\mathbf{V}} \int_r f \phi(\mathbf{v}, r) d\mathbf{v} dr + \nabla_{\mathbf{X}} \cdot \left(\int_{\mathbf{V}} \int_r f \mathbf{v} \phi(\mathbf{v}, r) d\mathbf{v} dr \right) \right] d\mathbf{x}\, dt \tag{4.10}$$

Assume for the sake of simplicity that during the interval of time $[t^n, t^{n+1}]$ the particles either do not enter the cell $\mathcal{C}_i$, either stay in the cell $\mathcal{C}_i$. Then, the integral of the divergence term in the last expression vanishes and we may write the following expression for Z_i:

$$\begin{aligned} \Omega_i \Delta t &\stackrel{def}{=} \int_{t^n}^{t^{n+1}} \int_{\mathcal{C}_i} (\mathbf{M}, \mathbf{I}, \mathbf{E})(\mathbf{x}, t) d\mathbf{x} dt \\ &= - \sum_{\mathbf{x}_k(t) \in \mathcal{C}_i} \left([g_k^{n+1}, g_k^{n+1} \mathbf{u}_k^{n+1}, g_k^{n+1} e_k^{n+1}] - [g_k^n, g_k^n \mathbf{u}_k^n, g_k^n e_k^n] \right) \end{aligned} \tag{4.11}$$

Next, the numerical particle $\mathbf{g}_k^n$ has a non zero diameter and lye in the ball B_k^n, of center $\mathbf{x}_k^n$ and diameter S_k^n. We have thus to consider the following events:

(i) During $[t^n, t^{n+1}]$, a numerical particle crosses more than one cell.

(ii) For some $t \in [t^n, t^{n+1}]$, $\mathbf{x}_k(t) \in \mathcal{C}_i$ but the ball B_k^n is no subset of $\mathcal{C}_i$.

The first event means that the center of a numerical particle may cross different cells during $[t^n, t^{n+1}]$ so that different values of the datas of the gas flow should be considered during one time step. However, if the length of the path of a numerical particle during one time step is of the same order as the size of a cell, only one value of the gas data may be considered. In order to ensure this we impose the following CFL-like condition for the droplets:

$$\sup_{i,k_i,n} \Delta t \frac{|\mathbf{u}_{k_i}^n|}{d_i} \leq 1 \tag{4.12}$$

where d_i is the diameter of the cell $\mathcal{C}_i$ and then, event (i) may be omitted.

Now, consider the second event. Actually, in the turbulent case, the diameter S_k^n of a numerical particle may increase indefinitely and this may be interpreted as follows: the pdf f, solution of the Fokker-Planck equation (2.12) represents the motion of the particle in a turbulent gas flow. However, the function f is a mean solution in a statistical sense. Consider indeed a single particle in a turbulent gas flow. Its motion is then a random walk. Here, the pdf f accounts for all the possible random walks of the particle. Hence, though a numerical particle may represent only one physical particle, that is $S_k(0) = 0$, we may have, for $t > 0$, $S_k(t) > 0$, accounting for the uncertainty about the position of the droplet at $t > 0$. More details concerning the statistics of the motion of the droplets in a turbulent gas flow field are available in ref. [2].

Finally, the exchange term in the scheme (4.3) for the gas are written as follows:

$$Z_i \Delta t = -\sum_k \frac{|B_k^n \cap \mathcal{C}_i|}{|\mathcal{C}_i|} \left([g_k^{n+1}, g_k^{n+1}\mathbf{u}_k^{n+1}, g_k^{n+1}e_k^{n+1}] - [g_k^n, g_k^n\mathbf{u}_k^n, g_k^n e_k^n] \right) \tag{4.13}$$

Hence, considering this coupling, the scheme for the whole system is "locally" conservative on a space scale of order $\max_{k,n} S_k^n$. Nevertheless the scheme for the whole system is globally conservative, since for any $n \in \mathbb{N}$, we have

$$\sum_i (W_i^{n+1} - W_i^n) + \sum_k \left([g_k^{n+1}, g_k^{n+1}\mathbf{u}_k^{n+1}, g_k^{n+1}e_k^{n+1}] - [g_k^n, g_k^n\mathbf{u}_k^n, g_k^n e_k^n] \right) = 0,$$

where we omitted the boundary conditions.

Remark 4.1 The motion of the numerical particule located at $\mathbf{x}_i(t)$ depends on the datas of the gas flow at position $\mathbf{x}_i(t)$ and time t. Since the gas is discretized by a finite volume approach, we had to interpolate the datas of the gas flow field on the particles, then project the datas of the particles on the mesh. Similar difficulties appear in the PIC methods. (see [15]).

5 Numerical results

• We first consider the case of the injection of droplets of water in a closed chamber. In this experiment we consider the non-turbulent equation for the spray, that is the diffusion coefficient D in Eq. (2.12) is zero. The chamber is $10cm$ long, $5cm$ high and contains air at the temperature $T = 300K$, at atmospheric pressure: $p = 10^5$Pa. We set here for the viscosity of the gas $\mu_g(\mathbf{x}) = \mu_g^0(T(\mathbf{x}))^{1/2}$ where $T(\mathbf{x})$ is the gas temperature and $\mu_g^0 = 1.26\ 10^{-6}$. Then, the volume is discretized by using square shaped cells of size $1.25mm$.

