

Constructions of simple kinetic equations for a dense gas

Takumu Miyauchi, Shigeru Takata, Masanari Hattori, and Aoto Takahashi

Abstract Constructions of simple kinetic equations for a dense gas are presented, with a special emphasis on a couple of modelling based on the Ellipsoidal-Statistical (ES)-type collision model. First, two previous models are reviewed: one based on a simple relaxation model with the isothermal assumption and the other based on the Bhatnagar–Gross–Krook (BGK)-type collision model. These models have a monotone functional that enables one to make thermodynamic interpretations on simulation results for phase change phenomena. They are, however, not designed so as to reproduce appropriate transport properties for a dense gas. Two types of the Ellipsoidal-Statistical (ES)-based model are proposed and described in detail. Both ES-based models reproduce appropriate transport properties, which is an advantage over the previous models. The difference of their monotone property in time is also discussed in detail.

Takumu Miyauchi

Department of Aeronautics and Astronautics, Kyoto University, Kyoto 615–8540, Japan, e-mail: miyauchi.takumu.23e@st.kyoto-u.ac.jp

Shigeru Takata

Department of Aeronautics and Astronautics & Advanced Engineering Research Center, Kyoto University, Kyoto 615–8540, Japan, e-mail: takata.shigeru.4a@kyoto-u.ac.jp

Masanari Hattori

Department of Aeronautics and Astronautics & Advanced Engineering Research Center, Kyoto University, Kyoto 615–8540, Japan, e-mail: hattori.masanari.4r@kyoto-u.ac.jp

Aoto Takahashi

Department of Aeronautics and Astronautics, Kyoto University, Kyoto 615–8540, Japan, e-mail: takahashi.aoto.63c@st.kyoto-u.ac.jp

1 Introduction

Phase transition is a common phenomenon and has been studied variously from a microscopic to a macroscopic point of view. In the kinetic theory, gas flows caused by the phase transition have been investigated, mostly assuming that the state of its condensed phase is specified, e.g., [1, 2, 3, 4, 5, 6, 7]. In the meantime, a new research direction that employs the real gas effect by the Enskog or the Enskog–Vlasov equation becomes common recently in the literature, thanks to the developments of a stochastic [8] and a deterministic [9] numerical algorithm for them. However, the studies based on those equations are still computationally demanding, even compared to the Boltzmann equation.

A construction of a simpler kinetic equation is thus worth exploring for accelerating that new direction of researches on non-ideal gas flows. It is also expected to advance our understanding of the kinetic theory approach for dense gases through close observations of the influence of the simplification procedure. Motivated by the research background described above, we have been trying to find a simple promising framework of a kinetic model for non-ideal gas phenomena. So far, the models making use of a simple relaxation term and the BGK-type collision term [10, 11] worked as desired in [12, 13, 14]. Nevertheless, they have a potential demerit in transport properties due to the specific choice of the collision model. In order to fix the demerit, a couple of models based on the Ellipsoidal-Statistical (ES)-type collision term [15, 16] will be introduced in the present paper.

The paper is organized as follows. Our previous models are briefly reviewed in Sec. 2. Then, a couple of new proposals based on the ES-model are presented in Sec. 3, where the first ES-based model is described in Sec. 3.1 and its potential limitation on the H theorem is explained in Sec. 3.2. Then, the second ES-based model is described in Sec. 3.3, where the H theorem for the second model is presented. The fluid dynamic limit of the proposed models is also discussed on the basis of the Chapman–Enskog method in the Appendix. Preliminary numerical tests are presented in Sec. 4. The paper is concluded in Sec. 5.

2 Previous models

2.1 Outline of previous models

Our attempts for the construction of a simple kinetic model started from the following simplest one under the isothermal assumption:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i^* \frac{\partial f}{\partial \xi_i} = C_*[f], \quad C_*[f] = A_*(\rho)(\rho M_* - f), \quad (1a)$$

$$F_i^* = -\frac{\partial}{\partial X_i}(\Phi_S^*(\rho) + \Phi_L[\rho]), \quad M_* = \frac{1}{(2\pi RT_*)^{3/2}} \exp\left(-\frac{\xi^2}{2RT_*}\right), \quad (1b)$$

where $f(t, \mathbf{X}, \boldsymbol{\xi})$ is the velocity distribution function (VDF) of molecules, with t , $\mathbf{X}$, and $\boldsymbol{\xi}$ being a time, a position, and a molecular velocity respectively; $m\mathbf{F}^*$ is a potential force acting on a molecule with a mass m , R is the specific gas constant, and $A_*(\rho)$ is a positive function of the gas density ρ defined by

$$\rho = \int f d\boldsymbol{\xi}. \quad (1c)$$

Here and in what follows, the integral with respect to $\boldsymbol{\xi}$ represents the definite one over its whole space, unless otherwise stated. With the density ρ , a uniform given temperature T_* , and two parameters a and b , the equation of state for the van der Waals fluids is written as

$$p = \frac{\rho RT_*}{1 - b\rho} - a\rho^2, \quad (1d)$$

under the isothermal assumption. The form of Φ_S^* is then determined as

$$\Phi_S^*(\rho) = \Phi_S(\rho, T_*) \equiv -RT_* \ln(1 - b\rho) + \frac{b\rho RT_*}{1 - b\rho} - 2a\rho, \quad (1e)$$

so as to recover the non-ideal gas effect in the equation of state (1d) through the relation

$$p = \rho RT_* + \int \rho \frac{d\Phi_S^*(\rho)}{d\rho} d\rho. \quad (1f)$$

Within the diffusive approximation, the form of Φ_L is reduced to

$$\Phi_L = -\kappa \Delta \rho, \quad (1g)$$

where $\Delta \equiv \partial^2 / \partial X_i^2$ is the Laplacian and κ is a given positive constant [17]. Once the collision frequency A_* is specified, the above system is closed. In what follows, let us call this system (1) the isothermal model. The isothermal model was considered to identify the key or minimum mechanism in the transition dynamics from a uniform equilibrium state to a phase separated equilibrium state (see [12, 13]).

Main features of the isothermal model are as follows. Firstly, a non-local effect of interaction is treated in $\Phi_L[\rho]$ as a long-range attractive term. It is localized only after applying a diffusive approximation. In contrast, short-range interactions of molecules are treated to be local from the beginning in the form of $\Phi_S^*(\rho)$ and $C_*[f]$ on the right-hand side. Secondly, the resting Maxwellian ρM_* with a given uniform temperature T_* is used in place of the local Maxwellian in $C_*[f]$. This feature implies that the system does not conserve the momentum nor energy. Thus, in the isothermal model, the main driving mechanism toward the equilibrium state is the interaction of molecules with a heat bath, not within themselves.

The next model developed from the system (1) adopts the BGK-type collision integral in place of $C_*[f]$ in (1a) and takes the following form:

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c[f] + Q_d[f], \quad (2a)$$

$$F_i = -\frac{\partial}{\partial X_i}(\Phi_S(\rho, T) + \Phi_L[\rho]), \quad (2b)$$

$$Q_c[f] = A(\rho, T)(f_e - f), \quad A(\rho, T) = \frac{A_c(T)\rho}{1 - b\rho} > 0, \quad (2c)$$

$$f_e = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{\mathbf{c}^2}{2RT}\right), \quad \mathbf{c} = \boldsymbol{\xi} - \mathbf{v}, \quad (2d)$$

$$Q_d[f] = -\frac{\partial}{\partial \xi_i}[(\alpha_i + \beta c_i)f], \quad \alpha_i = \frac{1}{\rho} \int \frac{\partial \Phi_S}{\partial T} d\rho \frac{\partial T}{\partial X_i}, \quad (2e)$$

$$\beta = \frac{1}{3R\rho} \left\{ \frac{\partial}{\partial t} \int \frac{\partial \Phi_S}{\partial T} d\rho + \frac{\partial}{\partial X_i} (v_i \int \frac{\partial \Phi_S}{\partial T} d\rho) \right\}, \quad (2f)$$

where $A_c(T) > 0$ (see the Appendix A of [14]), $\mathbf{v}$ and T are the gas flow velocity and temperature defined as

$$\mathbf{v} = \frac{1}{\rho} \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad T = \frac{1}{3R\rho} \int \mathbf{c}^2 f d\boldsymbol{\xi}. \quad (2g)$$

The indefinite integral with respect to ρ in (2) is taken along the isothermal process to give

$$\int \frac{\partial \Phi_S}{\partial T} d\rho = -\rho R \ln(1 - b\rho), \quad (3)$$

for the van der Waals fluids. Note that the equation of state takes the original form

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2 \left(= \rho RT + \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho \right), \quad (4)$$

in place of (1d), since the gas is no longer assumed to be isothermal. Hereafter, the system (2) – (4) is referred to as the BGK-based model.

