

Method of Kinetic Equations for Homogeneous and Multi-Phase Reactive Flows

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Abstract. The paper deals with the application of kinetic equations formalism to the description of homogeneous and multi-phase flows. In case of the homogeneous flow, the solution of the kinetic equation is treated as a fictitious one-particle distribution function for a set of notional particles. The low moments of the distribution function satisfy the fundamental conservation laws. In the case of the two-phase flows, two one-particle distribution functions are used. For various models of the two-phase flow, the corresponding closed-form kinetic equations are derived. In all cases, the kinetic equation can be represented by a set of Lagrange equations for notional particles. This allows one to apply particle methods to the numerical integration of the kinetic equations. The set of representative Lagrange equations differs from the standard set of equations applied when using the technique of probability density functions.

INTRODUCTION

The method of kinetic equations is one of the basic methods in the theory of nonequilibrium processes and is widely used in various fields of science [1, 2], e.g., gas dynamics, physics of condensed matter, plasma physics, biophysics, astrophysics, etc. The method is based on considering an evolution (kinetic) equation for one-particle distribution function with the type of particles specified for each application. In many cases, the solution of the evolution equation provides important characteristics of nonequilibrium processes. The opportunity of obtaining a closed-form kinetic equation for a nonequilibrium process is very attractive, since a single evolution equation can be used instead of an infinite chain of kinetic equations. A typical example is given by the Vlasov equation in plasma physics [1, 2]. Another example is the evolution equation for the one-particle probability density function (PDF) in the problem of turbulent combustion (see, e.g., [3, 4]). Evolution equations for a one-particle PDF governing a nonequilibrium process in a homogeneous flow with fluctuating characteristics are proposed in [3, 4].

This paper deals with a new type of kinetic equations for the one-particle distribution functions in homogeneous and heterogeneous flows. The main idea of the approach is to represent the evolution of a real flow by the kinetic equation for a fictitious distribution function. The only requirement set to the fictitious function is that its moments exactly correspond to physical variables of the real flow. This means that the fictitious distribution function does not necessarily correspond to the one-particle distribution function of a real flow; however, the moments of this function must satisfy the fundamental equations of gas dynamics. Thus, the objective of this paper is to generate a closed-form kinetic equation for a fictitious distribution function such that the solution of the equation is identical to the solution of fundamental conservation equations in terms of the moments of the fictitious function. The availability of this approach would allow to solve complicated problems of fluid dynamics by particle methods.

In Section 1, the method is illustrated for diverse flows, in particular homogeneous isothermal and nonisothermal, inviscid and viscous, single-component and multi-component, reactive and nonreactive. In Section 2 the analysis is carried over to two-phase flows.

1. KINETIC EQUATIONS AND THE SIMULATION OF HOMOGENEOUS FLOWS

1.1. *General Approach: Standard Euler Equations for Isothermal Flow*

It is assumed that, at any spatial point of physical space, there exists a large ensemble of notional particles constituting possible “internal states” of the matter. The “internal states” are represented by the number of particles in the ensemble, particle velocities, energies, species concentrations, etc. The evolution of the ensemble at each point in the physical space will be described by the evolution of a one-particle distribution function similarly to the transported PDF [3, 4] and cellular automata [5] approaches.

Let $F(t, x, v)$ be the one-particle distribution function of notional particles in the one-particle phase space at the time instant t and at the point (x, v) . Here x stands for the position and v for the particle velocity. In the following we assume that the function F rapidly decays to zero as $v \rightarrow \infty$. Then the local instantaneous density of the flow ρ is nothing but the number density of notional particles defined as

$$\rho = \rho(x, t) = \int F(t, x, v) dv. \quad (1)$$

It is further assumed that the local instantaneous flow velocity u is equal to the ensemble mean velocity for relevant notional particles, i.e., $u = u(x, t) = \langle v \rangle$. In terms of the function F , the flow velocity u is defined by the relation

$$\rho u = \rho \langle v \rangle = \int v F(t, x, v) dv. \quad (2)$$

Clearly, Eqs. (1) and (2) give the zero-order and first-order moments for the function F with respect to the variable v .

The next step in the analysis is the assumption that the evolution of the set of notional particles in the phase space is described by the following generalized kinetic equation of Vlasov type:

$$\partial_t F = -\partial_x (\langle v \rangle F) - \partial_v (AF). \quad (3)$$

In Eq. (3), A is both an unknown vector function of x and a functional of F (the explicit form of the function A will be specified below). The symbol $\partial_x(a(x, v))$ in Eq. (3) stands for the divergence of the vector a with respect to the spatial variable x for a chosen value of the variable v .