The nonevaporating droplets are injected during the interval of time $T = 1ms$ from the left side of the chamber, in the horizontal direction. The droplets that are injected all have the same radius $r = 5\mu m$: we say that the spray is monodispersed. The total mass of liquid is $M_T = 5\ 10^{-3}\ Kg$, and this mass is of the same order as the mass of the gas initially contained in the chamber. The droplets are injected with a velocity $V = 100m/s$. The vertical component V_y is randomly chosed in the interval $[-8m/s, +8m/s]$ with the uniform law. The horizontal component of the injection velocity is then $V_x = (100^2 - V_y^2)^{1/2}$. Now, let $K = 90$ be the number of numerical particles per cell near the injector. Then, the interval of time between the injection of two packets of particles is $\Delta t_i = \frac{\Delta x}{KV}$ where V is the injection velocity and Δx is the width of the cells. Finally, the mass flow of the injector is $Q = \frac{M_T}{T}$. Hence, every Δt_i second, a numerical particle is injected with a random velocity as described before. Each numerical particle represents a group of droplets of radius r with total mass $M_p = Q\Delta t_i = \frac{M_T}{T}\Delta t_i$.

The results of the computations are shown in Fig.1: we show the repartition of the computed mass of the droplets in the chamber every $.1ms$, between $.1ms$ and $1ms$.

We observe an instability of the liquid jet, due to the interaction with the gas phase. The diameter of the liquid jet increases with the distance from the injection point, due to the interaction between the droplets and gas. As usual when lagrangian methods are used, the interface between the liquid jet and the region with no droplets in the chamber is easily and precisely computed.

The mean velocity field at time $t = 1ms$ is shown in Fig.2. The maximal computed velocity is $93.2m/s$.

In this computation, taking the gas quantities as constant, we integrated exactly the trajectory of the numerical particles, thanks to formula (3.18). However, many popular methods use the following quadrature to determine the position of the numerical particles at time t^n, in function of the position in the phase space at time t^n:

$$\left\{ \begin{array}{l} \mathbf{x}(t^{n+1}) = \mathbf{x}(t^n) + \mathbf{v}(t^n)\ \Delta t \\ \mathbf{v}(t^{n+1}) = (1 - c\Delta t)\ \mathbf{v}(t^n) + c\Delta t\ \mathbf{u}_g^n \end{array} \right.$$

where $\Delta t = t^{n+1} - t^n$. Moreover, when $c\Delta t > 1$ we must impose $\mathbf{v}(t^{n+1}) = \mathbf{u}_g^n$. This means that when the time $t_{drag} = 1/c$ of capture of a droplet is larger than the time-step Δt, we impose that the velocity of the droplet equals that of the gas. In order to evaluate the differences between the two methods, we introduce the relative error $\frac{|m_1 - m_2|}{\max(m_1, m_2)}$. Here, m_1 is the mass of droplets computed by using the exact expressions given in formula (3.18), m_2 is the mass of droplets computed by using the approximation formula above. Hence, this error is a *local* measure of the differences between the two methods and ranges in the interval $[0, 1]$. We plotted this error in Fig.3 below. Note that the relative error equals 1 in a given cell when one of the two methods predicts a positive mass in the cell while the other method predicts that there are no droplets in that cell. Therefore, a significant "local" relative error between the two methods does not mean a significant difference between the aspects of the two-phase flow observed in the two methods. However, roughly speaking, this "local" error measures the ratio of mass that one should displace from a given cell to

