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Kinetic equations for spray behavior

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Abstract. In this work we are concerned with a kinetic description of a non-homogeneous system. The system is composed by a multi size set of droplets immersed in a multicomponent mixture of gases. In the preceding paper we studied this problem from a phenomenological point of view, here we assume both the droplets and the gases are described by the corresponding distribution functions. Those functions satisfy a modified Williams equation and the Boltzmann equation respectively. The set of equations are coupled through the interaction between droplets and the gases in the mixture. We found that the droplet vaporization rate is affected by the collision with the gas molecules. A force, caused by the gas-droplet collisions acting on the droplets appears. We identify the mass, momentum and energy sources, which were defined in a previous phenomenological treatment in order to have the conservation equations of the system as a whole.

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1. Introduction

Spray vaporization and combustion have several important practical consequences for some industrial processes. This fact has been a strong motivation to improve the knowledge of spray characteristics. The study about this problem has been done mainly along two lines: *i)* The experimental work has increased a lot since the laser technics were available, because those experiments allow a better observation of size and velocity distributions of droplets along the spray [1], *ii)* Computing facilities have also helped to study and predict the spray properties [2].

According to some recent reviews [3,4,5], the theoretical aspects of spray behavior have been studied from different points of view. For example, the isolated droplet vaporization, the internal motion in the droplets, some characteristics about the local heat transfer, have received a lot of efforts.

In contrast with these advances, the approach based on distribution functions seems to be underdeveloped. The classical work of Williams [6] established the basic ideas to study a spray from that point of view. Later Sirignano [7] took into account the droplets internal energy and he considered its contribution to the kinetic approach.

Williams assumed valid the statistical description and he considered a multidimensional distribution function which gives some information about size, velocity and position of droplets as a function of time. He derived the kinetic equation satisfied by such a function. The Williams kinetic equation considers the interaction of droplets and gases through an external drag force acting on them. This assumption allows to study the droplet evolution independently of the gases, and drives that approach to a "Separated Flow" view of the spray [3].

In this work we are concerned with the same problem as Williams and Sirignano, but we will describe the spray by means of $N+1$ distribution functions, one of them for the droplets and N for the N-component mixture of gases. There will be $N+1$ kinetic equations strongly coupled through the collision kernels, like in the Boltzmann equation [8]. However, we will simplify those collision terms through some approximations, which we consider valid for the particular spray problem.

The kinetic approach leads to a set of equations for some statistical averages, which can be identified with the macroscopic local variables. The set of equations we obtained by this method is compared to the phenomenological equations we derived in the preceding paper [9]. The mass, momentum and energy sources are also identified.

In Section 2 we establish the kinetic model we are interested in, we also make some approximations to obtain a modified kinetic equation for the droplets. In Section 3 the general balance equations are obtained while in Section 4 and 5 we take some particular cases for the mixture of gases and the droplets respectively. At last, in Section 6 we make a comparison with the phenomenological theory and we give some concluding remarks in Section 7.

2. Kinetic model

In this section we will sketch the kinetic model we use to study the spray. The spray contains a multicomponent mixture of gases and a large number of liquid droplets. They are immersed in the gases and move with them. We assume the gas species are described by the usual Boltzmann equation, each gas component will be characterized by the distribution function $f_i(\mathbf{c}_i, \mathbf{x}, t)$, where $\mathbf{c}_i$ is the molecular velocity of a molecule of the i-species with mass m_i, then $f_i(\mathbf{c}_i, \mathbf{x}, t)d\mathbf{c}_i d\mathbf{x}$ gives us the number of species-i molecules with velocity in the range $(\mathbf{c}_i, \mathbf{c}_i + d\mathbf{c}_i)$ in the volume element $d\mathbf{x}$ at time t.

The kinetic equations are:

$$\frac{\partial}{\partial t} f_i(\mathbf{c}_i, \mathbf{x}, t) + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{x}} f_i(\mathbf{c}_i, \mathbf{x}, t) + \mathbf{F}_{\text{ext}} \cdot \frac{\partial}{\partial \mathbf{c}_i} f_i(\mathbf{c}_i, \mathbf{x}, t) = \sum_{j=1}^{N} J_{ij}(f_i, f_j) + J_{id}(f_i, f_d) \quad i = 1, \ldots, N, \tag{1}$$

where $\mathbf{F}_{\text{ext}}$ is the bulk external force per unit mass acting on the system, $J_{ij}(f_i, f_j)$ are the usual Boltzmann collision kernels, which take into account the binary interaction between molecules of i, j species. The last term $J_{id}(f_i, f_d)$ measures the interaction between i-molecules and the droplets, it depends on the distribution function for i-molecules f_i and the distribution function of droplets f_d. There are N coupled equations like Eq. (1), because there are N chemical species in the mixture.