The Lagrange set of equations that corresponds to Eq. (3) is

$$\dot{x} = \langle v \rangle, \quad \dot{v} = A, \quad (4)$$

where the dot stands for the substantial derivative with respect to time.

Let us now determine the explicit form of the function A in Eqs. (3) and (4) such that the moments of the function F satisfy the standard Euler equations.

Integrating Eq. (3) with respect to v and taking into account the fact that $\int \partial_v (AF) dv = 0$ (this is equivalent to the assumption that $F \rightarrow 0$ as $v \rightarrow \infty$), we obtain

$$\partial_t \int F(t, x, v) dv = -\partial_x \left(\langle v \rangle \int F(t, x, v) dv \right).$$

The use of the form of Eqs. (1) and (2) enables us to rewrite this equation as follows:

$$\partial_t \rho = -\partial_x (\rho \langle v \rangle). \quad (5)$$

We now multiply Eq. (3) by v and integrate the resulting equation with respect to v . Applying the formula of integration by parts, $\int v \partial_v (AF) dv = -\int (AF) dv$, we obtain

$$\begin{aligned} \partial_t (\rho \langle v \rangle) &= -\partial_x (\rho \langle v \rangle \langle v \rangle) - \int v \partial_v (AF) dv \\ &= -\partial_x (\rho \langle v \rangle \langle v \rangle) + \int AF dv = -\partial_x (\rho \langle v \rangle \langle v \rangle) + \rho A. \end{aligned} \quad (6)$$

The standard Euler equations [6] become

$$\partial_t \rho = -\partial_x (\rho u), \quad \partial_t (\rho u) = -\partial_x (\rho u u) - \partial_x p, \tag{7}$$

where $p = p(\rho)$ is the pressure. In Eqs. (7), the symbol uu stands for the tensor multiplication of a vector u by itself, i.e., uu is the matrix with the (i, j) th element equal to the product of the i th and j th components of the vector u . Moreover, we denote by $\partial_x \mathbf{M}$ the divergence of a matrix \mathbf{M} , which is equal to the vector whose components are the divergences of the rows of the matrix.

Comparing Eqs. (7) with Eqs. (5) and (6), one finds that they are equivalent if

$$\rho A = -\partial_x p \quad \text{or} \quad A = -\frac{\partial_x p}{\rho}. \tag{8}$$

Thus, the standard Euler equations (7) can be derived from the kinetic equation (3) for the distribution function F by assuming that the function A is given by (8). To take into account possible source terms (like volume forces, etc.), the function A must be appropriately modified.

As is known, the transport-PDF method (see, e.g., [4]) can be applied to derive approximate governing equations for the flow dynamics with the subsequent use of Monte Carlo simulation. The current approach provides the exact governing equations for the flow dynamics by adopting a proper representation of the flow. In the transport-PDF method, the one-particle distribution function approximately represents flow realizations. In the method under consideration, the one-particle distribution function F does not necessarily represent flow realizations due to the condition $u = \langle v \rangle$. For this reason, the distribution function F can be treated as a fictitious one. Nevertheless, the moments of the function F are physical variables that satisfy the exact fundamental equations of the flow dynamics.

1.2. Discussion

The Lagrange equations (4) apparently differ from the standard equations of the transport PDF method by the fact that the first equation is written in terms of the local mean velocity $\langle v \rangle$ rather than the local instantaneous velocity v of notional particles. However, this modification follows from the very definition of a one-particle distribution function F .

If the kinetic equation (3) uses v instead of $\langle v \rangle$, then the equation for the first-order moment for the function F must contain a term with the second-order moment, and the resulting set of equations turns out to be nonclosed.