Due to the temperature dependence of Φ_S , a new term Q_d is added on the right-hand side for a well-balanced construction of the model. The BGK-based model conserves the mass, the momentum, and the energy and was used as well to study the dynamics of phase separation from a uniform equilibrium state in a periodic and an isolated system in [14]. Comparisons with simulation results for the isothermal model and related discussions can be found in the Appendix D of [14].

Besides their simplicity, both the isothermal and the BGK-based model have an advantage that there is a monotonically decreasing functional:

$$H^*(t) = \int_D \left(\int f \ln \frac{f}{\rho_0 M_*} d\boldsymbol{\xi} + \frac{1}{RT_*} \left\{ \int \Phi_S^* d\rho + \frac{\kappa}{2} (\nabla \rho)^2 \right\} \right) d\mathbf{X}, \quad (5a)$$

for the isothermal model [12, 13] and

$$H(t) = \int_D \left(\int f \ln \frac{f}{c_0} d\boldsymbol{\xi} + \frac{1}{R} \int \frac{\partial \Phi_S}{\partial T} d\rho \right) d\mathbf{X}, \quad (5b)$$

for the BGK-based model [14], where D is a unit region of a periodic domain, ρ_0 is a reference density, and c_0 is a positive constant with the same physical dimension as f . Occurrence of M_* and $\kappa(\nabla\rho)^2$ in (5a) is due to that the isothermal model is for the systems in contact with the heat bath, while the BGK-based model is for periodic (or isolated) systems. In other words, H^* corresponds to the free energy, while H the entropy in the thermodynamics. Note that the second term on the right-hand side of (5b) is a contribution of the dense gas effect. Equipped with the monotone functional, these models provided thermodynamically consistent discussions and interpretations to numerical simulation results for the phase change, e.g., [14]. It is a benefit in addition to their simple structures.

2.2 Fluid-dynamic limits and transport properties

The isothermal model leads to a Cahn–Hilliard-type equation:

$$\frac{\partial\rho}{\partial t} - \frac{\partial}{\partial X_j} \left[\frac{\rho}{A_*(\rho)} \frac{\partial}{\partial X_j} \left(\Phi - \kappa \frac{\partial^2 \rho}{\partial X_i^2} \right) \right] = 0, \quad (6a)$$

$$\Phi = -2a\rho + RT_* \left(\frac{1}{1-b\rho} + \ln \frac{b\rho}{1-b\rho} \right), \quad (6b)$$

in the fluid-dynamic limit, owing to a strong momentum-dissipation property of the collision term $C_*[f]$, see [12] for details. A derivation of the Cahn–Hilliard equation from the kinetic theory has been recently discussed as well in [18].

The BGK-based model yields the following balance laws of the mass, momentum, and energy:

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial X_i}(\rho v_i) = 0, \quad (7a)$$

$$\frac{\partial}{\partial t}(\rho v_j) + \frac{\partial}{\partial X_i}(\rho v_i v_j + p_{ij}) + \rho \frac{\partial \Phi_L}{\partial X_j} = 0, \quad (7b)$$

$$\frac{\partial}{\partial t}(\rho(e + \frac{1}{2}\mathbf{v}^2)) + \frac{\partial}{\partial X_i}(\rho v_i(e + \frac{1}{2}\mathbf{v}^2) + p_{ij}v_j + q_i) + \rho v_i \frac{\partial \Phi_L}{\partial X_i} = 0, \quad (7c)$$

where p_{ij} , q_i , and e are the stress tensor, the heat-flow vector, and the specific internal energy defined by

$$p_{ij} = p\delta_{ij} + \int (c_i c_j - \frac{1}{3}\mathbf{c}^2 \delta_{ij}) f d\boldsymbol{\xi}, \quad q_i = \frac{1}{2} \int c_i \mathbf{c}^2 f d\boldsymbol{\xi}, \quad (7d)$$

$$\rho e = \frac{3}{2}\rho RT + \int (\Phi_S - T \frac{\partial \Phi_S}{\partial T}) d\rho, \quad (7e)$$

and p is the pressure defined in (4). The derivation of (7) can be found in [14]. In the fluid-dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \frac{\rho RT}{A(\rho, T)} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right), \quad q_i = -\frac{5}{2} R \frac{\rho RT}{A(\rho, T)} \frac{\partial T}{\partial X_i}, \quad (8)$$

and accordingly the balance law of equation (7) is reduced to the Navier–Stokes set of equations with a self-consistent force term, see the Appendix. Here, as is seen from (8), the viscosity μ and the thermal conductivity λ are given respectively by $\mu = \rho RT/A(\rho, T)$ and $\lambda = (5/2)R\rho RT/A(\rho, T)$. These expressions imply that the Prandtl number $\text{Pr} \equiv (5R/2)(\mu/\lambda)$ is unity, inheriting a weakness of the BGK-type collision integral in the transport property. Another weakness is that the bulk viscosity predicted by the Enskog theory [19] is absent. In the next section, we propose a modification of the BGK-based model to fix its demerit in transport properties.

3 Modified models in terms of the Ellipsoidal-Statistical (ES)-type collision term

The key elements in the modification of the BGK-based model are, first, to use an ES-type collision term [15, 16] instead of the BGK-type term and, second, to add additional terms to Q_d . Here, two different ways of modification are presented.

3.1 The first ES-based model

The main idea of the first modified model proposed recently in [20] is to make the adjusting parameter ν in the ES-type collision integral dependent on ρ . The model is hereafter referred to as the first ES-based model and reads

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c^\sharp[f] + Q_d^\sharp[f], \quad (9a)$$

$$Q_c^\sharp[f] = A^\sharp(\rho, T)(\mathcal{G} - f), \quad \mathcal{G} = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}(\mathcal{T}^{-1})_{ij}c_i c_j\right), \quad (9b)$$

$$\mathcal{T}_{ij} = (1 - \nu(\rho))RT\delta_{ij} + \nu(\rho)\Theta_{ij}, \quad \Theta_{ij} = \frac{1}{\rho} \int c_i c_j f d\boldsymbol{\xi}, \quad (9c)$$

$$Q_d^\sharp[f] = -\frac{\partial}{\partial \xi_i} [(\alpha_i^\sharp + \beta^\sharp c_i) f], \quad (9d)$$

$$\alpha_i^\sharp = \alpha_i + \frac{1}{\rho} \frac{\partial}{\partial X_i} (\mu_B \frac{\partial v_k}{\partial X_k}), \quad \beta^\sharp = \beta + \frac{\mu_B}{3R\rho T} \left(\frac{\partial v_k}{\partial X_k} \right)^2, \quad (9e)$$

where F_i is the same as that in the BGK-based model, $\mathcal{T}^{-1}$ is the inverse of the tensor $\mathcal{T}$, μ_B and $A^\sharp$ are positive functions of ρ and T to be determined in accordance with the Enskog theory for the transport coefficients, and ν is an adjusting parameter function of ρ . The modified model keeps the set of balance equations (7) as it stands

by the following change of definition of the stress tensor:

$$p_{ij} = p\delta_{ij} + \int (c_i c_j - \frac{1}{3} c^2 \delta_{ij}) f d\xi - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}. \quad (10)$$

In the fluid-dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \frac{1}{1-\nu(\rho)} \frac{\rho RT}{A^\#(\rho, T)} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (11)$$

$$q_i = -\frac{5}{2} R \frac{\rho RT}{A^\#(\rho, T)} \frac{\partial T}{\partial X_i}. \quad (12)$$

See the Appendix for the derivation. Thus, μ_B introduced in (10) is the bulk viscosity, $\rho RT/((1-\nu)A^\#)$ the viscosity μ , and $(5/2)R(\rho RT/A^\#)$ the thermal conductivity λ . Hence, the Prandtl number is expressed in terms of ν as $\text{Pr}(\equiv (5/2)(R\mu/\lambda)) = 1/(1-\nu)$.