The droplets are atomized in such a way that there are a lot of them immersed in the gas, they vaporize with a vaporization rate $\dot{R}_{\text{vap}}$ and the vapors become one of the species of the gas. We will assume the droplets are spherical of radius R and move with velocity $\mathbf{v}$. The droplet properties are being described by a distribution function, so $f_d(R, \mathbf{v}, \mathbf{x}, t)dRd\mathbf{v}d\mathbf{x}$ gives us the number of droplets with radius in the range $(R, R + dR)$, velocity between $\mathbf{v}$ and $\mathbf{v} + d\mathbf{v}$ in the volume element $d\mathbf{x}$ at time t. The kinetic equation we will assume to be valid is like the Williams' equation [6]

$$\frac{\partial}{\partial t} f_d(R, \mathbf{v}, \mathbf{x}, t) + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} f_d(R, \mathbf{v}, \mathbf{x}, t) + \frac{\partial}{\partial R}[\dot{R}_{\text{vap}} f_d(R, \mathbf{v}, \mathbf{x}, t)] + \mathbf{F}_{\text{ext}} \cdot \frac{\partial}{\partial \mathbf{v}} f_d(R, \mathbf{v}, \mathbf{x}, t) = \sum_{i=1}^{N} J_{di}(f_d, f_i) + J_{dd}(f_d, f_d), \quad (2)$$

where $J_{di}(f_d, f_i)$ represents the interaction between the i-species in the gas and the droplets, consequently the summation gives us the contribution of all species. The term $J_{dd}(f_d, f_d)$ is the droplet-droplet interaction which we consider negligible for a dilute spray. In order to express the collision integrals in terms of the distribution functions we will follow the kinetic theory ideas [8]. First of all the collision kernels J_{ij} are the usual ones,

$$J_{ij} = \int [f_i(\mathbf{c}_i', \mathbf{x}, t) f_j(\mathbf{c}_j', \mathbf{x}, t) - f_i(\mathbf{c}_i, \mathbf{x}, t) f_j(\mathbf{c}_j, \mathbf{x}, t)] g_{ij} d\Gamma_{ij} d\mathbf{c}_j \quad (3)$$

where $\mathbf{c}_i', \mathbf{c}_j'$ are the velocities after the collision, $\mathbf{c}_i, \mathbf{c}_j$ are the velocities before the collision of particles i, j, g_{ij} is the magnitude of the relative velocity and $d\Gamma_{ij}$ the corresponding cross section. The distribution functions f_i, f_j satisfy Eq. (1), which is coupled with the kinetic equation for the droplets. The droplets affect the gas kinetic equation mainly through the collision integral $J_{id}(f_i, f_d)$, here we will assume there is a binary interaction between a gas molecule and the droplet. The dynamics of that interaction is given by a cross section which we call $d\Gamma_{id}$, the velocities after the collision are $\mathbf{c}_i'$ and $\mathbf{v}'$, and the corresponding velocities before the collision are unprimed, then,

$$J_{id} = \int [f_i(\mathbf{c}_i', \mathbf{x}, t) f_d(R', \mathbf{v}', \mathbf{x}, t) - f_i(\mathbf{c}_i, \mathbf{x}, t) f_d(R, \mathbf{v}, \mathbf{x}, t)] g_{id} d\Gamma_{id} dR d\mathbf{v}, \quad i = 1, \ldots, N, \quad (4)$$

here R' is the droplet radius after the collision. We recall that there is no nucleation nor coalescence of the molecules on the droplets, the change in the droplet radius is caused by vaporization. We simplify the collision integral in Eq. (4) by making some assumptions about the interaction of the gas molecules and the droplet. First, the droplet is very big compared with the molecule, the droplet distribution function is almost unaffected by one molecule collision, meaning that $f_d(R', \mathbf{v}', \mathbf{x}, t) \cong f_d(R, \mathbf{v}, \mathbf{x}, t)$ in Eq. (4). On the other hand the molecules suffer a big change and we will assume $\mathbf{c}'_i \cong -\mathbf{c}_i$ so the molecule is reflected by the droplet. Taking into account these assumptions, Eq. (4) can be written as follows

$$J_{id}(f_i, f_d) = \int f_d(R, \mathbf{v}, \mathbf{x}, t) \times [f_i(-\mathbf{c}_i, \mathbf{x}, t) - f_i(\mathbf{c}_i, \mathbf{x}, t)] g_{id} d\Gamma_{id} dR d\mathbf{v}, \quad i = 1, \ldots, N. \quad (5)$$