Let us illustrate this closure problem by trying to derive the set of equations of gas dynamics from the simplest kinetic equation

$$\partial_t F(t, x, v) = -\partial_x (vF(t, x, v)). \tag{9}$$

Integrating Eq. (9) with respect to v and taking into account that $\int \partial_v (F) dv = 0$, we obtain

$$\partial_t \int F(t, x, v) dv = -\partial_x \left(\int vF(t, x, v) dv \right),$$

and hence

$$\partial_t \rho = -\partial_x (\rho \langle v \rangle).$$

Next, after multiplying Eq. (9) by v and integrating the resulting equation with respect to v , we can write

$$\partial_t (\rho \langle v \rangle) = -\partial_x \left(\rho \int v v F dv \right) = -\partial_x (\langle v \rangle \rho \langle v \rangle) - \partial_x \int (v - \langle v \rangle) (v - \langle v \rangle) F dv = -\partial_x (\langle v \rangle \rho \langle v \rangle) - \partial_x P.$$

Here we used the fact that the mean value of the “thermal” velocity $(v - \langle v \rangle)$ is zero, and the stress tensor P is given by

$$P = \int (v - \langle v \rangle) (v - \langle v \rangle) F dv.$$

Similarly, after multiplying Eq. (9) by $v^2/2$ and integrating the resulting equation, we obtain

$$\partial_t(\rho E) = -\partial_x(\rho u E) - \partial_x(uP), \quad \text{where} \quad \rho E = \int \left(\frac{v^2}{2}\right) F dv.$$

The resulting set of differential equations resembles the equations of gas dynamics; however, it is not closed. It is impossible to define the stress tensor P in terms of the variables ρ , E , and $\langle v \rangle$. This means that this approach cannot lead to an equation of state of the form $P = P(\rho, E, \langle v \rangle)$.

The choice of the kinetic equation in the form of Eq. (3) avoids this closure problem because the derivation procedure involves the zero-order and first-order moments only, and the second-order moments do not occur at all. In this procedure, the equation of state is used when determining the function A in Eq. (8).

Note that the closure problem also arises if the Boltzmann equation is used instead of Eq. (9). The corresponding closure problem is discussed in [7]. If the function $F(t, x, v)$ is assumed to be isotropic with respect to v (i.e., F is a function of $|v|$ for any chosen t and x), then the second-order moments can be derived provided that the zero-order and first-order moments are known, and the resulting set of equations turns out to be closed. The Maxwell distribution function with parameters depending on t and x is considered in [7] as an example; strictly speaking, this application of [7] is incorrect because the isotropy of the function F with respect to v (even if it holds initially) can fail in the course of time. However, the isotropy condition (with respect to v) for the function F used in [7] can hold after passing to the well-known limit $\delta \rightarrow 0$, where the parameter $1/\delta$ is the multiplier of the collision integral on the right-hand side of the Boltzmann equation. This limiting procedure results in a rapid decay to isotropy due to the large number of collisions (of order $1/\delta$). The justification of this limiting procedure is a rather complicated mathematical problem. The equation of state thus obtained is known to correspond to ideal gas. It should be noted that the current approach using the kinetic equation (3) requires no limiting procedure and is applicable without any constraints on the equation of state.

1.3. Standard Euler Equations for Nonisothermal Flow

In the set of gas dynamic equations (7), the equation of state was taken in the form $p = p(\rho)$. For the more general case $p = p(\rho, s)$, where s is the entropy, we face a substantial difficulty, which is illustrated below by a simple example.

It seems natural to assume that the total energy $E = E_i + u^2/2$ is given by

$$\rho E = \int \left(\frac{v^2}{2}\right) F dv = \frac{\rho \langle v \rangle^2}{2} + \rho E_i, \quad (10)$$

where E_i is the internal energy. Let us derive the corresponding equation for the function E defined by Eq. (10). Multiplying Eq. (3) by $v^2/2$, integrating the resulting equation with respect to v , and using the formula of integration by parts, we obtain

$$\begin{aligned} \partial_t(\rho E) &= -\partial_x(\rho \langle v \rangle E) - \int \left(\frac{v^2}{2}\right) \partial_v(AF) dv \\ &= -\partial_x(\rho \langle v \rangle E) + \int vAF dv = -\partial_x(\rho \langle v \rangle E) + \rho \langle v \rangle A. \end{aligned}$$

Taking into account Eq. (8), we see that

$$\partial_t(\rho E) = -\partial_x(\rho \langle v \rangle E) - \langle v \rangle \partial_x p. \quad (11)$$

If we assume that $p = p(\rho, E_i)$, then the resulting set of equations for the zero-, first-, and second-order moments is closed. However, this set of equations differs from the set of fundamental equations of gas dynamics (see, e.g., [4]). The following equation is valid instead of Eq. (11):

$$\partial_t(\rho E) = -\partial_x(\rho u E) - \partial_x(up). \quad (12)$$

To find a correct set of equations of gas dynamics in the case of a more general equation of state, e.g., for $p = p(\rho, s)$, one must extend the phase space by adding a supplementary variable E . In this case, the function F becomes $F = F(t, x, v, E)$, and the particle number density, the mean velocity, and the total energy are then defined as

$$\rho = \int F(t, x, v, E) dv dE, \quad \rho \langle v \rangle = \int v F(t, x, v, E) dv dE, \quad \rho \langle E \rangle = \int E F(t, x, v, E) dv dE,$$

and the kinetic equation becomes

$$\partial_t F = -\partial_x(\langle v \rangle F) - \partial_v(AF) - \partial_E(BF),$$

and contains an additional unknown function B . The explicit form of B is determined below.