In order to make the model equipped with the desired transport properties, it is necessary to determine $\nu(\rho)$ in accordance with the Enskog theory for transport properties. In the Enskog theory, the viscosity μ , bulk viscosity μ_B , and the thermal conductivity λ are expressed as [19, 21]

$$\mu = \frac{\mu_0}{\chi} \left(1 + \frac{16}{5} \phi \chi + 12.2(\phi \chi)^2 \right), \quad \mu_B = \frac{\mu_0}{\chi} (4\phi \chi)^2, \quad (13a)$$

$$\lambda = \frac{\lambda_0}{\chi} \left(1 + \frac{24}{5} \phi \chi + 12.1(\phi \chi)^2 \right), \quad (13b)$$

where μ_0 and λ_0 are respectively the viscosity and thermal conductivity of the gas in the dilute gas limit, while ϕ and χ are dense gas factors that can be related to the exclusion parameter b in the equation of state for the van der Waals fluids, i.e.,

$$\phi = \frac{1}{4} b \rho, \quad \chi = \frac{1}{1 - b \rho}; \quad (14)$$

see the discussions in the Appendix A of [14] for details. Hence, substituting (14) into (13), $A^\#$ and ν in the system (9) as well as the transport coefficients are all expressed in terms of the exclusion parameter b , ρ , and T :

$$A^\#(\rho, T) = \frac{5}{2} \frac{\rho RT}{1 - b\rho} \frac{R/\lambda_0(T)}{g_2(\frac{b\rho}{1-b\rho})}, \quad (15a)$$

$$\nu(\rho) = 1 - \frac{2}{5} \frac{1}{R} \frac{\lambda_0(T)}{\mu_0(T)} \frac{g_2(\frac{b\rho}{1-b\rho})}{g_1(\frac{b\rho}{1-b\rho})} = 1 - \frac{1}{\text{Pr}_0} \frac{g_2(\frac{b\rho}{1-b\rho})}{g_1(\frac{b\rho}{1-b\rho})}, \quad (15b)$$

$$\mu(\rho, T) = (1 - b\rho) g_1\left(\frac{b\rho}{1 - b\rho}\right) \mu_0(T), \quad (15c)$$

$$\mu_B(\rho, T) = (1 - b\rho) \left(\frac{b\rho}{1 - b\rho}\right)^2 \mu_0(T), \quad (15d)$$

$$\lambda(\rho, T) = (1 - b\rho)g_2\left(\frac{b\rho}{1 - b\rho}\right)\lambda_0(T), \quad (15e)$$

where

$$g_1(x) = 1 + \frac{4}{5}x + \frac{6.1}{8}x^2, \quad g_2(x) = 1 + \frac{6}{5}x + \frac{12.1}{16}x^2, \quad (15f)$$

and Pr_0 is the Prandtl number in the dilute gas limit, which is usually set as $\text{Pr}_0 = 2/3$ for monatomic gases. The system (9) with (15) thus forms a closed kinetic model with appropriate transport coefficients. Note that the model recovers the BGK-based model with $A_c = (5/2)R^2T/\lambda_0(T)$ as a special case by discarding (15d) and (15f) and putting $g_1 = g_2 = 1$, $\mu_B = 0$, and $\text{Pr}_0 = 1$ (see Sec. 2.1).

3.2 A slight limitation on the monotonicity of the first ES-based model

We shall discuss the monotone property of the model (9) with (15) in a periodic domain. Let D denote a unit region of the periodic domain. Multiplying (9a) by $1 + \ln(f/c_0)$ and integrating the result over the whole range of ξ and over the unit region D yield

$$\begin{aligned} \frac{d}{dt} \int_D \int f \ln \frac{f}{c_0} d\xi d\mathbf{X} &= \int_D \int (Q_c^\sharp[f] + Q_d^\sharp[f]) \ln \frac{f}{c_0} d\xi d\mathbf{X} \\ &= \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} - 3 \int_D \beta^\sharp \rho d\mathbf{X}, \end{aligned} \quad (16)$$

where the second and the third term of (9a) do not contribute because of the periodic condition in space and the rapid decay of VDF in molecular speed. Then, after a few manipulations making use of (2f) and the periodic condition,

$$\begin{aligned} \frac{d}{dt} H(t) &= \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} - \int_D \frac{\mu_B}{RT} \left(\frac{\partial v_k}{\partial X_k} \right)^2 d\mathbf{X} \\ &\leq \int_D \int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi d\mathbf{X}, \end{aligned}$$

is obtained. Therefore, if

$$\int Q_c^\sharp[f] \ln \frac{f}{c_0} d\xi \leq 0, \quad (17)$$

holds, the monotonic property is retained as well in the first ES-based model.

Although the property (17) is one of merits to use the ES-type collision model, it should be reminded that (17) holds unconditionally only when the adjusting parameter ν is in the range $[-1/2, 1)$, i.e., the Prandtl number $\text{Pr}(\equiv \frac{5}{2} \frac{R\mu}{\lambda}) = 1/(1 - \nu)$ should be in the range $[2/3, \infty)$ [16]. In the present case, it is seen from (15) that

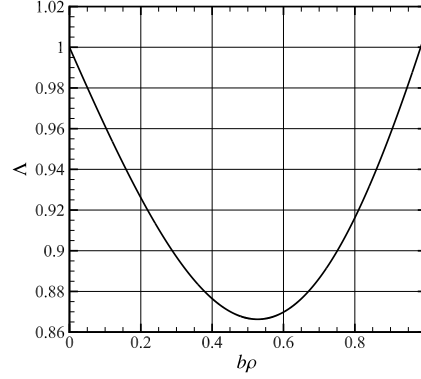


Fig. 1 $A(\frac{b\rho}{1-b\rho})$ versus a rescaled density $b\rho$. See (18).

$$\text{Pr} = \text{Pr}_0 A\left(\frac{b\rho}{1-b\rho}\right), \quad A(x) = \frac{g_1(x)}{g_2(x)} = 1 - \frac{\frac{2}{5}x(1 - \frac{x}{64})}{g_2(x)}. \quad (18)$$

Since $\text{Pr}_0 = 2/3$ is the usual setting for monatomic gases, $A \geq 1$ is required for (17) to hold unconditionally. However, A decreases from unity as $b\rho$ increases, reaches its minimum 0.8663 at $b\rho = 0.5274$, and then increases, as shown in Fig. 1. When A takes its minimum, the corresponding values of Pr and ν are respectively 0.5775 and -0.7315 . Therefore, the monotonicity of H is not guaranteed in the first ES-based model. Nevertheless, by a close examination of the original proof of the H theorem for $\nu \geq -1/2$ in [16], it was made clear in [22] that (17) still holds, provided that (i) $\mathcal{T}$ is positive definite and (ii) $\det \mathcal{T} \geq \det \Theta$. A similar discussion on a Fokker-Planck model can be found in [23]. Below is the quantitative criterion obtained in [22] for $\int \ln(f/c_0) Q_c^\sharp[f] d\xi \leq 0$ to hold:

Proposition 1. *Let $\lambda_1 \leq \lambda_2 \leq \lambda_3$ be the positive real eigenvalues of Θ that is a symmetric positive definite tensor by definition. If three eigenvalues are the same, $\mathcal{T}$ and Θ are identical, so that $\mathcal{T} = \Theta = RT\mathbb{I}$, where $\mathbb{I}$ is the identity tensor. The two conditions (i) and (ii) are then automatically satisfied. Next suppose that $\lambda_1 \neq \lambda_3$, and introduce additional notation $\epsilon \equiv 1 - \lambda_1/\lambda_3$ and $\theta = (1 - \lambda_2/\lambda_3)/(1 - \lambda_1/\lambda_3)$. Note that $0 < \epsilon < 1$ and $0 \leq \theta \leq 1$ by construction. Then, for $-1 \leq \nu < -1/2$, which corresponds to $1/2 \leq \text{Pr} < 2/3$, the following criterion must be fulfilled for (17) to hold $\int \ln(f/c_0) Q_c^\sharp[f] d\xi \leq 0$:*

$$\begin{cases} 0 < \epsilon < 1, & \text{for } 0 \leq \theta \leq \frac{2+\nu}{1-\nu}, \\ 0 < \epsilon < \frac{9(1+\nu)(\theta^2 - \theta + 1)}{(1+\theta)(1-\nu)^2(\frac{2\nu+1}{1-\nu} + \theta)(\frac{2\nu+1}{1-\nu}\theta + 1)}, & \text{for } \frac{2+\nu}{1-\nu} < \theta \leq 1. \end{cases} \quad (19)$$

The criterion (19) is of posteriori condition, and its practical restriction should be checked carefully. Numerical assessment of the criterion can be found in [22], where (17) is shown to hold except for highly anisotropic non-equilibrium states.

3.3 The second ES-based model

The second ES-based model is motivated by the slight limitation of the first ES-based model on the monotonicity described in Sec. 3.2. The main idea is to keep the adjusting parameter ν in the range $[-1/2, 1)$, thereby keeping the monotonic property of $H(t)$ by modifying $Q_d^\sharp$ term. The second ES-based model reads

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = Q_c^\flat[f] + Q_d^\flat[f], \quad (20a)$$

$$Q_c^\flat[f] = A^\flat(\rho, T)(\mathcal{G} - f), \quad \mathcal{G} = \frac{\rho}{\sqrt{\det(2\pi\mathcal{T})}} \exp(-\frac{1}{2}(\mathcal{T}^{-1})_{ij}c_i c_j), \quad (20b)$$

$$\mathcal{T}_{ij} = (1 - \nu)RT\delta_{ij} + \nu\Theta_{ij}, \quad \Theta_{ij} = \frac{1}{\rho} \int c_i c_j f d\xi, \quad (20c)$$

$$Q_d^\flat[f] = -\frac{\partial}{\partial \xi_i} [(\alpha_i^\flat + \beta^\flat c_i)f], \quad (20d)$$

$$\begin{aligned} \alpha_i^\flat &= \alpha_i + \frac{1}{\rho} \frac{\partial}{\partial X_j} [\mu_P (\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij}) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}] \\ &= \alpha_i^\sharp + \frac{1}{\rho} \frac{\partial}{\partial X_j} [\mu_P (\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij})], \end{aligned} \quad (20e)$$

$$\begin{aligned} \beta^\flat &= \beta + \frac{1}{3R\rho T} \left\{ \frac{\partial}{\partial X_k} (\lambda_P \frac{\partial T}{\partial X_k}) \right. \\ &\quad \left. + \frac{\partial v_i}{\partial X_j} [\mu_P (\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij}) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}] \right\} \\ &= \beta^\sharp + \frac{1}{3R\rho T} \left\{ \frac{\partial}{\partial X_k} (\lambda_P \frac{\partial T}{\partial X_k}) + \mu_P \frac{\partial v_i}{\partial X_j} (\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij}) \right\}, \end{aligned} \quad (20f)$$

where μ_B is the same as before and

$$A^\flat(\rho, T) = \frac{5}{2} \frac{\rho R T}{1 - b\rho} \frac{R}{\lambda_0(T)} \left(= g_2(\frac{b\rho}{1 - b\rho}) A^\sharp(\rho, T) \right), \quad (21a)$$

$$\nu = 1 - \frac{2}{5} \frac{1}{R} \frac{\lambda_0(T)}{\mu_0(T)} = 1 - \frac{1}{\text{Pr}_0}, \quad (21b)$$

$$\mu_P(\rho, T) = (1 - b\rho) g_1^\flat(\frac{b\rho}{1 - b\rho}) \mu_0(T), \quad (21c)$$

$$\lambda_P(\rho, T) = (1 - b\rho) g_2^\flat(\frac{b\rho}{1 - b\rho}) \lambda_0(T), \quad (21d)$$

$$g_1^\flat(x) = g_1(x) - 1, \quad g_2^\flat(x) = g_2(x) - 1. \quad (21e)$$

Comparing (21e) with (15f), it is seen that $g_1^\flat(x) > 0$ and $g_2^\flat(x) > 0$ for $x > 0$; thus $\mu_P > 0$ and $\lambda_P > 0$ for $0 \leq b\rho < 1$. Then, by the following change of the definitions of p_{ij} and q_i :

$$p_{ij} = p\delta_{ij} + \int (c_i c_j - \frac{1}{3} c^2 \delta_{ij}) f d\mathbf{\xi} - \mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (22)$$

$$q_i = \frac{1}{2} \int c_i c^2 f d\mathbf{\xi} - \lambda_P \frac{\partial T}{\partial X_i}, \quad (23)$$

the second ES-based model retains the set of conservation laws (7) as it stands. Furthermore, in the fluid dynamic limit, the stress tensor and heat-flow vector are reduced to

$$p_{ij} = p\delta_{ij} - \mu \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}, \quad (24a)$$

$$q_i = -\lambda \frac{\partial T}{\partial X_i}, \quad (24b)$$

where μ and λ are the same as those in (15); see the Appendix for the derivation. Substitution of (24) to (7) gives the Navier–Stokes set of equations with a self-consistent force term.

In contrast to the first ES-based model, ν is a constant parameter in the second ES-based model and it can be set as $\nu = -1/2$. Thus,

$$\int Q_c^b[f] \ln \frac{f}{c_0} d\mathbf{\xi} \leq 0, \quad (25)$$

holds unconditionally. This is an advantage over the first ES-based model, because with this property, $H(t)$ can be shown monotonically decreasing.

Proposition 2. *For the system (20) with (21), $H(t)$ defined by (5b) in a spatially periodic domain monotonically decreases in time t . Furthermore, $H(t)$ reaches a stationary state if and only if f is a Maxwellian with a uniform temperature and a uniform flow velocity.*

Proof. By following the calculations in (16),

$$\begin{aligned} \frac{d}{dt} \int_D \int f \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} &= \int_D \int (Q_c^b[f] + Q_d^b[f]) \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} \\ &= \int_D \int Q_c^b[f] \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} - 3 \int_D \beta^b \rho d\mathbf{X}. \end{aligned} \quad (26)$$

Since the β -part in β^b gives rise the second term of (5b), the above is reduced to

$$\frac{d}{dt} H(t) = \int_D \int Q_c^b[f] \ln \frac{f}{c_0} d\mathbf{\xi} d\mathbf{X} - 3 \int_D (\beta^b - \beta) \rho d\mathbf{X}. \quad (27)$$

Note that the first term in (27) is designed to be nonpositive as far as $\nu \in [-1/2, 1)$, which is a marked contrast to the case of the first ES-based model. As to the second term of (27), the following transformation from the definition of β^b is possible:

$$\begin{aligned}
(\beta^b - \beta)\rho &= \frac{1}{3RT} \left\{ \frac{\partial}{\partial X_k} \left(\lambda_P \frac{\partial T}{\partial X_k} \right) \right. \\
&\quad \left. + \frac{\partial v_i}{\partial X_j} \left[\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij} \right] \right\} \\
&= \frac{1}{3R} \left\{ \frac{\partial}{\partial X_k} \left(\frac{\lambda_P}{T} \frac{\partial T}{\partial X_k} \right) + \frac{\lambda_P}{T^2} \left(\frac{\partial T}{\partial X_k} \right)^2 \right. \\
&\quad \left. + \frac{1}{2} \frac{\mu_P}{T} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right)^2 + \frac{\mu_B}{T} \left(\frac{\partial v_k}{\partial X_k} \right)^2 \right\}. \quad (28)
\end{aligned}$$