Now we will discuss the collision integral $J_{di}(f_d, f_i)$ which collects the effects of the molecule collision with the droplet. The cross section for such a collision is $d\Gamma_{di}$, the relative velocity is g_{di} so

$$J_{di} = \int [f_d(R', \mathbf{v}', \mathbf{x}, t) f_i(\mathbf{c}', \mathbf{x}, t) - f_d(R, \mathbf{v}, \mathbf{x}, t) f_i(\mathbf{c}_i, \mathbf{x}, t)] g_{di} d\Gamma_{di} d\mathbf{c}_i, \quad i = 1, \ldots, N. \quad (6)$$

The radius of the droplet after the collision is calculated through the vaporization rate $\dot{R}_{\text{vap}}$ which can be obtained by means of an independent model or from experimental data, it can be written as

$$R' = R + \int_t^{t+\tau} \dot{R}_{\text{vap}} dt = R + \alpha(t, \tau), \quad (7)$$

where R is the radius before the collision and τ is a characteristic collision time.

The droplets velocity after collision $\mathbf{v}'$, is calculated from a momentum balance. The momentum change for a droplet is

$$(\Delta \mathbf{P})_d = \frac{4}{3}\pi \rho_L R^3 (\mathbf{v}' - \mathbf{v}) + \frac{4}{3}\pi \rho_L R^2 \alpha \mathbf{v}', \quad (8)$$

where ρ_L is the liquid density and $(\Delta \mathbf{P})_d$ is calculated up to first order in α. The change of momentum for the gas molecules is given by the momentum change of one molecule multiplied by $\nu_i \tau$, where ν_i is the number of collisions of molecules of species i with the droplet per unit time.

According to the hypothesis about the momentum transfer given prior to Eq. (5), the change of momentum for a molecule is $2m_i\mathbf{c}_i$, therefore the momentum conservation gives us

$$\mathbf{v}' = \mathbf{v} - \frac{3\alpha}{R}\mathbf{v} + \frac{3}{2}\frac{m_i\nu_i\tau}{\pi\rho_L R^3}\mathbf{c}_i \tag{9}$$

We substitute Eqs. (7) and (9) into (6) and we expand in Taylor series up to the first order to obtain

$$\begin{aligned} J_{di}(f_d, f_i) = (\gamma_{1i} - \gamma_{2i}) f_d(R, \mathbf{v}, \mathbf{x}, t) + \gamma_{1i}\left[-\frac{3\alpha}{R}\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{v}} f_d(R, \mathbf{v}, \mathbf{x}, t)\right. \\ \left. + \alpha\frac{\partial}{\partial R} f_d(R, \mathbf{v}, \mathbf{x}, t)\right] + \frac{3}{2}\frac{m_i\nu_i\tau}{\pi\rho_L R^3}\boldsymbol{\gamma}_{3i}\cdot\frac{\partial}{\partial\mathbf{v}} f_d(R, \mathbf{v}, \mathbf{x}, t), \end{aligned} \tag{10}$$

where the quantities γ_{1i}, γ_{2i} and $\boldsymbol{\gamma}_{3i}$ depending on $R, \mathbf{v}$ and the gas properties are given by

$$\gamma_{1i}(R, \mathbf{v}, \{\text{gas}\}) = \int f_i(-\mathbf{c}_i, \mathbf{x}, t) g_{di} d\Gamma_{di} d\mathbf{c}_i, \tag{11}$$

$$\gamma_{2i}(R, \mathbf{v}, \{\text{gas}\}) = \int f_i(\mathbf{c}_i, \mathbf{x}, t) g_{di} d\Gamma_{di} d\mathbf{c}_i, \tag{12}$$

$$\boldsymbol{\gamma}_{3i}(R, \mathbf{v}, \{\text{gas}\}) = \int \mathbf{c}_i f_i(-\mathbf{c}_i, \mathbf{x}, t) g_{di} d\Gamma_{di} d\mathbf{c}_i, \tag{13}$$

