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Derivation of the macroscopic continuum equations for multiphase flow

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Macroscopic continuum equations for multiphase flow are derived from a modified Boltzmann equation using the Chapman-Enskog expansion technique. Phase separation and interface formation are naturally driven by an intermolecular interaction. At the equilibrium state, these equations reduce to previous results of thermodynamical studies. This work provides a solid physical foundation for the continuum descriptions of surface tension and will be useful for studying multiphase flow. [S1063-651X(99)03601-6]

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Numerical simulation of multiphase flow is of great significance in both fundamental research and industrial applications. The most challenging part in simulation of multiphase flows is to model interfaces between different phases and the associated surface tensions. One of the commonly used approaches, which will be specifically addressed in this paper, is the front capturing technique.

In the front capturing technique an interface is regarded as a transient region where physical properties vary significantly but still smoothly. In other words, the interface itself is treated as a part of the flow domain. The front capturing has been successfully applied to capture the shock wave (see, e.g., the review in [1]), in which flow is governed by the same Euler equation throughout the whole flow field. When the same idea is used to study multiphase flows, the Euler and Navier-Stokes equations are no longer valid because flow in an interface region evolves quite differently from those in the homogeneous region due to the existence of surface tension.

In the literature several techniques have been proposed [2] for incorporation of the surface tension effect into the Euler or Navier-Stokes equations. Most of these approaches start from phenomenological reasonings: An interface is artificially smeared into a transient region with a finite thickness and the surface tension is subsequently converted into an effective volumetric force. A common difficulty in these approaches is how to calculate correctly the curvature of an interface, which the volumetric force is proportional to. Previous studies usually introduced an artificial label function to describe the interface and the associated curvature. Even if the curvature can be accurately calculated, there is still no rigorous way to convert the surface tension into the corresponding volumetric force.

Recently, Nadiga and Zaleski [3] proposed the following continuum equations for the multiphase flow by directly inserting a new stress tensor into the momentum equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{\Pi}^{(v)} + \nabla \cdot \mathbf{\Pi}^{(1)}, \tag{2}$$

where $\mathbf{\Pi}^{(v)}$ is the ordinary viscous stress tensor and $\mathbf{\Pi}^{(1)}$ is a new term representing the surface tension effect

$$\mathbf{\Pi}^{(1)} = \kappa[(\tfrac{1}{2}|\nabla \rho|^2 + \rho \nabla^2 \rho)\mathbf{I} - \nabla \rho \nabla \rho], \tag{3}$$

where the parameter κ controls the strength of the surface tension effect. The temperature in the equation of state is fixed for simplicity.

The direct insertion of the stress tensor $\mathbf{\Pi}^{(1)}$ into the Navier-Stokes equations is somewhat phenomenological because it is based on the *equilibrium* state (see, e.g., [4]). To give a solid foundation to the equations, we will show in this paper that the continuum equations (1) and (2) indeed can be directly derived from the kinetic theory. Therefore, they are valid for describing multiphase flows.

Swift *et al.* [5] also introduced a lattice-Boltzmann Bhatnagar-Gross-Krook (BGK) model [6] to account for liquid-gas mixture. The resulting macroscopic equation has terms in the stress tensor similar to that in $\mathbf{\Pi}^{(1)}$. In their paper the equilibrium distribution was constructed to be consistent with the thermodynamical theory of nonuniform fluids at equilibrium state. For an idea gas, the validation of the BGK model can be justified by the recovery of the Boltzmann-BGK equation to the Navier-Stokes equation under the Chapman-Enskog expansion. For a multiphase fluid, however, there is no *a priori* macroscopic equation that can be used. Whether the BGK model is correct for multiphase flow remains unproved in their paper. This paper fills such a gap.

We start our analysis from the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f + \mathbf{F} \cdot \nabla_{\xi} f = \frac{\partial_e f}{\partial t}, \tag{4}$$

where f is the single-particle distribution function for a one-chemical-component system, $\boldsymbol{\xi}$ is the microscopic particle velocity, $\mathbf{F}$ is the force experienced by molecules, and $\partial_e f/\partial t$ is the collision term as used in [7].