Here, the following identities have been used:

$$\left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) \delta_{ij} = 0, \quad (29a)$$

$$\frac{\partial v_i}{\partial X_j} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) = \frac{1}{2} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right)^2. \quad (29b)$$

Coming back to (28), the contribution of the first term in the curly brackets vanishes, thanks to the periodic condition and the divergence theorem. Therefore, $\int_D (\beta^b - \beta) \rho d\mathbf{X} \geq 0$, and

$$\frac{d}{dt} H(t) = \int_D \int Q_c^b[f] \ln \frac{f}{c_0} d\xi d\mathbf{X} - 3 \int_D (\beta^b - \beta) \rho d\mathbf{X} \leq 0. \quad (30)$$

The last equality holds if and only if $\int_D \int Q_c^b[f] \ln(f/c_0) d\xi d\mathbf{X} = 0$ and $\int_D (\beta^b - \beta) \rho d\mathbf{X} = 0$. The former condition requires that f is a Maxwellian, while the latter condition requires a uniform temperature and $\partial v_i / \partial X_j + \partial v_j / \partial X_i = 0$. Then, the last condition on the velocity gradients admits a flow field that is a superposition of a uniform flow and a rigid body rotation. However, the rigid body rotation conflicts with the periodic condition, and the flow velocity is uniform in the present case. $\square$

Remark 1. The density is not necessarily uniform in a stationary state.

4 Preliminary tests

Numerical simulations have been conducted to check quantitative differences between two ES-based models. In each simulation, a dense gas is confined in a spatially one-dimensional periodic domain with D being its unit region, and a time evolution from a uniform equilibrium state at rest by an initial sinusoidal perturbation

$$\rho(0, X_1) = \rho_0(1 + \omega \sin(2\pi X_1/L)), \quad (31)$$

is studied, where ρ_0 is the average density of the gas, L is the length of the unit region, and ω is a factor of the initial perturbation size. Because of the total mass, momentum, and energy constraints [see (7)], the initial disturbance of density is given

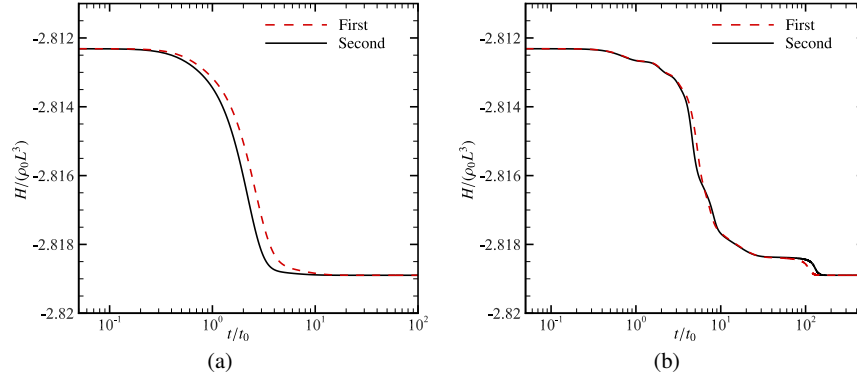


Fig. 2 Time evolution of $H(t)$ from the perturbed uniform state with $\omega = 0.1$ in the case $b\rho_0 = 1/3$, $c \equiv a/(bRT_0) = 3.8$, and $K \equiv \kappa/(2bRT_0L^2) = 1.0 \times 10^{-4}$. (a) $k^b = 0.1$ and (b) $k^b = 0.01$. The solid line indicates the result of the second ES-based model, while the dashed red line indicates the result of the first ES-based model. $t_0 = L/\sqrt{2RT_0}$.

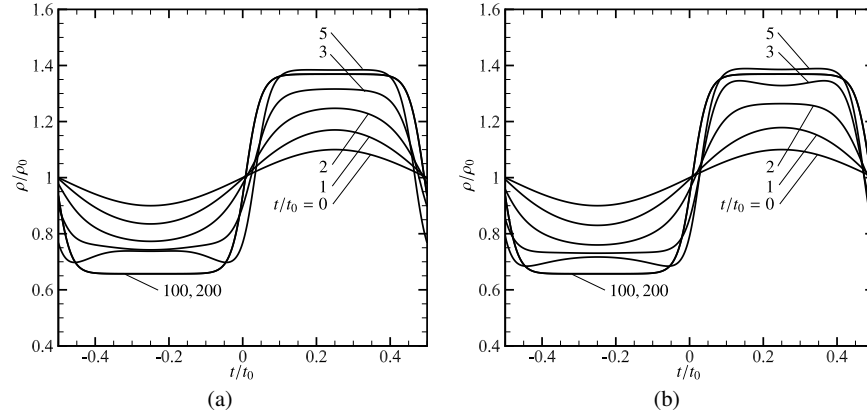


Fig. 3 Time evolution of the density profile from the initial disturbed state with $\omega = 0.1$ for the case $b\rho_0 = 1/3$, $c = 3.8$, $K = 1.0 \times 10^{-4}$, and $k^b = 0.1$. (a) the first ES-based model, (b) the second ES-based model. See also the caption of Fig. 2.

in such a way that the initial uniform temperature is different from the temperature T_0 of the undisturbed uniform equilibrium state, while the initial flow velocity is zero. Since comparisons between the BGK-based and the first ES-based model can be found in [20], we report preliminary results of comparisons between the first and the second ES-based model. In the numerical results to be presented below, the first ES-based model is well inside the valid range of the H theorem.

Figure 2 shows time evolutions of the function $H(t)$ from the initial disturbed state with $\omega = 0.1$ for the case $b\rho_0 = 1/3$, $c \equiv a/(bRT_0) = 3.8$, $K \equiv \kappa/(2bRT_0L^2) = 1.0 \times 10^{-4}$, and $k^b \equiv \sqrt{2RT_0}/(A^b(\rho_0, T_0)L) = 0.1$ and 0.01 , where $\text{Pr}_0 = 2/3$ and $\lambda_0(T)$ is chosen as the one for hard-sphere molecules in the dilute gas limit.

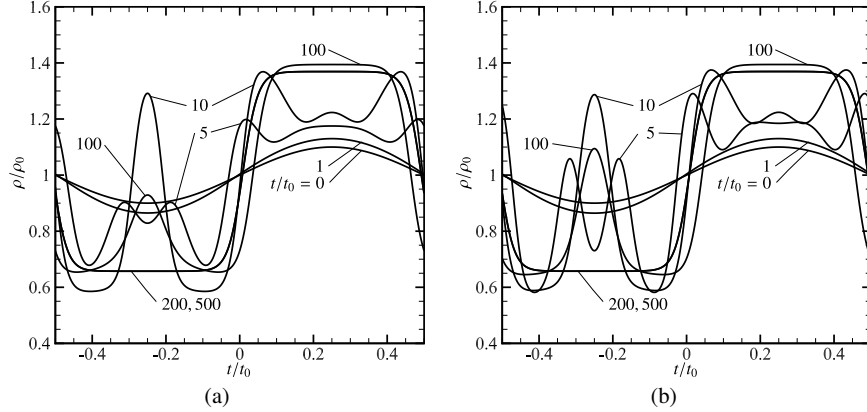


Fig. 4 Time evolution of the density profile from the initial disturbed state with $\omega = 0.1$ for the case $b\rho_0 = 1/3$, $c = 3.8$, $K = 1.0 \times 10^{-4}$, and $k^b = 0.01$. (a) the first ES-based model, (b) the second ES-based model. See also the caption of Fig. 2.