Using a procedure similar to that used above, we obtain the equation

$$\partial_t \int E F(t, x, v, E) dv dE = -\partial_x(\langle v \rangle \int E F(t, x, v, E) dv dE) - \int E \partial_v(AF) dv dE - \int E \partial_E(BF) dv dE,$$

and therefore

$$\partial_t(\rho \langle E \rangle) = -\partial_x(\rho \langle v \rangle \langle E \rangle) + B\rho. \tag{13}$$

With regard for Eq. (8), the last equation is equivalent to Eq. (12) if the function $E = E(t, x)$ in Eq. (12) is replaced by $\langle E \rangle$ and B is taken in the form $B = -\partial_x(p\langle v \rangle)/\rho$.

Thus, the introduction of an additional scalar variable E enables us to obtain the set of equations of gas dynamics with a more general equation of state. In other words, to obtain the conservation law of entropy, one must specify the additional variable E for each notional particle.

1.4. Standard Euler Equations for a Multi-Component Reactive Flow

For the general case in which there are many scalar variables along with the entropy (e.g., the species concentrations), the dimension of the phase space must be increased by adding supplementary variables $\Phi_1, \Phi_2, \dots, \Phi_k$; we introduce the notation $\Phi = (\Phi_1, \Phi_2, \dots, \Phi_k)$. The function F becomes $F = F(t, x, v, E, \Phi)$, and the particle number density, the mean velocity, the mean energy $\langle E \rangle$, and the mean scalar $\langle \Phi \rangle$ are defined as follows:

$$\begin{aligned} \rho &= \int F(t, x, v, E, \Phi) dv dE d\Phi, & \rho u &= \int v F(t, x, v, E, \Phi) dv dE d\Phi, \\ \rho \langle E \rangle &= \int E F(t, x, v, E, \Phi) dv dE d\Phi, & \rho \langle \Phi \rangle &= \int \Phi F(t, x, v, E, \Phi) dv dE d\Phi. \end{aligned} \tag{14}$$

Consider the corresponding set of Euler equations. An equation describing the evolution of scalars ϕ must be added to the set of Eqs. (7), (12),

$$\partial_t \phi + u \partial_x \phi = S, \tag{15}$$

where S is the source term. The kinetic equation is taken in the form

$$\partial_t F = -\partial_x(\langle v \rangle F) - \partial_v(AF) - \partial_E(BF) - \partial_\Phi(CF). \tag{16}$$

The derivation of equations for $\rho, u = \langle v \rangle$ and $e = \langle E \rangle$ is similar to that presented above if the additional term is assumed to have a negligible contribution due to the rapid decay at infinity of the function F with respect to the variables v, E , and Φ .

Let us derive the equation for the evolution of $\langle \Phi \rangle$. Multiplying Eq. (16) by Φ and integrating the resulting equation with respect to v, E , and Φ , we see that

$$\begin{aligned} \partial_t \int \Phi F(t, x, v, E, \Phi) dv dE d\Phi &= -\partial_x \left(\langle v \rangle \int \Phi F(t, x, v, E, \Phi) dv dE d\Phi \right) \\ &\quad - \int \Phi \partial_v(AF) dv dE d\Phi - \int \Phi \partial_E(BF) dv dE d\Phi - \int \Phi \partial_\Phi(CF) dv dE d\Phi, \end{aligned}$$

and therefore

$$\partial_t(\rho\langle\Phi\rangle) = -\partial_x(\rho\langle v\rangle\langle\Phi\rangle) + C\rho$$

or (with regard to Eq. (5))

$$\partial_t\phi + u\partial_x\phi = C, \quad (17)$$

where ϕ stands for $\langle\Phi\rangle$. Clearly, to satisfy Eq. (15), one must take $C = S$.