They contain the collision dynamics and the properties of the gas. Substitution of Eq. (10) in Eq. (2) allows a great simplification in the kinetic equation for the spray, *i.e.*

$$\begin{aligned} \frac{\partial}{\partial t} f_d + \mathbf{v}\cdot\frac{\partial}{\partial\mathbf{x}} f_d + \frac{\partial}{\partial R}\left[(\dot{R}_{\text{vap}} - \alpha\sum_{i=1}^{N}\gamma_{1i}) f_d\right] + \left[\mathbf{F}_{\text{ext}} + \sum_{i=1}^{N}\gamma_{1i}\frac{3\alpha}{R}\mathbf{v}\right. \\ \left. - \frac{1}{R^3}\sum_{i=1}^{N}\beta_i m_i \boldsymbol{\gamma}_{3i}\right]\cdot\frac{\partial}{\partial\mathbf{v}} f_d = \sum_{i=1}^{N}(\gamma_{1i} - \gamma_{2i}) f_d - f_d\left(\frac{\partial}{\partial R}\alpha\sum_{i=1}^{N}\gamma_{1i}\right) \end{aligned} \tag{14}$$

To obtain this equation we have defined $\beta_i = 3\nu_i\tau/2\pi\rho_L$ and assumed the spray is diluted enough to neglect the interaction between droplets, represented by the collision integral J_{dd}. Now it is possible to look at the modified equation for the spray, Eq. (14), in a different way: the first two terms are the usual ones in all kinetic equations, the third term gives an effective vaporization rate

$$\dot{R}_{\text{eff}} = \dot{R}_{\text{vap}} - \alpha\sum_{i=1}^{N}\gamma_{1i}, \tag{15}$$

which is the vaporization rate for an isolated droplet modified by the collision with the gas molecules. The fourth term in Eq. (14) is a very interesting one because it is given by the external bulk force $\mathbf{F}_{\text{ext}}$ modified by collisions between the gas molecules and the droplets, it depends on the droplet characteristics as well as the gas properties. We hope the additional terms in this force will render us a drag force

$$\mathbf{F}_{\text{eff}} = \mathbf{F}_{\text{ext}} + \sum_{i=1}^{N} \gamma_{1i} \frac{3\alpha}{R} \mathbf{v} - \frac{1}{R^3} \sum_{i=1}^{N} \beta_i m_i \boldsymbol{\gamma}_{3i}, \tag{16}$$

Finally, the right hand side of that equation is a linearized collision term in a Williams-like kinetic equation, which looks like a Bhatnagar, Gross, Krook [10] approximation for the droplets, with a relaxation time given by

$$\Theta^{-1}(R, \mathbf{v}, \{\text{gas}\}) = -\sum_{i=1}^{N} (\gamma_{1i} - \gamma_{2i}) + \frac{\partial}{\partial R} \left(\alpha \sum_{i=1}^{N} \gamma_{1i} \right), \tag{17}$$

The spray kinetic equations are then written as:

$$\frac{\partial}{\partial t} f_d + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} f_d + \frac{\partial}{\partial R} [\dot{R}_{\text{eff}} f_d] + \mathbf{F}_{\text{eff}} \cdot \frac{\partial}{\partial \mathbf{v}} f_d = -\Theta^{-1} f_d, \tag{18}$$

$$\begin{aligned} \frac{\partial}{\partial t} f_i + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{x}} f_i + \mathbf{F}_{\text{ext}} \cdot \frac{\partial}{\partial \mathbf{v}} f_i &= \sum_{j=1}^{N} J_{ij}(f_i, f_j) + \\ &+ \int f_d [f_i(-\mathbf{c}_i, \mathbf{x}, t) - f_i(\mathbf{c}_i, \mathbf{x}, t)] g_{id} d\Gamma_{id} dR d\mathbf{v}, \quad (i = 1, \ldots, N). \end{aligned} \tag{19}$$

They are coupled equations but the droplets distribution function only appears in a linear way.

3. General balance equations

In order to obtain the balance equation for the spray we need a definition for the average quantities. Let $\phi_i(\mathbf{c}_i, \mathbf{x}, t)$ be any function of the species variables in the gas, its average given by

$$\{\phi_i(\mathbf{c}_i, \mathbf{x}, t)\} = \frac{1}{n_i} \int d\mathbf{c}_i f_i(\mathbf{c}_i, \mathbf{x}, t) \phi_i(\mathbf{c}_i, \mathbf{x}, t), \tag{20}$$

where

$$n_i = \int d\mathbf{c}_i f_i(\mathbf{c}_i, \mathbf{x}, t) \tag{21}$$

is the number density for the i component in the mixture.

If we want to obtain the average of a function of the droplets variables $\phi_d(R,\mathbf{v},\mathbf{x},t)$, we will use the corresponding average

$$\langle \phi_d(R,\mathbf{v},\mathbf{x},t)\rangle = \frac{1}{\langle N\rangle}\int f_d(R,\mathbf{v},\mathbf{x},t)\phi_d((R,\mathbf{v},\mathbf{x},t)d\mathbf{v}, \tag{22}$$

where

$$\langle N\rangle = \int f_d(R,\mathbf{v},\mathbf{x},t)d\mathbf{v} \tag{23}$$

is the number of droplets of radius R in the volume $d\mathbf{x}$ at time t.