In both ES-based model, the function $H(t)$ monotonically decreases as the time increases. However, the evolution in the first model is delayed for $k^b = 0.1$. Indeed, instantaneous density profiles do not necessarily agree between the two models during the time evolution, though the time evolution of density profile is similar as a whole irrespective of $k^b = 0.1$ or 0.01 ; see Figs. 3 and 4. The final stationary states are not influenced by the difference of models, which also applies to the BGK-based model [20].

5 Conclusion

In the present paper, our constructions of simple kinetic models are presented, including a couple of new proposals based on the ES-type collision integral. The ES-based models have an advantage over our previous models in that they reproduce transport properties appropriately. The two models have a difference in the monotone property that is also desired as a kinetic model. The first ES-based model does not fully satisfy the H theorem, while the second ES-based model satisfies it unconditionally. In this sense, the latter has a better property qualitatively. In order to assess the quantitative difference between them, numerical simulations of the one-dimensional phase separation problem have been conducted for the parameter setting that falls into the thermodynamically unstable regime. Thermodynamically stable, metastable, and unstable regimes were not influenced by the change of the kinetic model presented in this paper. As a whole, the two ES-based models behave similarly, but do not achieve the perfect agreement in the time evolution of density profile. Further numerical assessment is needed, but is left for future works.

Appendix

In this Appendix, the fluid-dynamic limit of the second ES-based model will be studied based on the Chapman–Enskog (CE) method along the lines of Harold Grad [24, 25]. The case of the first ES-based model is similar, and the case of the BGK-based model is much simpler.

In order to avoid unnecessary increase of notations and to indicate the scaling, we shall artificially multiply μ_P , λ_P , and μ_B by a small parameter ε and Q_c^b by $1/\varepsilon$ instead of making (20) dimensionless. After the analysis, the artificial parameter ε is removed or set as unity.

Since μ_P , λ_P , and μ_B are all confined in the difference between Q_d^b and Q_d , we denote it by $\varepsilon\tilde{Q}_d^b$, i.e., $Q_d^b = Q_d + \varepsilon\tilde{Q}_d^b$, rewrite (20) as

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial X_i} + F_i \frac{\partial f}{\partial \xi_i} = \frac{1}{\varepsilon} Q_c^b[f] + Q_d[f] + \varepsilon \tilde{Q}_d^b[f], \quad (32)$$

and consider a solution of this equation in the form $f = f(\rho_r, \nabla \rho_r, \boldsymbol{\xi})$, where and hereafter $\rho_r = \int \psi_r f d\boldsymbol{\xi}$ ($r = 0, 1, \dots, 4$) with $\psi_0 = 1$, $\psi_i = \xi_i$ ($i = 1, 2, 3$), $\psi_4 = \boldsymbol{\xi}^2/2$, and, unlike the usual notation, $\nabla \rho_r$ represents a spatial derivative of ρ_r of arbitrary order. Note that $\{\rho_0, \rho_i, \rho_4\} = \{\rho, \rho v_i, (3/2)\rho RT + (1/2)\rho v^2\}$ ($i = 1, 2, 3$) and that the present form of f depends on t and $\mathbf{X}$ only through ρ_r and $\nabla \rho_r$. By multiplying (32) with ψ_r and integrating the result with respect to $\boldsymbol{\xi}$, the time derivative of ρ_r can be expressed in the form

$$\frac{\partial \rho_r}{\partial t} + \mathcal{F}_r(\rho_r, \nabla \rho_r, \varepsilon) = 0, \quad (r = 0, 1, \dots, 4). \quad (33)$$

From now on, we seek the solution f in a series of ε :

$$f = \sum_{n=0}^{\infty} \varepsilon^n f^{(n)}(\rho_r, \nabla \rho_r, \boldsymbol{\xi}). \quad (34)$$

Substitution of (34) into (33) gives

$$\frac{\partial \rho_r}{\partial t} + \sum_{n=0}^{\infty} \varepsilon^n \mathcal{F}_r^{(n)}(\rho_r, \nabla \rho_r) = 0, \quad (r = 0, 1, \dots, 4), \quad (35)$$

and accordingly the time derivative of f is expressed as

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial \rho_r} \frac{\partial \rho_r}{\partial t} + \frac{\partial f}{\partial \nabla \rho_r} \frac{\partial \nabla \rho_r}{\partial t} = - \sum_{n=0}^{\infty} \varepsilon^n \left(\frac{\partial f}{\partial \rho_r} \mathcal{F}_r^{(n)} + \frac{\partial f}{\partial \nabla \rho_r} \nabla \mathcal{F}_r^{(n)} \right). \quad (36)$$

Here and hereafter the summation convention rule is applied to the repeated r and ∇ . The form of $\mathcal{F}_r^{(n)}$ will be determined in the course of analysis that follows.

Substitution of (34) and (36) into (32) gives the following series of equations:

$$A^{b(0)}(f^{(0)} - \mathcal{G}[f]^{(0)}) = 0, \quad (37a)$$

$$\begin{aligned} A^{b(0)}(f^{(1)} - \mathcal{G}[f]^{(1)}) = & \left(\frac{\partial f^{(0)}}{\partial \rho_r} \mathcal{F}_r^{(0)} + \frac{\partial f^{(0)}}{\partial \nabla \rho_r} \nabla \mathcal{F}_r^{(0)} \right) \\ & - \xi_i \frac{\partial f^{(0)}}{\partial X_i} - F_i^{(0)} \frac{\partial f^{(0)}}{\partial \xi_i} + Q_d[f]^{(0)}, \end{aligned} \quad (37b)$$

$$\begin{aligned} A^{b(0)}(f^{(2)} - \mathcal{G}[f]^{(2)}) \\ = A^{b(1)}(\mathcal{G}[f]^{(1)} - f^{(1)}) + \sum_{\ell=0}^1 \left(\frac{\partial f^{(\ell)}}{\partial \rho_r} \mathcal{F}_r^{(1-\ell)} + \frac{\partial f^{(\ell)}}{\partial \nabla \rho_r} \nabla \mathcal{F}_r^{(1-\ell)} \right) \\ - \xi_i \frac{\partial f^{(1)}}{\partial X_i} - F_i^{(0)} \frac{\partial f^{(1)}}{\partial \xi_i} - F_i^{(1)} \frac{\partial f^{(0)}}{\partial \xi_i} + Q_d[f]^{(1)} + \tilde{Q}_d^b[f]^{(0)}, \end{aligned} \quad (37c)$$

and so on, where

$$\mathcal{G}[f] = \sum_{n=0}^{\infty} \mathcal{G}[f]^{(n)} \varepsilon^n, \quad F_i = \sum_{n=0}^{\infty} F_i^{(n)} \varepsilon^n, \quad (38a)$$

$$A^b(\rho, T) = \sum_{n=0}^{\infty} A^{b(n)} \varepsilon^n, \quad Q_d^b[f] = \sum_{n=0}^{\infty} (Q_d[f]^{(n)} + \varepsilon \tilde{Q}_d^b[f]^{(n)}) \varepsilon^n. \quad (38b)$$

Under the conventional condition

$$\int \psi_r f d\boldsymbol{\xi} = \int \psi_r f^{(0)} d\boldsymbol{\xi}, \quad (39)$$

we solve (37) from the lowest order. Before going into details, it should be noted that, by (39) and the property of the ES collision integral [16]:

$$\int \psi_r \mathcal{G}[f] d\boldsymbol{\xi} = \int \psi_r f d\boldsymbol{\xi}, \quad (r = 0, 1, \dots, 4), \quad (40a)$$

$$\int c_i c_j \mathcal{G}[f] d\boldsymbol{\xi} = \rho \mathcal{T}_{ij} = (1 - \nu) \rho R T \delta_{ij} + \nu \rho \Theta_{ij}, \quad (40b)$$

it holds that

$$\int \psi_r \mathcal{G}[f]^{(0)} d\boldsymbol{\xi} = \int \psi_r f^{(0)} d\boldsymbol{\xi}, \quad (41a)$$

$$\int \psi_r f^{(n+1)} d\boldsymbol{\xi} = 0, \quad \int \psi_r \mathcal{G}[f]^{(n+1)} d\boldsymbol{\xi} = 0, \quad (41b)$$

where $r = 0, 1, \dots, 4$ and $n = 0, 1, 2, \dots$.