As a special example, consider the flow of a multi-component reactive mixture of ideal gases disregarding the transport processes (viscosity, thermal conductivity, and diffusion). In this case, the vector Φ is represented by the vector $Y = (Y_1, Y_2, \dots, Y_{N-1})$, where Y_1, Y_2, \dots, Y_{N-1} are the mass fractions of the components with indices $1, 2, \dots, N-1$ in the mixture. The mass fraction of the N th component can be found from the relationship

$$\sum_{i=1}^N Y_i = 1.$$

The source term S is equal to the vector w/ρ , where w is the vector of chemical reaction rates (see, e.g., [8]). The equation of state is given by

$$p = \rho R^0 T \sum_{i=1}^N \frac{Y_i}{W_i},$$

where W_i is the molecular mass of the i th component.

Thus, the kinetic equation (16) results in the set of Euler equations for the multi-component reactive mixture of ideal gases [6].

1.5. Effect of Transport Processes

The effect of transport processes can readily be taken into account. For example, we can illustrate it for thermal conductivity. It is necessary to modify the function B in the kinetic equation (16) by setting

$$B = -\frac{\partial_x(pu)}{\rho} - \frac{\partial_x q}{\rho},$$

where q is the vector of heat flux (for the specific form of q , see [6]). A similar procedure of modifying the function B can be used to consider the effect of viscosity.

It should be noted that, for an incompressible fluid, there is another way of introducing the viscosity effect, which requires a more substantial modification of the kinetic equation. The analysis starts from the Navier–Stokes equations

$$\partial_t\rho = -\partial_x(\rho u), \quad \partial_t(\rho u) = -\partial_x(\rho u u) - \partial_x p + \nu\partial_x^2(\rho u). \quad (18)$$

For $\rho = \text{const}$, the kinetic equation can be considered in the form

$$\partial_t F = -\partial_x(\langle v\rangle F) - \partial_v(AF) + \partial_x^2(CF), \quad (19)$$

where the function A is given by Eq. (8), and the function C is to be determined.

Let us derive the set of equations (18) from Eq. (19). We begin by deriving the second equation of (18). For this purpose, multiply Eq. (19) by v . Then, by using the formula of integration by parts, we see that

$$\begin{aligned} \partial_t(\rho\langle v\rangle) &= -\partial_x(\rho\langle v\rangle\langle v\rangle) - \int v\partial_v(AF) dv + \partial_x^2 \int vCF dv \\ &= -\partial_x(\rho\langle v\rangle\langle v\rangle) + \int AF dv + \partial_x^2 \int vCF dv = -\partial_x(\langle v\rangle\rho\langle v\rangle) + \rho A + \partial_x^2(C\rho\langle v\rangle). \end{aligned}$$

Assuming that $C = \nu$, one arrives at the equation

$$\partial_t(\rho u) = -\partial_x(\rho u u) + \rho A + \nu \partial_x^2(\rho u),$$

which is similar to the second equation of system (18). The first equation of system (18) can be obtained by integrating Eq. (19) with respect to variable v . The contribution of the viscous term is zero because C and ρ are constant and

$$\int \partial_x^2(CF) dv = \partial_x^2 \left(\int CF dv \right) = \partial_x^2 \left(C \int F dv \right) = \partial_x^2(C\rho) = 0.$$

Hence, Eqs. (18) have been derived from the kinetic equation (19). The derivation procedure shows that the condition $\rho = \text{const}$ is of importance. Equation (19) corresponds to the ‘‘Langevin Lagrange system’’

$$\dot{x} = \langle v \rangle + \sqrt{2\nu} \xi(t), \quad \dot{v} = A, \quad (20)$$

where $\xi(t)$ is the vector of Gauss white noise with the standard covariant function $\overline{\xi(t)\xi(s)} = \delta(t-s)I$ (I is the identity matrix) [9]. This is entirely similar to the correspondence between the Fokker–Plank equation (the forward Kolmogorov equation) and the stochastic differential equation. The solution of the Fokker–Plank equation with the help of stochastic differential equations is similar to the solution of a hyperbolic partial differential equation by using the method of characteristics. This approach can be referred to as the method of stochastic characteristics followed by averaging over the ensemble of characteristics. In our case, Eq. (20) provides stochastic characteristics for the kinetic equation (19).