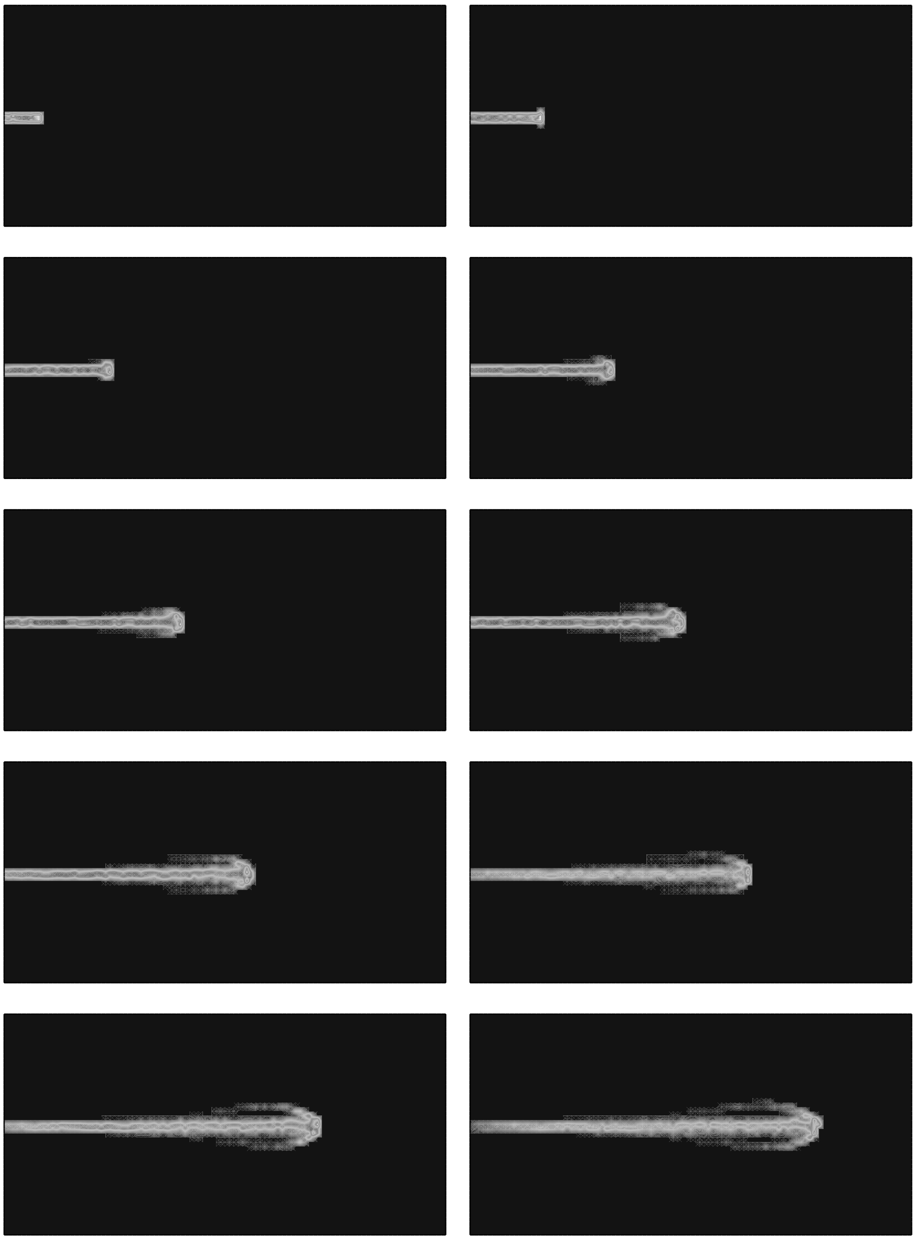

Figure 1: Mass of the liquid.

a neighbouring cell in order to obtain the spray observed in a first experiment when given the spray in a second experiment. Finally, we expect that the error increases when the drag coefficient c increases, that is when we consider smallest droplets. We observe here that the local relative error concentrates in the recirculation zone. Finally, we computed the total mass displaced when computing the spray with one method or the other. This total mass equals only 1% of the total mass injected which is not very much. We believe that the coupling with the gas stabilizes the two-phase fluid flow and therefore limitates the effect of the local relative errors in the global behavior of the spray.

• In a second experiment, we consider small scale turbulence in the gas flow, which means that we take a nonzero diffusion coefficient D in the spray equation (2.12). Following [2], we know that the diffusion coefficient D may be computed in terms of the gas phase turbulent kinetic energy and the correlation time of the turbulence. More precisely, the diffusion in the spray equation accounts for the effects of the small scale turbulent structures in the gas velocity field while the large structures should be taken into account seperately, for instance by means of a random component in the gas velocity. We thus need for a model that gives the turbulent kinetic energy in the gas flow and the correlation time of the turbulence that should be considered to compute D.

Very few two-phase flow turbulence models are available. The presence of the dispersed phase should indeed deeply influence the Kolmogorov's cascade: some characteristics length scales of the turbulence spectrum should be attenuated, which means that the presence of the particles induce a sink in some part of the energy spectrum, while small eddies are expected in the wake of the particles. Here, omiting the small scale turbulent structures produced by the Kolmogorov's cascade, we may try to evaluate that small scale turbulent structures directly induced by the presence of the particles. Then, according to a dimensional analysis, we expect that the associated gas phase turbulent kinetic energy has the following form:

$$\mathcal{K}^{1/2} = C(1-\alpha)\|\mathbf{u}_p - \mathbf{u}_g\|$$

where $1-\alpha$ is the volume fraction of the dispersed phase, $\mathbf{u}_p$ is the mean velocity of the dispersed phase, $\mathbf{u}_g$ is the mean gas velocity and C is an unknown coefficient. We shall take here:

$$\mathcal{K} = (1-\alpha)^2(\mathbf{u}_p - \mathbf{u}_g)^2. \tag{5.1}$$

where we set $C = 1$. Of course, more elaborate two-phase turbulence models, that compare to experiments should be used but, as a first step towards more realistic computations, and in order to test the capabilities of our numerical method, we shall use such a simple law (5.1) in the sequel.

Indeed, at time $t = 0$, we set the internal kinetic energy E_k and the size S_k of each numerical particle as $E_k = 0$ and $S_k = 0.3mm$. The correlation time of the small eddies is taken as $t_d = 0.1(1/c(r))$ where $t_{drag} = 1/c(r) \simeq 2.5\ 10^{-4}s$ is the "capture time" of a droplet. That is we consider that the turbulent correlation time is smaller than the capture time. Accordingly to the discussion above, the specific turbulent kinetic energy of the small eddies is taken as $\mathcal{K}(\mathbf{x}) = 10^{-6}\ (\mathbf{u}_g(\mathbf{x}) - \mathbf{u}_p(\mathbf{x}))^2$ where $\mathbf{u}_p$ is the mean velocity of the droplets in the cell containing the point $\mathbf{x}$.