Let us now start with the solution of (37a). Since $\mathcal{G}[f]^{(0)} = \lim_{\varepsilon \rightarrow 0} \mathcal{G}[f] = \mathcal{G}[f^{(0)}]$, (37a) is reduced to

$$f^{(0)} = \mathcal{G}[f^{(0)}],$$

and thus $f^{(0)}$ is a local Maxwellian:

$$f^{(0)} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \mathbf{v}|^2}{2RT}\right),$$

where the condition (39) has been used. By the same condition, it is also seen that

$$F_i^{(0)} = F_i, \quad A^{b(0)} = A^b, \quad Q_d^b[f]^{(0)} = Q_d[f^{(0)}], \quad (42a)$$

$$F_i^{(n+1)} = 0, \quad A^{b(n+1)} = 0, \quad Q_d^b[f]^{(n+1)} = Q_d[f^{(n+1)}] + \tilde{Q}_d^b[f^{(n)}], \quad (42b)$$

where $n = 0, 1, \dots$, since F_i , A^b , Q_d , and $\tilde{Q}_d^b$ are all expressed in terms of ρ_r and $\nabla\rho_r$ and thus Q_d and $\tilde{Q}_d^b$ can be treated as linear operators acting on the expanded VDF $f^{(n)}$. Furthermore, (37b) is reduced to

$$f^{(1)} = \mathcal{G}[f]^{(1)} + \frac{1}{A^b} \left(\frac{\partial f^{(0)}}{\partial \rho_r} \mathcal{F}_r^{(0)} - \xi_i \frac{\partial f^{(0)}}{\partial X_i} - F_i \frac{\partial f^{(0)}}{\partial \xi_i} + Q_d[f^{(0)}] \right), \quad (43)$$

since $f^{(0)}$ is independent of $\nabla\rho_r$. From (41b) with $n = 0$, the ψ_s -moment of (43) ($s = 0, 1, \dots, 4$) gives the following constraint for (37b) to be solvable:

$$\mathcal{F}_s^{(0)} = \int \xi_i \psi_s \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} - F_i \int \frac{\partial \psi_s}{\partial \xi_i} f^{(0)} d\boldsymbol{\xi} - \int \psi_s Q_d[f^{(0)}] d\boldsymbol{\xi}. \quad (44)$$

The above constraint is consistent with the definition of $\mathcal{F}_s$ at the leading order ($n = 0$) [see (33) or (35)] and eventually leads to the following expressions of $\mathcal{F}_s^{(0)}$:

$$\mathcal{F}_0^{(0)} = \int \xi_i \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} = \frac{\partial \rho_i}{\partial X_i} = \frac{\partial \rho v_i}{\partial X_i}, \quad (45a)$$

$$\begin{aligned} \mathcal{F}_j^{(0)} &= \int \xi_i \xi_j \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} - F_j \rho - \alpha_j \rho \\ &= \frac{\partial}{\partial X_i} \left(\rho v_i v_j + (\rho RT + \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho) \delta_{ij} \right) + \rho \frac{\partial \Phi_L}{\partial X_j} \\ &= \frac{\partial}{\partial X_i} (\rho v_i v_j + p \delta_{ij}) + \rho \frac{\partial \Phi_L}{\partial X_j}, \quad (j = 1, 2, 3), \end{aligned} \quad (45b)$$

$$\begin{aligned} \mathcal{F}_4^{(0)} &= \frac{1}{2} \int \xi_i \xi^2 \frac{\partial f^{(0)}}{\partial \rho_r} d\boldsymbol{\xi} \frac{\partial \rho_r}{\partial X_i} - F_i \rho v_i - (\alpha_i \rho v_i + 3\beta \rho RT) \\ &= \frac{\partial}{\partial X_i} \left(\left(\frac{5}{2} RT + \frac{1}{2} \mathbf{v}^2 \right) \rho v_i \right) + \frac{\partial}{\partial t} \int (\Phi_S - T \frac{\partial \Phi_S}{\partial T}) d\rho \\ &\quad + \frac{\partial}{\partial X_i} \left(v_i \int (\Phi_S - T \frac{\partial \Phi_S}{\partial T}) d\rho + v_i \int \rho \frac{\partial \Phi_S}{\partial \rho} d\rho \right) + \rho v_i \frac{\partial \Phi_L}{\partial X_i} \\ &= \frac{\partial}{\partial X_i} \left(\left(e + \frac{1}{2} \mathbf{v}^2 \right) \rho v_i + p v_i \right) + \frac{\partial}{\partial t} \int (\Phi_S - T \frac{\partial \Phi_S}{\partial T}) d\rho + \rho v_i \frac{\partial \Phi_L}{\partial X_i}. \end{aligned} \quad (45c)$$

If we stop the solution procedure at this stage and substitute (45) into (35) truncated at $n = 0$, the Euler set of equations, i.e., (7) with $p_{ij} = p \delta_{ij}$ and $q_i = 0$, is obtained.

In order to complete the solution of $f^{(1)}$, it is necessary to evaluate $\mathcal{G}[f]^{(1)}$. The evaluation needs some direct calculations to conclude

$$\mathcal{G}[f]^{(1)} = \frac{2\nu}{(2RT)^2} \Theta_{k\ell}^{(1)} c_k c_\ell f^{(0)}, \quad (46a)$$

where

$$\rho \Theta_{ij}^{(1)} = \int c_i c_j f^{(1)} d\boldsymbol{\xi}. \quad (46b)$$

Then, taking the $c_i c_j$ -moment of (43) eventually lead to

$$\int c_i c_j f^{(1)} d\boldsymbol{\xi} (= \rho \Theta_{ij}^{(1)}) = -\frac{\rho RT}{(1-\nu)A^b} \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right), \quad (47)$$

with the aid of (46a). Substitution of (46a) and (47) into (43) completes the solution of $f^{(1)}$. With thus obtained $f^{(1)}$, it is also seen that

$$\frac{1}{2} \int c_i c^2 f^{(1)} d\boldsymbol{\xi} = -\frac{5}{2} \frac{R}{A^b} \rho RT \frac{\partial T}{\partial X_i}. \quad (48)$$

Finally, let us consider (37c), which is slightly simplified as

$$\begin{aligned} f^{(2)} = \mathcal{G}[f]^{(2)} + \frac{1}{A^b} & \left(\frac{\partial f^{(0)}}{\partial \rho_r} \mathcal{F}_r^{(1)} + \frac{\partial f^{(1)}}{\partial \rho_r} \mathcal{F}_r^{(0)} + \frac{\partial f^{(1)}}{\partial \nabla \rho_r} \nabla \mathcal{F}_r^{(0)} \right. \\ & \left. - \xi_i \frac{\partial f^{(1)}}{\partial X_i} - F_i \frac{\partial f^{(1)}}{\partial \xi_i} + Q_d[f^{(1)}] + \tilde{Q}_d^b[f^{(0)}] \right), \end{aligned} \quad (49)$$

by using the results obtained so far in the Appendix. Because of (41b) with $n = 1$, the ψ_s -moment of (49) gives the following constraint for (37c) to be solvable:

$$\mathcal{F}_s^{(1)} = \frac{\partial}{\partial X_i} \int \xi_i \psi_s f^{(1)} d\boldsymbol{\xi} - \int \psi_s Q_d[f^{(1)}] d\boldsymbol{\xi} - \int \psi_s \tilde{Q}_d^b[f^{(0)}] d\boldsymbol{\xi}, \quad (50)$$

which is again consistent with the definition of $\mathcal{F}_s$ at the order $n = 1$. (50) is further reduced to

$$\mathcal{F}_0^{(1)} = 0, \quad (51a)$$

$$\mathcal{F}_j^{(1)} = \frac{\partial}{\partial X_i} \int c_i c_j f^{(1)} d\boldsymbol{\xi} - \rho(\alpha_j^b - \alpha_j), \quad (j = 1, 2, 3), \quad (51b)$$

$$\begin{aligned} \mathcal{F}_4^{(1)} = \frac{\partial}{\partial X_i} & \left(\frac{1}{2} \int c_i c^2 f^{(1)} d\boldsymbol{\xi} + v_j \int c_i c_j f^{(1)} d\boldsymbol{\xi} \right) \\ & - \rho(\alpha_i^b - \alpha_i) v_i - 3(\beta^b - \beta) \rho RT. \end{aligned} \quad (51c)$$