2. KINETIC EQUATIONS AND SIMULATION OF MULTI-PHASE FLOWS

2.1. General Approach: Euler Equations for Two-Phase Flow

In addition to notional particles representing the ‘‘internal states’’ of the gas phase (phase 1), one can introduce another set of particles which represent the dispersed phase (phase 2). The latter particles are regarded as solid spheres of diameter d . Both sets of particles are described by single-point distribution functions denoted as $F_1(t, v, x)$ and $F_2(t, v, x)$, respectively. Then the following relationships hold:

$$\alpha \rho_1 = \int F_1(t, x, v) dv, \quad (1 - \alpha) \rho_2 = \int F_2(t, x, v) dv, \quad (21)$$

where α is the volume fraction of particles of phase 1 at the time instant t and at the point x , the function ρ_1 gives the number density of particles of phase 1 per unit ‘available’ volume, and ρ_2 is the volume density of the solid sphere material. The ‘available’ volume is the volume occupied by phase 1; this is a part of the total volume. In principle, one can place an arbitrary number of particles of phase 1 into the ‘available’ volume with the constraint $\rho_2 = \text{const}$. In the following, the functions F_1 and F_2 are assumed to rapidly decay as $v \rightarrow \infty$.

We further assume that the distribution functions $F_1(t, x, v)$ and $F_2(t, x, v)$ satisfy the following set of kinetic equations:

$$\partial_t F_1 = -\partial_x(\langle v \rangle_1 F_1) - \partial_v(A F_1), \quad \partial_t F_2 = -\partial_x(\langle v \rangle_2 F_2) - \partial_v(B F_2), \quad (22)$$

where

$$\alpha \rho_1 \langle v \rangle_1 = \int v F_1(t, x, v) dv, \quad (1 - \alpha) \rho_2 \langle v \rangle_2 = \int v F_2(t, x, v) dv. \quad (23)$$

The functions $A = A(x, F_1, F_2)$ and $B = B(x, F_1, F_2)$ are vector functions of the point x and functionals of F_1 and F_2 . The explicit form of these functions must be determined.

Let us derive the set of Euler equations corresponding to Eqs. (22). For this purpose, we integrate the first equation of system (22) with respect to v and use the relation $\int \partial_v(AF_1) dv = 0$. This yields

$$\partial_t \int F_1(t, x, v) dv = -\partial_x \left(\langle v \rangle_1 \int F_1(t, x, v) dv \right),$$

and therefore

$$\partial_t (\alpha \rho_1) = -\partial_x (\alpha \rho_1 \langle v \rangle_1).$$

One can similarly prove that

$$\partial_t ((1 - \alpha) \rho_2) = -\partial_x ((1 - \alpha) \rho_2 \langle v \rangle_2).$$

Multiply the first equation of system (22) by v and integrate the resulting equation with respect to v . The repeated use of the formula of integration by parts yields

$$\begin{aligned} \partial_t (\alpha \rho_1 \langle v \rangle_1) &= -\partial_x (\alpha \rho_1 \langle v \rangle_1) - \int v \partial_v (AF_1) dv \\ &= -\partial_x (\alpha \rho_1 \langle v \rangle_1) + \int AF_1 dv = -\partial_x (\langle v \rangle_1 \alpha \rho_1 \langle v \rangle_1) + \alpha \rho_1 A. \end{aligned}$$

Similarly,

$$\partial_t (1 - \alpha) \rho_2 \langle v \rangle_2 = -\partial_x (\langle v \rangle_2 (1 - \alpha) \rho_2 \langle v \rangle_2) + (1 - \alpha) \rho_2 B.$$

Introduce the notation $u_1 = \langle v \rangle_1$ and $u_2 = \langle v \rangle_2$. As a result of the above transformations, we arrive at the following set of equations:

$$\begin{aligned} \partial_t (\alpha \rho_1) &= -\partial_x (\alpha \rho_1 u_1), & \partial_t ((1 - \alpha) \rho_2) &= -\partial_x ((1 - \alpha) \rho_2 u_2), \\ \partial_t (\alpha \rho_1 u_1) &= -\partial_x (\alpha \rho_1 u_1 u_1) + \alpha \rho_1 A, & \partial_t ((1 - \alpha) \rho_2 u_2) &= -\partial_x ((1 - \alpha) \rho_2 u_2 u_2) + (1 - \alpha) \rho_2 B. \end{aligned} \tag{24}$$

The set of Lagrange equations corresponding to Eqs. (22) is

$$\begin{aligned} \dot{x}^{(1)} &= u_1, & \dot{v}^{(1)} &= A, \\ \dot{x}^{(2)} &= u_2, & \dot{v}^{(2)} &= B. \end{aligned} \tag{25}$$