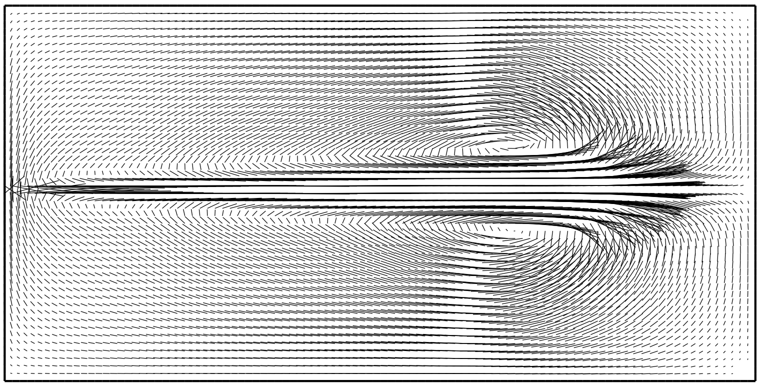

Figure 2: Velocity of the gas at time $t = 1ms$.

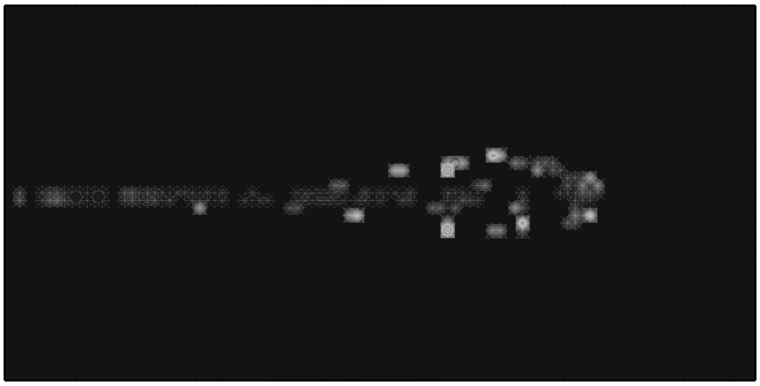

Figure 3: Local relative error at time $t = 1ms$.

The shape of the spray as well as the velocity field of the gas are very similar to that obtained in the first experiment, with no turbulence modeling. The maximal velocity of the gas at time $1ms$ is now $92.8m/s$ that is a little bit smaller than in the first experiment. Actually, it seems to us important to remark that introducing the effect of the small scale turbulent structures introduces a new term of energy exchange between the two phases (compare Eqs. (2.7) and (2.14)). In other words, we may consider that some energy of the gas is transfered to the physical droplets of any given numerical particle.

Now, even if the general aspects of the two-phase fluid flow in the two experiments are very similar, we may look at the local relative error for the mass of the liquid between the two methods. This error still ranges in the interval $[0, 1]$ and is quite important (compare with Fig.3). Moreover we notice that the error is larger at the interface between the jet of droplets and the gas:

Then, though the shape of the spray is very similar to that obtained in the first experiment, the total mass displaced between the two methods is now 7% of the total mass injected and is thus quite important.

Finally, in our calculations the size of the numerical particles at the final time $t = 1ms$ ranges from $0.3mm$ to $0.7mm$. The biggest numerical particles concentrate in the recirculation zone.

• In a third experiment, we consider a two-meter long and one-meter high chanel containing air at a temperature of 300 Kelvin and at atmospheric pressure. The top and bottom boundaries of the chanel are walls. The gas is injected on the left boundary of the chanel with a velocity of one hundred meters per second and goes out through the right boundary of the chanel. The mesh consists in square-shaped cells of size $2cm$.

At time $t = 0$, we begin the injection of non vaporazing droplets. Here, the spray is polydisperse and the liquid is water. The injector is located at the center of the bottom wall. The direction of injection is 45^o towards the left and the injection lasts for $0.1s$. The injection velocity is $100m/s$ with a transverse component ranging in the interval $[-20m/s, +20m/s]$. The total mass injected is $M_T = 10Kg$, and, setting here $K = 20$, $\Delta t_i = \frac{\Delta x}{KV}$ is the interval of time between the injection of two numerical particles. Following Dukowicz, the distribution of radii of the polydisperse spray is given by the following exponential law: $F(r) = \frac{3}{r_S} exp(-\frac{3r}{r_S})$ where $r_S = 5mm$ is the Sauter radius. Since we consider a finite number N of radii, we introduce the equiprobable family $(r_k)_{k=1,N}$ of radii where $r_k = \frac{r_S}{3} Log(\frac{N+1}{N+1-k})$. In the limit where N goes to infinity the family $(r_k)_{k=1,N}$ reproduces the exponential law. However, the smaller radius of a numerical particle is here $r_1 = \frac{r_S}{3} Log(\frac{N+1}{N}) \simeq \frac{r_s}{3N}$ and it is necessary to bound N so that r_1 remains physically acceptable.