Noting that

$$\rho(\alpha_i^b - \alpha_i) = \frac{\partial}{\partial X_j} [\mu_P \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3} \frac{\partial v_k}{\partial X_k} \delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k} \delta_{ij}], \quad (52a)$$

$$3(\beta^b - \beta)\rho RT + \rho(\alpha_j^b - \alpha_j)v_j = \frac{\partial}{\partial X_k}(\lambda_P \frac{\partial T}{\partial X_k}) + \frac{\partial}{\partial X_j}[\mu_P(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij})v_i + \mu_B \frac{\partial v_k}{\partial X_k}v_j], \quad (52b)$$

(51b) and (51c) are finally expressed as

$$\mathcal{F}_j^{(1)} = -\frac{\partial}{\partial X_i} \left(\mu \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij} \right) + \mu_B \frac{\partial v_k}{\partial X_k}\delta_{ij} \right), \quad (53)$$

$$\mathcal{F}_4^{(1)} = -\frac{\partial}{\partial X_i} \left(\lambda \frac{\partial T}{\partial X_i} + \mu v_j \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij} \right) + \mu_B v_i \frac{\partial v_k}{\partial X_k} \right), \quad (54)$$

where

$$\mu = \mu_P + \frac{\rho RT}{(1-\nu)A^b}, \quad \lambda = \lambda_P + \frac{5}{2}\frac{R}{A^b}\rho RT. \quad (55)$$

Thus, (35) truncated at $n = 1$ gives the Navier–Stokes set of equations, i.e., (7) with

$$p_{ij} = p\delta_{ij} - \mu \left(\frac{\partial v_i}{\partial X_j} + \frac{\partial v_j}{\partial X_i} - \frac{2}{3}\frac{\partial v_k}{\partial X_k}\delta_{ij} \right) - \mu_B \frac{\partial v_k}{\partial X_k}\delta_{ij}, \quad (56)$$

$$q_i = -\lambda \frac{\partial T}{\partial X_i}. \quad (57)$$

Acknowledgments

The present work has been supported in part by the JSPS KAKENHI Grants (No. 17K18840 and 22K03923), the Kyoto University Foundation, the HPCI system Research Projects hp210007 and hp220077, and the research grant from the Mori Manufacturing Research and Technology Foundation to T. M. The authors thank Luc Mieussens for calling their attention to [23].

References

1. Y. Sone, K. Aoki, and I. Yamashita, A study of unsteady strong condensation on a plane condensed phase with special interest in formation of steady profile, in *Rarefied Gas Dynamics*, V. Boffi and C. Cercignani eds., Vol. II, Teubner, Stuttgart, pp. 323–333 (1986).
2. K. Aoki, S. Sone, and T. Yamada, Numerical analysis of gas flows condensing on its plane condensed phase on the basis of kinetic theory, *Phys. Fluids A* **2**, 1867–1878 (1990).
3. Y. Sone and H. Sugimoto, Strong evaporation from a plane condensed phase, in *Adiabatic Waves in Liquid-Vapor Systems*, G. E. A. Meier and P. A. Thompson, eds., Springer-Verlag, Berlin, pp. 293–304 (1990).
4. M. N. Kogan, Kinetic theory in aerothermodynamics, *Prog. Aerospace Sci.* **29**, 271–354 (1992).
5. S. Ukai, T. Yang, and S.-H. Yu, Nonlinear boundary layers of the Boltzmann equation I. Existence, *Commun. Math. Phys.* **236**, 373–393 (2003).

6. C. Bardos, F. Golse, and Y. Sone, Half-space problems for the Boltzmann equation: A survey, *J. Stat. Phys.* **124**, 275–300 (2006).
7. T.-P. Liu and S.-H. Yu, Invariant manifolds for steady Boltzmann flows and applications, *Arch. Rational Mech. Anal.* **209**, 869–997 (2013).
8. A. Frezzotti, Monte Carlo simulation of the heat flow in a dense hard sphere gas, *Eur. J. Mech. B/Fluids* **18**, 103–119 (1999).
9. L. Wu, Y. Zhang, and J. M. Reese, Fast spectral solution of the generalized Enskog equation for dense gases, *J. Comput. Phys.* **303**, 66–79 (2015).
10. P. L. Bhatnagar, E. P. Gross, and M. Krook, A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems, *Phys. Rev.* **94**, 511–525 (1954).
11. P. Welander, On the temperature jump in a rarefied gas, *Arkiv fysik* **7**, 507–553 (1954).
12. S. Takata and T. Noguchi, A simple kinetic model for the phase transition of the van der Waals fluid, *J. Stat. Phys.* **172**, 880 (2018).
13. S. Takata, T. Matsumoto, A. Hirahara, and M. Hattori, Kinetic theory for a simple modeling of a phase transition: Dynamics out of local equilibrium, *Phys. Rev. E* **98**, 052123 (2018).
14. S. Takata, T. Matsumoto, and M. Hattori, Kinetic model for the phase transition of the van der Waals fluid, *Phys. Rev. E* **103**, 062110 (2021).
15. L. H. Holway, New statistical models for kinetic theory: Methods of construction, *Phys. Fluids* **9**, 1658–1673 (1966).
16. P. Andries, P. Le Tallec, J.-P. Perlat, and Benoît Perthame, The Gaussian-BGK model of Boltzmann equation with small Prandtl number, *Eur. J. Mech. B-Fluids* **19**, 813–830 (2000).
17. κ can be related to a in the equation of state, once the long-range attractive potential is specified. Here κ and a are regarded as independent parameters. This reflects a degree of freedom on the choice of attractive potential.
18. V. Giovangigli, Kinetic derivation of Cahn-Hilliard fluid models, *Phys. Rev. E* **104**, 054109 (2021).
19. D. Enskog, Kinetic theory of heat conduction, viscosity, and self-diffusion in compressed gases and liquids, in *Kinetic Theory*, Vol. 3, S. G. Brush ed., Pergamon Press, Oxford, Part 2, pp. 226–259, 1972.
20. T. Miyauchi, S. Takata, and M. Hattori, An attempt on an ES-model-based construction of a kinetic equation for a dense gas, in *AIP conference Proceedings: 32nd International Symposium on Rarefied Gas Dynamics*, (submitted).
21. R. Soto, *Kinetic Theory and Transport Phenomena*, Oxford University Press, Oxford, 2016.
22. S. Takata, M. Hattori, and T. Miyauchi, On the entropic property of the ellipsoidal statistical model with the Prandtl number below $2/3$, *Kinetic & Related Models* **13**, 1163–1174 (2020).
23. J. Mathiaud and L. Mieussens, A Fokker–Planck model of the Boltzmann equation with correct Prandtl number, *J. Stat. Phys.* **162**, 397–414 (2016).
24. Y. Sone, *Molecular Gas Dynamics*, Birkhäuser, Boston, 2007, Appendix B.4.
25. H. Grad, Principles of the kinetic theory of gases, in *Handbuch der Physik*, Band XII, S. Flügge ed., Springer–Verlag, Berlin, pp. 205–294, 1958, Sec. 25.