When the quantity we are interested in does not depend on the radius of the droplets, we can also average over them, thus obtaining the corresponding local quantity, *i.e.*

$$\langle\langle \phi_d\rangle\rangle = \frac{1}{\langle\langle N\rangle\rangle}\int f_d(R,\mathbf{v},\mathbf{x},t)\phi_d(R,\mathbf{v},\mathbf{x},t)d\mathbf{v}dR, \tag{24}$$

where

$$\langle\langle N\rangle\rangle = \int \langle N\rangle dR \tag{25}$$

is the number of droplets in $d\mathbf{x}$ at time t.

The general balance equation for any physical variable associated with the i-component of the gas mixture is obtained multiplying Eq. (19) by the corresponding function $\phi_i(\mathbf{c}_i,\mathbf{x},t)$ and integrating over $\mathbf{c}_i$, the result is

$$\frac{\partial}{\partial t}n_i\{\phi_i\} + \nabla\cdot[n_i\{\phi_i\}\mathbf{U} + n_i\{\mathbf{c}_i\phi_i\}] - n_i\left[\{\frac{\partial}{\partial t}\phi_i\} + \{\mathbf{c}_i\cdot\nabla\phi_i\} + \mathbf{F}_{\text{ext}}\cdot\{\nabla_{\mathbf{c}_i}\phi_i\}\right]$$
$$= \sum_{j=1}\int \phi_i J_{ij}(f_i,f_j)d\mathbf{c}_i + \langle\langle \mu_i\phi_i\rangle\rangle, \tag{26}$$

where $\mathbf{U}$ is the hydrodynamic velocity of the whole system and it is given in terms of the gases velocities $\mathbf{u}_j$,

$$\mathbf{U} = \frac{n\mathbf{u}_g + \langle\langle N\rangle\rangle\,\langle\langle \mathbf{v}\rangle\rangle}{n + \langle\langle N\rangle\rangle}, \tag{27}$$

$$\mathbf{u}_g = \frac{1}{n}\sum_{j=1}^{N} n_j\mathbf{u}_j, \tag{28}$$

$$\mathbf{u}_j = \frac{1}{n_j}\int \mathbf{c}_j f_j(\mathbf{c}_j, \mathbf{x}, t) d\mathbf{c}_j, \tag{29}$$

The quantity μ_i is given by

$$\mu_i(R, \mathbf{v}, \{\text{gas}\}) = \int [f_i(-\mathbf{c}_i, \mathbf{x}, t) - f_i(\mathbf{c}_i, \mathbf{x}, t)] g_{id} d\Gamma_{id} \tag{30}$$

and it depends on the droplets' variables and the properties of the mixture.

On the other hand, the general balance equation for any function of the droplets variables is given by

$$\begin{aligned}
&\frac{\partial}{\partial t}(\langle N\rangle\langle\phi_d\rangle) + \frac{\partial}{\partial \mathbf{x}}\cdot[\langle N\rangle\langle\mathbf{v}\phi_d\rangle] + \frac{\partial}{\partial R}[\langle N\rangle\langle\dot{R}_{\text{eff}}\phi_d\rangle] \\
&- \langle N\rangle\left[\left\langle\frac{\partial}{\partial t}\phi_d\right\rangle + \left\langle\frac{\partial}{\partial \mathbf{x}}\cdot\mathbf{v}\phi_d\right\rangle + \left\langle\dot{R}_{\text{eff}}\frac{\partial}{\partial R}\phi_d\right\rangle\left\langle\frac{\partial}{\partial \mathbf{v}}\cdot\phi_d\mathbf{F}_{\text{eff}}\right\rangle\right] \\
&= -\langle N\rangle\langle\Theta^{-1}\phi_d\rangle.
\end{aligned} \tag{31}$$

All variables in this equations are functions of $\mathbf{x}, t$ and the radius R of the droplets.

4. Balance equations in the mixture of gases

In this Section we will consider some special cases of the balance equations we wrote in Section 3. We begin with the mass equation and to obtain it, we choose $\phi_i = m_i$ and substitute in Eq. (26). The result is given by

$$\frac{\partial}{\partial t}\rho_i + \nabla\cdot(\rho_i\mathbf{u}_i) = \sum_{j=1}^{N}{}' \int m_i J_{ij}(f_i, f_j) d\mathbf{c}_i + m_i\langle\langle\mu_i\rangle\rangle, \tag{32}$$

where the symbol $\sum_{j=1}^{N}{}'$ means that the term $i = j$ is absent and $\rho_i = n_i m_i$. That term is zero because the conservation of mass, momentum and energy is valid in a $i - i$ molecular collision

$$\int J_{ii}(f_i, f_i)\begin{pmatrix} m_i \\ m_i c_i \\ \frac{1}{2}m_i c_i^2 \end{pmatrix} d\mathbf{c}_i = 0. \tag{33}$$

Eq. (32) can be written as a concentration balance equation for i-species but we do not need it explicitly.