In a one-particle phase space (x_1, v_1, x_2, v_2) of a two-phase system, the kinetic equation for system (25) obviously is

$$\partial_t F = -\partial_{x_1}(u_1 F) - \partial_{x_2}(u_2 F) - \partial_{v_1}(AF) - \partial_{v_2}(BF). \tag{26}$$

If the functions F_1 and F_2 are solutions of Eqs. (22), then it can be proved directly that the function

$$F(t, x_1, v_1, x_2, v_2) = F_1(t, x_1, v_1) F_2(t, x_2, v_2)$$

is a solution of Eq. (26). Moreover, the mean velocities u_1 and u_2 obtained from F turn out to be equal to those obtained from F_1 and F_2 . Here we consider only the above product solutions of Eq. (26). In this sense only, the Lagrange system (25) corresponds to the kinetic system of Eqs. (22).

2.2. *Wijnngarden's Model*

Consider the model of two-phase flow suggested in [10]. In our notation,

$$\begin{aligned}\partial_t(\alpha\rho_1) &= -\partial_x(\alpha\rho_1u_1), & \partial_t((1-\alpha)\rho_2) &= -\partial_x((1-\alpha)\rho_2u_2), \\ \partial_t(\alpha\rho_1u_1) &= -\partial_x(\alpha\rho_1u_1u_1) + \alpha\partial_xp, & \partial_t((1-\alpha)\rho_2u_2) &= -\partial_x((1-\alpha)\rho_2u_2u_2) - (1-\alpha)\partial_xp.\end{aligned}\quad (27)$$

In addition, it is assumed that $\partial p/\partial\rho_1 = c^2$, where c is the sound velocity in phase 1. This relationship enables one to rewrite the equation of state in the form $p = p(\rho_1)$. Then Eqs. (27) can be regarded as a set of equations for the functions ρ_1 , α , u_1 , and u_2 . Comparing Eqs. (24) and (27), we see that $\alpha\rho_1A = -\alpha\partial_xp$ and $(1-\alpha)\rho_2B = -(1-\alpha)\partial_xp$, i.e.,

$$A = -\frac{\partial_xp}{\rho_1}, \quad B = -\frac{\partial_xp}{\rho_2}.\quad (28)$$

Thus, the set of equations (27) has been derived from the set of kinetic equations (22) for one-particle distribution functions under the assumption that the functions A and B are given by Eqs. (28). We stress that the ‘‘exact’’ equations of the two-phase flow model have been derived by using the method of kinetic equations.

The method suggested here is very flexible. If one needs to calculate, for example, the drag force between phases, then one needs to modify the functions A and B somewhat. The viscosity can be taken into account in a similar way.

2.3. *Nigmatulin's Model*

Consider the model of two-phase flow suggested in [11]. In the above notation,

$$\begin{aligned}\partial_t(\alpha\rho_1) &= -\partial_x(\alpha\rho_1u_1), \\ \partial_t((1-\alpha)\rho_2) &= -\partial_x((1-\alpha)\rho_2u_2), \\ \partial_t(\alpha\rho_1u_1) &= -\partial_x(\alpha\rho_1u_1u_1) - \alpha\partial_xp - F_d, \\ \partial_t((1-\alpha)\rho_2u_2) &= -\partial_x((1-\alpha)\rho_2u_2u_2) - (1-\alpha)\partial_xp + F_d, \\ \partial_t(\alpha\rho_1E) &= -\partial_x(\alpha u_1(\rho_1E + p)) - p\partial_t\alpha - F_du_2,\end{aligned}\quad (29)$$

where the inter-phase drag force F_d is given by

$$F_d = C_x \frac{(1-\alpha)\rho_1(u_1 - u_2)|u_1 - u_2|}{2}.$$

Here C_x is the dimensional function proportional to the drag coefficient of a solid particle and to the local particle concentration. In this model, the equation of state is

$$p = (\gamma - 1)\rho_1E_i,$$

where E_i stands for the internal energy and γ for the ratio of specific heats. The term $-p\partial_t\alpha$ in the last equation of (29) is due to the contribution of the work of pressure on the compression or expansion of the gas phase [11]. Since Eqs. (29) contain the equation for total energy E , we follow the approach of Subsection 2.1 and introduce two distribution functions $F_1(t, x, v, E)$ and $F_2(t, x, v, E)$. In this case, the following relations hold:

$$\alpha\rho_1 = \int F_1(t, x, v, E) dv dE, \quad (1-\alpha)\rho_2 = \int F_2(t, x, v, E) dv dE.$$