Let us precise the numerical injection of droplets: the time interval between two injections is Δt_i and may differ from Δt. When $n\Delta t \le p\Delta t_i < (n+1)\Delta t$ for some pair of integers (n, p) an injection of droplets occurs between t^n and t^{n+1}. We randomly choose a radius r_k with $1 \le k \le N$ and we decide that every droplet injected at time $p\Delta t_i$ has radius r_k. In order to determine the mass of the numerical particle injected at time $p\Delta t_i$ (or equivalently, the number of droplets taken into

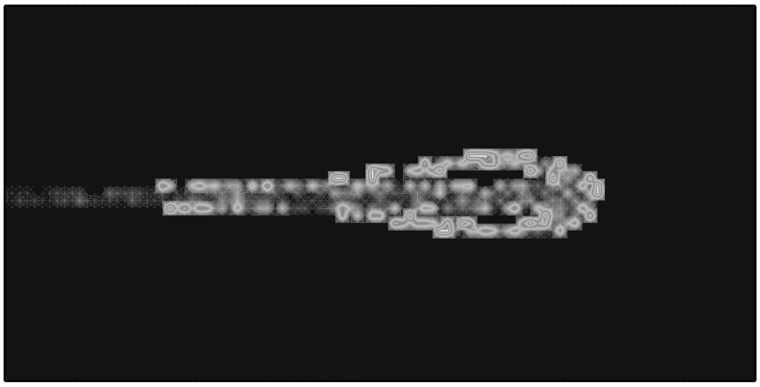

Figure 4: Local relative error between the first two methods, at time $t = 1ms$.

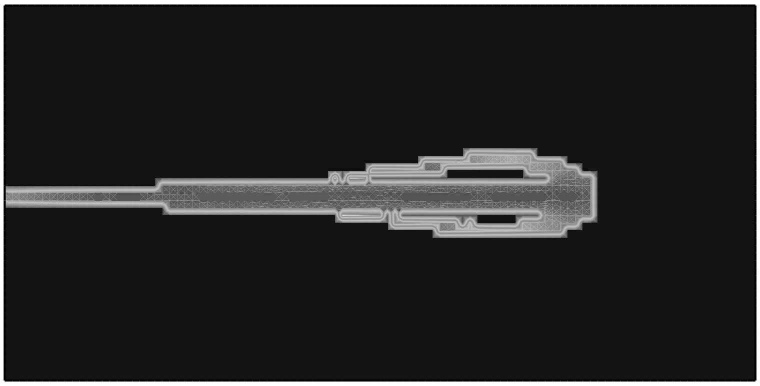

Figure 5: Size of the numerical particles at time $t = 1ms$.

account in the numerical particle), we require that the mass flux of the liquid phase is constant: denote by $M(t)$, the total mass of liquid already injected at time t. If the injection process were continuous we could impose $M(t) = M_T \frac{t}{T}$ where M_T denotes the total mass of droplets injected at the end of the experiment. Here, the injection process is a discrete one and, in order to approximate the continuous law, the mass of particles injected at time $(p\Delta t_i)$ is given by the following expression:

$$m = \max(M_T \frac{(p\Delta t_i)}{T} - M\big((\Delta t_i)^-\big), 0), \tag{5.2}$$

and the total mass of droplets at time $(p\Delta t_i)^+$ is thus exactly $M_T \frac{(p\Delta t_i)}{T}$. With this algorithm, we injected a total mass $M_i = 9.99976Kg$ instead of $M_T = 10Kg$, which proves the accuracy of the injection method. Finally, the injected mass of liquid is very important since it corresponds to $100Kg$ per second. This computation was performed in order to check the robustness of the whole numerical method.

Moreover, we take into consideration the possible break-up of the droplets thanks to a simple phenomenological model: let We denote the Weber number of a droplet with radius r_k,

$$We = \frac{\rho_g |\Delta \mathbf{u}|^2 r_k}{\sigma}$$

where ρ_g is the gas mass density at the position of the droplet, $\Delta \mathbf{u}$ the relative velocity between the droplet and the surrounding gas, and $\sigma = .073$ is the surface tension of water at a temperature of 300 K. When a droplet's Weber number becomes larger than a critical number (usually between 7 and 10), the droplet breaks up after a time interval that depends itself on the Weber number (see [16]). The result of the break up is difficult to predict. However we shall assume here that the droplets obtained from the breaking drop all have the same radius and a Weber number less or equal to 1. Of course a more realistic break-up model should be used in practicle approximations but such a simplified model allows to obtain physically meaningfull results.

We show on Fig.6 below the mass of the droplets inside the chanel at time $t = 10ms$. We observe the curvature of the droplets jet due to interaction with the gas velocity field. The velocity field at time $t = 10ms$ ranges between $2m/s$ and $170m/s$. It is shown in Fig.7 below. We note that the presence of the droplets induces an important perturbation of the gas flow and a recirculation behind the liquid jet. Finally, the relative error between the droplets mass distributions, obtained thanks to the exact integration formula of the characteristics on the one hand and thanks to Euler's explicit first order integration formula on the other hand is given on Fig.8 below. Here the total mass displaced between the two methods is about 1.5% of the total mass injected.