To obtain the momentum balance we choose $\phi_i = m_i\mathbf{c}_i$ to sustitute in Eq. (26), then

$$\frac{\partial}{\partial t}\rho_i\mathbf{u}_i + \nabla\cdot[\rho_i(\mathbf{u}_i\mathbf{U}+\mathbf{U}\mathbf{u}_i-\mathbf{U}\mathbf{U})+\mathbb{P}_i] = \rho_i\mathbf{F}_{\text{ext}} + \sum_{j=1}^{N}{}' \int J_{ij}m_i\mathbf{c}_i d\mathbf{c}_i + \langle\langle m_i\mathbf{c}_i\mu_i\rangle\rangle\,, \tag{34}$$

where $\mathbb{P}_i$ is the pressure tensor defined as

$$\mathbb{P}_i = \int m_i\mathbf{c}_i\mathbf{c}_i f_i(\mathbf{c}_i,\mathbf{x},t)d\mathbf{c}_i. \tag{35}$$

In a similar way we obtain the energy balance equation, in that case $\phi_i = (1/2)m_ic_i^2$ is the total energy because we assumed the molecules have no internal degrees of freedom. The macroscopic variable corresponding to that function is given by

$$n_ie_i = \int \tfrac{1}{2}m_ic_i^2 f_i(\mathbf{c}_i,\mathbf{x},t)d\mathbf{c}_i. \tag{36}$$

The balance equation we obtain is the following one

$$\frac{\partial}{\partial t}\rho_ie_i + \nabla\cdot[\rho_ie_i\mathbf{U}+\mathbf{q}_i] = \sum_{j=1}^{N}\int \tfrac{1}{2}m_ic_i^2 J_{ij}(f_i,f_j)d\mathbf{c}_i + \left\langle\left\langle \tfrac{1}{2}m_ic_i^2\mu_i\right\rangle\right\rangle, \tag{37}$$

where we have defined the heat flux $\mathbf{q}_i$

$$\mathbf{q}_i = \int \frac{1}{2}m_ic_i^2\mathbf{c}_i f_i(\mathbf{c}_i,\mathbf{x},t)d\mathbf{c}_i, \tag{38}$$

All balance equations we constructed here are similar to those used in kinetic theory of gases, but they have an additional source term coming from the interaction with the droplet immersed in the gas mixture.

5. Droplet balance equations

To study the droplets behavior we will take some particular cases of the general balance equation given in Eq. (39). First of all we are interested in the number of droplets in a volume $d\mathbf{x}$ at time t with radius between R and $R+dR$. That information is obtained by taking $\phi_d = 1$ in Eq. (39)

$$\frac{\partial}{\partial t}\langle N\rangle + \frac{\partial}{\partial\mathbf{x}}(\langle N\rangle\langle\mathbf{v}\rangle) = -\frac{\partial}{\partial R}(\langle N\rangle\langle\dot{R}_{\text{eff}}\rangle) + \langle N\rangle\left[\left\langle\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{F}_{\text{eff}}\right\rangle - \langle\Theta^{-1}\rangle\right]. \tag{39}$$

We immediately see that the number of droplet does not obey a conservation equation as one would expect, there are changes caused by the effective vaporization rate, the effective force acting on the droplets and the relaxation due to the interaction with the gas molecules.

We define the droplets mass density as

$$\rho_d(R,\mathbf{x},t) = \tfrac{4}{3}\pi\rho_L R^3 \langle N\rangle. \tag{40}$$

The balance equation is obtained by making $\phi_d = \frac{4}{3}\pi\rho_L R^3$ in Eq. (31), or multiplying Eq. (39) by ϕ_d, since the average in velocities does not affect that function,

$$\frac{\partial}{\partial t}\rho_d + \frac{\partial}{\partial \mathbf{x}}\cdot\rho_d\langle\mathbf{v}\rangle = \rho_d\left[-\frac{\partial}{\partial R}\langle\dot{R}_{\text{eff}}\rangle + \left\langle\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{F}_{\text{eff}}\right\rangle - \langle\Theta^{-1}\rangle\right]. \tag{41}$$