The distribution functions F_1 and F_2 must satisfy the following set of equations of Vlasov type:

$$\partial_tF_1 = -\partial_x(\langle v \rangle_1 F_1) - \partial_v(AF_1) - \partial_E(CF_1), \quad \partial_tF_2 = -\partial_x(\langle v \rangle_2 F_2) - \partial_v(BF_2).$$

The first four equations in system (29) can be obtained from the set of kinetic equations by a procedure similar to that used in Subsection 2.1 with regard for the rapid decay of the functions F_1 and F_2 as v and E tend to infinity. The calculation of the drag force F_d results in the following expressions for the functions A and B :

$$A = -\frac{\partial_x p}{\rho_1} - \frac{F_d}{\alpha\rho_1}, \quad B = -\frac{\partial_x p}{\rho_2} - \frac{F_d}{(1-\alpha)\rho_2}.$$

Let us derive the last equation of system (29). For this purpose, multiply the equation for F_1 by E and integrate the resulting equation with respect to v and E . This gives

$$\begin{aligned} \partial_t \int E F_1(t, x, v, E) dv dE &= -\partial_x \left(\langle v \rangle \int E F_1(t, x, v, E) dv dE \right) \\ &\quad - \int E \partial_v (A F_1) dv dE - \int E \partial_E (C F_1) dv dE. \end{aligned}$$

Thus,

$$\partial_t (\alpha\rho_1 \langle E \rangle) = -\partial_x (\alpha\rho_1 \langle v \rangle_1 \langle E \rangle) + C\alpha\rho_1. \quad (30)$$

Comparing Eq. (30) with Eqs. (29), we finally obtain

$$C = \frac{-p\partial_t \alpha - F_d u_2}{\alpha\rho_1}.$$

CONCLUSION

This paper proposes an approach for obtaining a new type of kinetic equations describing the dynamics of a continuous medium in terms of a fictitious one-particle distribution function. The approach enables one to derive exact equations of gas dynamics as the equations for lower-order moments of the distribution function, and to solve the well-known closure problem arising in the method of kinetic equations. Kinetic equations for various flows (homogeneous and heterogeneous, inviscid and viscous, single-component and multi-component, reactive and nonreactive) are derived and analyzed. The kinetic equations can be used to develop new hybrid computational algorithms based on the Monte Carlo and cellular automata methods for solving complicated problems of homogeneous and multi-phase reactive flows.

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REFERENCES

1. Balescu, R., *Equilibrium and Nonequilibrium Statistical Mechanics*, New York: John Wiley, 1975.
2. Lifsič [Lifshits], E. M. and Pitaevskii, L. P., *Physical Kinetics*, Moscow: Nauka, 1979.
3. Frost, V. A., Mathematical Model of Turbulent Combustion, in *Proc. 3rd All-Union Conf. on Combustion Theory*, Moscow: Acad. Sci., 1960, pp. 121–125.
4. Pope, S. B., PDF Methods for Turbulent Reactive Flows, *Prog. Energy Combust. Sci.*, 1985, vol. 11, pp. 119–151.
5. Frisch, U., Lectures on Turbulence and Lattice Gas Hydrodynamics, in *Lecture Notes on Turbulence*, Herring, J. R. and McWilliams, J. C., Eds., NCAR-GTP, Summer School, June 1987, pp. 219–371.
6. Landau, L. D. and Lifshits, E. M., *Hydrodynamics*, Moscow: Nauka, 1986.
7. D'yachenko, V. F., *Ten Lectures on Physical Mathematics*, Moscow: Factorial, 1998.
8. Williams, F. A., *Combustion Theory*, MenloPark: Benjamin/Cummings, 1985.
9. Gihman, I. I. and Skorohod, A. V., *The Theory of Stochastic Processes*, Berlin: Springer, 1974–1979, vols. 1–3.
10. Van Wijngaarden, L., Some Problems in the Formulation of the Equations for Gas/Liquid Flow, in *Theoretical and Applied Mechanics. Proc. 14th IUTAM Congress Delft, the Netherlands, August 30–September 4, 1976*, Koiter, W. T., Ed., Amsterdam: North-Holland, 1977, pp. 528–552.
11. Nigmatulin, R. I., *Dynamics of Multiphase Media*, Moscow: Nauka, 1987, vols. 1–2.