6 Conclusion

The semi-fluid model allowed us to give more insight in the meaning of numerical particles in the domain of spray computation. We underlined the general hypothesis that permit to treat a numerical particle like a physical one. This was possible in this study first, since the velocity distribution of the droplets is assumed to be

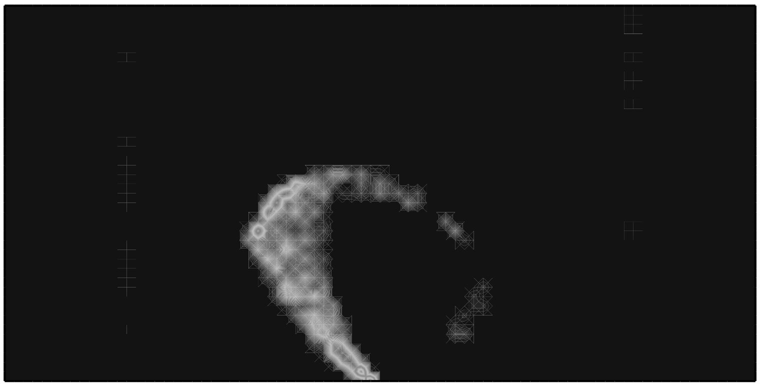

Figure 6: Mass of the liquid at time $t = 10ms$.

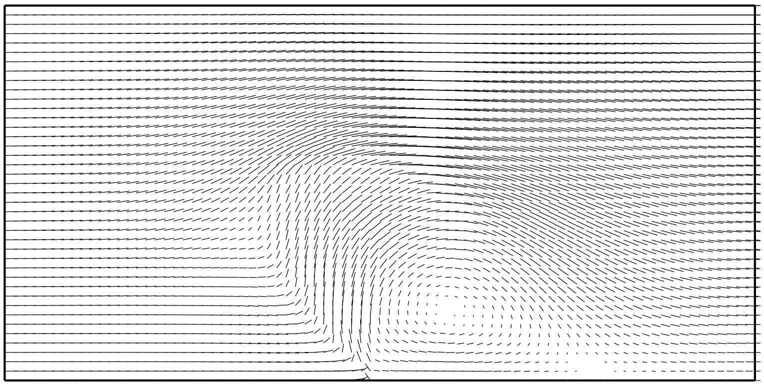

Figure 7: Velocity of the gas at time $t = 10ms$.

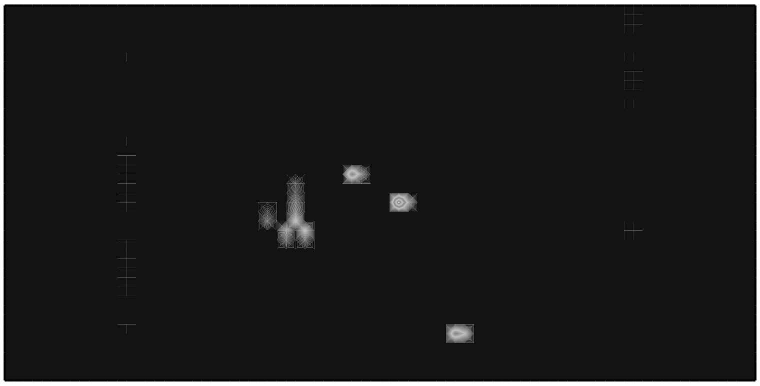

Figure 8: Relative error at time $t = 10ms$.

isotropic, second, because the spray obeys the linear transport equation (without collision terms), third, because the datas of the gas flow are supposed to be constant in each cell of the computational domain when we compute the unknowns for the spray and four, because we used the simple Stokes drag force. Finally, we insisted on the fact that it may be important to take into account the size of the numerical particles since it introduces a coupling between the two phases.

We believe that using exact expressions for the characteristics of the droplets as well as taking into account the size of the numerical particle is important since large local relative errors are obtained between the different methods. Indeed, concerning the computation of the motion of the droplet, the use of a time step small enough in order that the particles trajectory is accurately computed would dramatically increase the computational cost. However, we keep in mind that of course this is not the main source of errors when computing realistic two-phase fluid flows. Indeed, one must first write more complex and realistic physical laws for the motion of the droplets while we used here the simplest ones.

The numerical scheme that we introduced to discretize the semi-fluid model is elegant and efficient. The extension to second order is in progress. The other points that we are currently improving concern the modeling of the two-phase turbulence and the computation of droplets heating and vaporization.

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A Appendix: Mathematical results

This appendix is devoted to the derivation of some mathematical properties of the Fokker-Planck equation (2.12) which we recall below for the sake of completeness:

$$\partial_t f + \nabla_{\mathbf{X}} \cdot (f\mathbf{v}) + \nabla_{\mathbf{V}} \cdot (f\beta) + \partial_r(f\mathcal{R}) - \nabla_{\mathbf{V}} \cdot (D\nabla_{\mathbf{V}} f) = 0.$$

where $\beta = \beta(\mathbf{v}, r)$ and $D = D(r)$ are defined by (2.4) and (2.13) repectively. Its solution writes explicitly as follows:

Theorem A.1 (Solution of the Fokker-Plank equation)
Let f_0 be given. The solution f of the Fokker-Planck equation (2.12) with initial data f_0 writes:

$$f(\mathbf{x}, \mathbf{v}, r, t) = (S_t f_0) = \frac{1}{J_r(t)} \int_{\mathbf{X}'} \int_{\mathbf{V}'} \mathcal{G}_{R^-}(\mathbf{X}^- - \mathbf{x}', \mathbf{V}^- - \mathbf{v}', t) f_0(\mathbf{x}', \mathbf{v}', R^-) d\mathbf{x}' d\mathbf{v}' \tag{A.1}$$

where $1/J_r(t)$ is the Jacobian $\dfrac{\partial(\mathbf{X}^-, \mathbf{V}^-, R^-)(t)}{\partial(\mathbf{x}, \mathbf{v}, r)}$ and,

$$\mathcal{G}_r(\mathbf{x}, \mathbf{v}, t) = \frac{1}{(2\pi)^d \Delta_r^{\frac{d}{2}}(t)} exp(-(a_r(t)\mathbf{x}^2 + 2h_r(t)\mathbf{x} \cdot \mathbf{v} + b_r(t)\mathbf{v}^2)/2\Delta_r(t)).$$

Here,

$$\begin{cases} a_r(t) = 2\displaystyle\int_0^t \psi_r^2(s)ds, & b_r(t) = 2\displaystyle\int_0^t \phi_r^2(s) \\ h_r(t) = 2\displaystyle\int_0^t \phi_r(s)\psi_r(s)ds, & \Delta_r(t) = a_r(t)b_r(t) - h_r(t) \end{cases} \tag{A.2}$$

where,

$$\begin{cases} \psi_r(t) = \left(\dfrac{D(R(t;r,0))}{\eta_1^2(t)}\right)^{\frac{1}{2}} \\ \phi_r(t) = \left(\dfrac{D(R(t;r,0))\alpha_1^2(t)}{\eta_1^2(t)}\right)^{\frac{1}{2}} \end{cases}$$

The numbers $\alpha_1(t)$ and $\eta_1(t)$ in the above expressions are the coefficients of the characteristics defined in Eq. (3.9).

Proof: Let us define the function $\tilde{f}$ by

$$\tilde{f}(\mathbf{x}, \mathbf{v}, r, t) = J_r(t) f(\mathbf{X}^+, \mathbf{V}^+, R^+, t). \tag{A.3}$$

where $J_r(t)$ is the following function:

$$J_r(t) = exp\left(\int_0^t (\partial_r \mathcal{R} + \nabla_{\mathbf{V}} \cdot \beta)(R(s;r,0))ds\right), \tag{A.4}$$

A straightforward computation proves that $\tilde{f}$ is solution of

$$(\partial_t \tilde{f})(\mathbf{x},\mathbf{v},r,t) = J_r(t)D(R(t;r,0))(\Delta_{\mathbf{V}} f)(\mathbf{X}^+,\mathbf{V}^+,R^+,t). \tag{A.5}$$

Thanks to Eq. (A.3) and the expression of the characteristics, the second term of Eq.(A.5) may be rewritten in terms of derivatives of $\tilde{f}$, so that:

$$\partial_t \tilde{f}(\mathbf{x},\mathbf{v},r,t) = \frac{D(R(t;r,0))}{\eta_1^2(t)} \left(\alpha_1^2(t)\Delta_{\mathbf{X}}\tilde{f} - 2\alpha_1(t)(\nabla_{\mathbf{X}}\cdot\nabla_{\mathbf{V}})\tilde{f} + \Delta_{\mathbf{V}}\tilde{f}\right)(\mathbf{x},\mathbf{v},r,t) \tag{A.6}$$

where α_1 and η_1 are the coefficients of the characteristics, defined in Eq. (3.9). Setting indeed:

$$\psi_r(t) = \sqrt{D(R(t;r,0))/\eta_1^2} \quad , \quad \phi_r(t) = \sqrt{D(R(t;r,0))\alpha_1^2/\eta_1^2},$$

one recovers the expressions of ϕ_r and ψ_r defined in Theorem **A.1**. Hence, we are left to solving Eq. (A.6) in each of the d directions of $\mathbb{R}_x^d \times \mathbb{R}_v^d$, and we only need the following lemma:

Lemma A.2 *Let $\phi(t)$ and $\psi(t)$ be two arbitrary functions of time. The solution in 1D of*

$$\begin{cases} \partial_t \mathcal{G} = \phi_r^2(t)\partial_{xx}\mathcal{G} - 2\phi_r(t)\psi_r(t)\partial_{xv}\mathcal{G} + \psi_r^2(t)\partial_{vv}G \\ \mathcal{G}(x,v,0) = \delta(x)\otimes\delta(v), \end{cases}$$

where δ denotes Dirac's δ function, is given by:

$$\mathcal{G}(x,v,t) = \frac{1}{2\pi\Delta^{\frac{1}{2}}} exp(-(a(t)x^2 + 2h(t)xv + b(t)v^2)/2\Delta(t)).$$

with

$$\begin{cases} a(t) = 2\int_0^t \psi^2(s)ds \quad , \; b(t) = 2\int_0^t \phi^2(s)ds \\ h(t) = 2\int_0^t \phi(s)\psi(s)ds \quad , \; \Delta(t) = a(t)b(t) - h(t) \end{cases}$$

Proof: The proof of Lemma **A.2** may be found in Chapter II of the article of S.Chandrasekhar (see [9]). □

In other words, the solution $\tilde{f}(\mathbf{x},\mathbf{v},r,t)$ of (A.3) writes in terms of a convolution operator in $(\mathbb{R}_{\mathbf{X}} \times \mathbb{R}_{\mathbf{V}})$:

$$\tilde{f}(\mathbf{x},\mathbf{v},r,t) = \int_{\mathbf{X}'}\int_{\mathbf{V}'} G_r(\mathbf{x}-\mathbf{x}',\mathbf{v}-\mathbf{v}',r,t) f_0(\mathbf{x}',\mathbf{v}',r) d\mathbf{x}' d\mathbf{v}'$$

where G_r is defined in Theorem **A.1**. Thanks to Eq. (A.3), this means that the solution f of the Fokker-Planck equation (2.12) is exactly given by the expressions in Eq. (A.1). Note that the solution f does not write in terms of a convolution operator.