Following with the scheme of balance equations, we now construct the momentum balance by taking $\phi_d = \frac{4}{3}\pi\rho_L R^3\mathbf{v}$ in Eq. (31)

$$\begin{aligned}\frac{\partial}{\partial t}(\rho_d\langle\mathbf{v}\rangle) + \frac{\partial}{\partial\mathbf{x}}\cdot[\rho_d\langle\mathbf{v}\rangle\langle\mathbf{v}\rangle + \rho_d\langle\dot{\mathbf{V}}\dot{\mathbf{V}}\rangle] &= -\operatorname{grad}\left(\rho_d\left\langle\frac{V^2}{3}\right\rangle\right) + \rho_d\mathbf{F}_{\text{eff}}\\ &+ \rho_d\left[-\langle\mathbf{v}\dot{R}_{\text{eff}}\rangle\frac{\partial}{\partial R}\ln\langle N\rangle + \left\langle\mathbf{v}\left(\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{F}_{\text{eff}}\right)\right\rangle - \langle\mathbf{v}\Theta^{-1}\rangle\right],\end{aligned} \tag{42}$$

where $\mathbf{V} = \mathbf{v} - \langle\mathbf{v}\rangle$ and $\dot{\mathbf{V}}\dot{\mathbf{V}}$ means traceless $\mathbf{VV}$ tensor. Eq. (42) looks like an usual momentum equation provided we can interpret the tensor $\rho_d\langle\dot{\mathbf{V}}\dot{\mathbf{V}}\rangle$ as the viscous tensor and $\rho_d\langle V^2/3\rangle$ as the pressure, we observe that both terms are in fact the correlation of the droplets velocities. The last three terms are the momentum sources also caused by vaporization, the effective force and relaxation respectively.

In a similar way we obtain the energy equation with a function $\phi_d = \frac{4}{3}\pi\rho_L R^3\frac{v^2}{2}$

$$\begin{aligned}\frac{\partial}{\partial t}e_d + \frac{\partial}{\partial\mathbf{x}}\cdot[e_d\langle\mathbf{v}\rangle + \mathbf{q}_d + \mathbb{P}_d\cdot\langle\mathbf{v}\rangle] &= \rho_d\left[\left\langle\frac{v^2}{2}\dot{R}_{\text{eff}}\right\rangle\frac{\partial}{\partial R}\ln\langle N\rangle\right.\\ &\left. + \left\langle\frac{\partial}{\partial\mathbf{v}}\cdot\frac{v^2}{2}\mathbf{F}_{\text{eff}}\right\rangle - \left\langle\frac{v^2}{2}\Theta^{-1}\right\rangle\right],\end{aligned} \tag{43}$$

where e_d is the total energy, $\mathbf{q}_d$ the heat flux associated with the droplets and $\mathbb{P}_d$ the pressure tensor, they are given by

$$e_d = \tfrac{1}{2}\rho_d(\langle\mathbf{v}\rangle^2 + \langle v^2\rangle), \tag{44}$$

$$\mathbf{q}_d = \rho_d\left\langle\frac{V^2}{2}\mathbf{V}\right\rangle, \tag{45}$$

$$\mathbb{P}_d = \rho_d \langle \dot{\mathbf{V}}\dot{\mathbf{V}} \rangle + \rho_d \left\langle \frac{V^2}{3} \right\rangle \mathbb{I}. \tag{46}$$

The pressure tensor written here is the same we identified in the momentum Eq. (42), it i.e. it gives us the droplets velocity correlation function. We wrote it in terms of the contributions coming from the symmetric part and the isotropic one, to compare with the corresponding hydrostatic pressure and the viscous part.

6. Comparison with the phenomenological theory

Now we compare the balance equations we obtained in the last two sections with the corresponding ones in the phenomenological theory [9] developed to study this kind of systems. First of all, our kinetic treatment allows us to identify the relevant variables to be used and afterwards the mass, momentum and energy sources, in such a way that we have now a kinetic expression for them and we know their origin. On the other hand, in the phenomenological work we assumed the total system obeys the usual conservation equations, that assumption implying some restrictions on the sources.