The same Boltzmann equation is valid for general fluids, but there are two important facts that must be taken into account [8]. First, the collision term $\partial_e f/\partial t$ needs to be modified because the particle size becomes comparable to the free path of molecules for a dense gas or a liquid. Second, the intermolecular attraction may become important especially for fluids involved in phase separations and transitions such as multiphase flows.

Based on Enskog's elastic particle model [7], the collision term for a dense gas can be approximated as

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$$\frac{\partial_e f}{\partial t}=\left(\frac{\partial_e f}{\partial t}\right)_0-b\rho\chi f^{\mathrm{eq}}\{(\boldsymbol{\xi}-\mathbf{u})\cdot[\boldsymbol{\nabla}\ \ln(\rho^2\chi T)+\tfrac{3}{5}(C^2-\tfrac{5}{2})\boldsymbol{\nabla}\ \ln T]+\tfrac{2}{5}[2\mathbf{CC}:\boldsymbol{\nabla}\mathbf{u}+(C^2-\tfrac{5}{2})\boldsymbol{\nabla}\cdot\mathbf{u}]\},\tag{5}$$

where $(\partial_e f/\partial t)_0$ is the ordinary collision term when the particle size can be neglected; $\mathbf{C}=(\boldsymbol{\xi}-\mathbf{u})/\sqrt{2RT}$ and C is its magnitude; the colon represents the scalar product of two tensors; and χ is the increase in collision probability due to increase in density,

$$\chi=1+\frac{5}{8}b\rho+0.2869(b\rho)^2+0.1103(b\rho)^3+0.0386(b\rho)^4+\cdots,\tag{6}$$

where

$$b=\frac{2\pi d^3}{3m},\tag{7}$$

with d and m being the diameter and mass of particles, respectively.

In Enskog's original work, particles are assumed only to experience external forces such as gravity or electromagnetic forces. In real dense gas, especially for those involved in phase transitions, particles also experience intermolecular attractions. In the framework of the mean-field theory [9], the intermolecular attraction can be modeled by the mean field potential

$$V_m=-2a\rho-\kappa\nabla^2\rho.\tag{8}$$

The coefficients a and κ relate to the intermolecular potential u_{attr} by

$$a=-\frac{1}{2}\int_{r>d}u_{attr}(r)d\mathbf{r},$$

$$\kappa=-\frac{1}{6}\int_{r>d}r^2u_{attr}(r)d\mathbf{r}.$$

They can be treated as constant parameters in the model. Ignoring the external forces, the total force experienced by particles to be used in Eq. (4) can hence be expressed as

$$\mathbf{F}=-\boldsymbol{\nabla}V_m.\tag{9}$$

The macroscopic fluid density ρ, velocity $\mathbf{u}$, and temperature T can be calculated as the velocity moments of the distribution function

$$\rho=\int f\ d\boldsymbol{\xi},\tag{10}$$

$$\rho\mathbf{u}=\int \boldsymbol{\xi}f\ d\boldsymbol{\xi},\tag{11}$$

$$3\rho RT=\int(\boldsymbol{\xi}-\mathbf{u})^2f\ d\boldsymbol{\xi}.\tag{12}$$

Following Chapman and Enskog, we expand the distribution function and time derivative in series of the Knudsen number ϵ (ratio of the mean free path to the macroscopic characteristic length):

$$f=\sum_{n=0}^{\infty}\epsilon^n f^n,\tag{13}$$

$$\partial_t=\sum_{n=0}^{\infty}\epsilon^n\partial_{t_n}.\tag{14}$$

The rest of the procedure of the Chapman-Enskog expansion is straightforward. For simplicity, we focus only on the mass and momentum conservations in this paper and neglect the temperature variation. The first-order approximation yields the macroscopic equation

$$\partial_{t_0}\rho+\boldsymbol{\nabla}\cdot(\rho\mathbf{u})=0,\tag{15}$$

$$\partial_{t_0}(\rho\mathbf{u})+\boldsymbol{\nabla}\cdot(\rho RT\mathbf{I}+\rho\mathbf{uu})+\rho\boldsymbol{\nabla}V_m=-\boldsymbol{\nabla}(b\rho^2\chi RT)+\kappa\rho\boldsymbol{\nabla}\nabla^2\rho,\tag{16}$$

or

$$\partial_{t_0}(\rho\mathbf{u})+\boldsymbol{\nabla}\cdot(\rho\mathbf{uu})=-\boldsymbol{\nabla}p+\kappa\rho\boldsymbol{\nabla}\nabla^2\rho,\tag{17}$$

where the pressure is related to the density and temperature by

$$p=\rho RT(1+b\rho\chi)-a\rho^2.\tag{18}$$

Equation (18) is the general equation of state for fluids.