Now, let us indentify the function $J_r(t)$. We note that the characteristics defined in Eq. (3.8) may be written as the solution of the following system of ODEs:

$$\frac{d}{dt}\begin{bmatrix} \mathbf{X}_t \\ \mathbf{V}_t \\ R_t \end{bmatrix} = \mathbf{F}(\mathbf{X}_t, \mathbf{V}_t, R_t, t),$$

with obvious notations for $\mathbf{F}$. Then, it is well known that the jacobian $\partial(\mathbf{X}, \mathbf{V}, R)(t;s)/\partial(\mathbf{x}, \mathbf{v}, r)$ of the transformation $(\mathbf{x}, \mathbf{v}, r) \longrightarrow (\mathbf{X}, \mathbf{V}, R)(t;s)$ equals 1 at $t = s$ and is solution of the following ODE:

$$\frac{d}{dt}\left[\frac{\partial(\mathbf{X}, \mathbf{V}, R)(t;s)}{\partial(\mathbf{x}, \mathbf{v}, r)}\right] = \left(\begin{pmatrix} \nabla_{\mathbf{X}} \\ \nabla_{\mathbf{V}} \\ \partial_r \end{pmatrix} \cdot \mathbf{F}\right)\left[\frac{\partial(\mathbf{X}, \mathbf{V}, R)(t;s)}{\partial(\mathbf{x}, \mathbf{v}, r)}\right]$$

so that

$$\frac{\partial(\mathbf{X}, \mathbf{V}, R)(t;s)}{\partial(\mathbf{x}, \mathbf{v}, r)} = exp\left(\int_s^t (\partial_r \mathcal{R} + \nabla_{\mathbf{V}} \cdot \beta)(R(\theta; r, s))d\theta\right).$$

Take $s = 0$: we obtain the expression (A.4) of $J_r(t)$. In other words, $1/J_r(t)$ is indeed the jacobian associated to the flow of the reverse characteristics. This concludes the proof of Theorem **A.1**. □

References

[1] F.A.Williams. *Combustion Theory, 2nd edition.* Benjamin Cummings, 1985.

[2] J.F.Clouet and K.Domelevo. Solution of a kinetic stochastic equation modeling a spray in a turbulent gas flow. *To appear in M3AS*, 2(7), 1997.

[3] P.D.Lax A.Harten and B.Van Leer. On upstream differencing and godunov-type schemes for hyperbolic conservation laws. *SIAM Rev.*, 25:35–61, 1983.

[4] S.M.Deshpande. Kinetic theory based new upwind methods for inviscid compressible flows. *AIAA paper 86-0275*, American Institute of Aeronautics and Astronautics, New York, 1986.

[5] B.Perthame. Boltzmann type schemes for gas dynamics and the entropy property. *SIAM J. Numer. Anal.*, 27(6):1405–1421, December 1990.

[6] C.Cercignani. *The Boltzmann equation and its Applications*, volume 67 of *Applied Mathematics.* Springer Verlag, 1988.

[7] J.K.Dukowicz. A particle-fluid numerical model for liquid sprays. *J. Comp. Physics*, 35:229–253, 1980.

[8] P.J.O'Rourke. Statistical properties and numerical implementation of a model for droplets dispersion in a turbulent gas. *J. Comp. Physics*, 83:345–360, 1989.

[9] S.Chandrasekhar. Stochastic problems in physics and astronomy. *Rev. Mod. Ph.*, 15(1), January 1943.

[10] M.W.Reeks. On a kinetic equation for the transport of particles in turbulent flows. *Phys. Fluids A*, 3(3), March 1991.

[11] J.J. Monaghan and R.A. Gingold. Shock simulation by the particle method SPH. *J. Comp. Physics*, 52:374–389, 1983.

[12] S. Mas-Gallic and P.A. Raviart. A particle method for first-order symmetric systems. *Numer. Math.*, 51:323–352, 1987.

[13] Bernard Larrouturou. On the relation between finite-volume simulations of multi-dimensionnal and multi-species flow. *Internal Report. CERMICS, INRIA, Sophia-Antipolis, 06560 Valbonne, France*, unpublished.

[14] P.L.Roe. Some contributions to the modelling of discontinuous flow. *in Lectures in Applied Mathematics*, 22:163–193, 1985.

[15] J.U. Brackbill P.J. O'Rourke and B. Larrouturou. On particle-grid interpolation and calculating chemistry in particle-in-cell methods. *J. Comp. Physics*, 109:37–52, 1992.

[16] F.V. Bracco. Modelling of engine sprays. *SAE 850394*, pages 144–167.