From the point of view of kinetic theory it is not necessary to impose such restrictions, but we will do it in order to have a complete comparison between both approaches, at least for spray behavior. For the mass sources we have

$$\sum_{i=1}^{N}\sum_{j=1}^{N}{}' \int m_i J_{ij}(f_i, f_j) d\mathbf{c}_i + \sum_{i=1}^{N} m_i \langle\langle \mu_i \rangle\rangle \\ + \int \rho_d \left[-\frac{\partial}{\partial R} \langle \dot{R}_{\text{eff}} \rangle + \left\langle \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{F}_{\text{eff}} \right\rangle - \langle \Theta^{-1} \rangle \right] dR = 0. \tag{47}$$

The first term in Eq. (47) is identically equal to zero because the mass of molecules is invariant in the $i-j$ collision, in fact the collisional invariants satisfy the following equation

$$\sum_{i=1}^{N}\sum_{j=1}^{N}{}' \int \begin{pmatrix} m_i \\ m_i \mathbf{c}_i \\ \frac{1}{2} m_i c^2 \end{pmatrix} J_{ij}(f_i, f_j) d\mathbf{c}_i = 0. \tag{48}$$

The last term in Eq. (47) can be simplified by means of Eq. (24), then

$$\sum_{i=1}^{N} m_i \langle\langle \mu_i \rangle\rangle + \langle\langle N \rangle\rangle \left\langle \left\langle \rho_d \left[-\frac{\partial}{\partial R} \langle \dot{R}_{\text{eff}} \rangle + \left\langle \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{F}_{\text{eff}} \right\rangle - \langle \Theta^{-1} \rangle \right] \right\rangle \right\rangle = 0. \tag{49}$$

In a similar way we obtained the restriction equations in the momentum and energy balance, they are the following ones:

$$\sum_{i=1}^{N}\langle\langle m_i \mathbf{c}_i \mu_i\rangle\rangle + \langle\langle N\rangle\rangle \left\langle\left\langle \rho_d \left[-\langle \mathbf{v}\dot{R}_{\text{eff}}\rangle \frac{\partial}{\partial R}\ln\langle N\rangle + \left\langle \mathbf{v}\left(\frac{\partial}{\partial \mathbf{v}}\cdot \mathbf{F}_{\text{eff}}\right)\right\rangle - \langle \mathbf{v}\Theta^{-1}\rangle\right]\right\rangle\right\rangle = 0, \tag{50}$$

$$\sum_{i=1}^{N}\langle\langle \tfrac{1}{2} m_i c_i^2 \mu_i\rangle\rangle + \langle\langle N\rangle\rangle \left\langle\left\langle \rho_d \left[\left\langle \frac{v^2}{2}\dot{R}_{\text{eff}}\right\rangle \frac{\partial}{\partial R}\ln\langle N\rangle + \left\langle \frac{\partial}{\partial \mathbf{v}}\cdot \frac{v^2}{2}\mathbf{F}_{\text{eff}})\right\rangle - \left\langle \frac{v^2}{2}\Theta^{-1}\right\rangle\right]\right\rangle\right\rangle = 0, \tag{51}$$

for the momentum and energy sources respectively.

A close comparison of the set of phenomenological equations [9] and the kinetic ones, shows us the role played by the interaction between the mixture of gases and the droplets. This interaction is very important to study the behavior of a spray and our kinetic model will allow us to calculate some of its characteristics.

7. Concluding remarks

In this work we studied a kinetic model for a spray, which is based on the Boltzmann and Williams equations, strongly coupled to take into account the interaction between the mixture of gases and the droplets. We obtained a modified kinetic equation valid for the droplets which rendered us an effective vaporization rate and an effective force acting on the droplets as well as a relaxation time. Those quantities depend on the gas and droplets properties, their calculation requiring a solution for the distribution functions. The solution of the equations is far from being a trivial one, we hope to solve them in an approximate way in a future work.

We used the kinetic equations to obtain the mass, momentum and energy balance equations for the mixture of gases and droplets. The corresponding sources were identified and we wrote the restrictions for them in order to have the conservation of mass, energy and the balance equation for the momentum for the whole system, as we did in the phenomenological theory developed to study this system.

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Resumen. En este trabajo se desarrolla la descripción cinética de un sistema inhomogéneo. El sistema está constituido por un conjunto de gotas de tamaños diferentes y que están inmersas en una mezcla multicomponente de gases. En un trabajo anterior estudiamos este problema desde el punto de vista fenomenológico, aquí suponemos que tanto las gotas como los gases están descritos por funciones de distribución. Dichas funciones satisfacen las ecuaciones de Williams y de Boltzmann respectivamente. El conjunto de ecuaciones se acoplan mediante la interacción entre las gotas y los gases. Encontramos que la razón de evaporación se ve afectada por las colisiones con las moléculas de los gases. También aparece una fuerza que actua sobre las gotas, causada por las colisiones con el gas. Se identifican las fuentes de masa, momento y energía que fueron definidas en un tratamiento fenomenológico previo, con el objeto de obtener las ecuaciones de conservación del sistema como un todo.