The second-order Chapman-Enskog expansion leads to

$$\partial_{t_1}\rho=0,\tag{19}$$

$$\partial_{t_1}(\rho\mathbf{u})=\boldsymbol{\nabla}\cdot\boldsymbol{\Pi}^{(v)},\tag{20}$$

where

$$\boldsymbol{\Pi}^{(v)}=\mu(\boldsymbol{\nabla}\mathbf{u}+\mathbf{u}\boldsymbol{\nabla})\tag{21}$$

is the viscous stress tensor. In our model, the intermolecular attraction does not change the viscosity that has been derived by Enskog [7] for dense gases:

$$\mu=b\rho[(b\rho\chi)^{-1}+0.8+0.7614b\rho\chi]\rho RT.\tag{22}$$

In practice, we can always measure the viscosity by experiments.

The combination of the first- and second-order approximations of the Chapman-Enskog expansion leads to the macroscopic continuum equations (1) and (2) for multiphase flows. Notice that the following equation is used in this procedure:

$$\kappa\rho\boldsymbol{\nabla}\nabla^2\rho=\kappa\boldsymbol{\nabla}\cdot[(\tfrac{1}{2}|\boldsymbol{\nabla}\rho|^2+\rho\nabla^2\rho)\mathbf{I}-\boldsymbol{\nabla}\rho\boldsymbol{\nabla}\rho]=\boldsymbol{\nabla}\cdot\boldsymbol{\Pi}^{(1)}.\tag{23}$$

Two remarks are due at this point. First, at the equilibrium, the momentum equation (2) reduces to

$$\nabla p = \nabla \cdot \mathbf{\Pi}^{(1)}. \tag{24}$$

Equation (24) is consistent with the thermodynamical results for nonuniform fluids in an equilibrium state [4]. As shown in classic thermodynamical studies, the phase separation is driven by the intermolecular interaction through the equation of state.

Second, in our formulation, the interface is captured by the spatial distribution of density and the surface tension effect is automatically distributed in space. No artificial smearing is necessary and calculation of the local curvature is avoided. The total force acting on a unit area of an interface can be given by the integration of $\nabla \cdot \mathbf{\Pi}^{(1)}$ over a thin volume Ω containing a small part of a curved interface with area A:

$$\begin{aligned}
&\lim_{A\to 0} \frac{1}{A} \int_{\Omega} \kappa \rho \nabla \nabla^2 \rho \\
&\quad = \lim_{A\to 0} \frac{1}{A} \int_{\partial\Omega} \kappa\left(\rho \nabla^2 \rho + \tfrac{1}{2}|\nabla \rho|^2 - \nabla \rho \nabla \rho\right) \cdot \mathbf{S}\, dl \\
&\quad = \sigma \kappa_c \mathbf{n},
\end{aligned} \tag{25}$$

where $\partial\Omega$ is the surface of Ω with outnormal $\mathbf{S}$, κ_c is the local curvature of the interface, $\mathbf{n}$ is the normal direction of the interface, and σ is the surface tension

$$\sigma = \kappa \int_{-\infty}^{\infty} |\nabla \rho|^2 dz,$$

as in [9]. Equations (24) and (25) yield the Laplace law.

In conclusion, we have derived the macroscopic continuum equations for multiphase flow from the microscopic Boltzmann equation using the Chapman-Enskog expansion technique. Phase separation and interface formation are naturally driven by intermolecular interaction. The resulting equations are consistent with those proposed by Nadiga and Zaleski [3]. This work provides a solid foundation for continuum descriptions of interfaces and surface tension effects in multiphase flows.

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