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Some comments on modeling the linearized Boltzmann equation

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Abstract

Some exact solutions of the homogeneous and the inhomogeneous linearized Boltzmann equation (LBE) for rigid-sphere collisions are used to define two model equations in the general area of rarefied-gas dynamics. These equations are obtained from a systematic development of two synthetic scattering kernels that yield model equations that have as exact solutions certain known exact solutions of the homogeneous and of the inhomogeneous LBE. The first model established is defined in terms of the collisional invariants and the Chapman–Enskog integral equations for viscosity and for heat conduction. An extended model is defined also in terms of the collisional invariants and the Chapman–Enskog functions for viscosity and heat conduction, but the first and second Burnett functions are also included in the model. The variable collision frequency or generalized BGK model is also obtained as a special case. In addition, the exact mean-free paths defined, for rigid-sphere collisions and the LBE, in terms of viscosity or heat conduction are employed to define approximations of these quantities that are consistent with the use of the variable collision frequency model.

Keywords: Boltzmann equation; Rarefied-gas dynamics; Synthetic kernels

1. Introduction

Internal rarefied-gas flows define a field of major interest in the general area of rarefied-gas dynamics, and so the contributions to this body of knowledge are many. The books of Cercignani [1,2] and Williams [3] provide excellent material relevant to this field and a comprehensive review recently reported by Sharipov and Seleznev [4] also is a useful up-to-date source that pays much attention to comparing different computational methods as well as different mathematical formulations basic to rarefied-gas dynamics. In recent years, we have seen an increased interest in the general

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area of rarefied-gas dynamics essentially because of applications in nanotechnology (for example, as related to micro-machines and high-speed disk drives) where the Boltzmann equation or a model equation is required in order to describe well gas-flow and heat-flow mechanisms. It was also pointed out in Ref. [4] that the thermal transpiration phenomena, which exist in internal flows produced by a temperature or pressure gradient, continue to attract the attention of scientists. Moreover, there is additional recent interest in these effects due to applications in micro-electro-mechanical systems (MEMS), and so we believe there is need for further improvements in computational methods and mathematical modeling for the flow of microfluids. In many cases the flow conditions are in the transition regime and as a result the well-known and commonly used Navier–Stokes equations can not be applied. In these cases the Boltzmann equation or suitable kinetic models should be utilized.

In regard to improvements in computational methods in the general area of rarefied-gas dynamics, we note that our analytical discrete-ordinates (ADO) method [5] has been shown [6–9] to be a useful method for solving a class of basic problems in this field. For example, many of the classical problems based on the BGK model [10] have been solved in a unified and especially accurate way with the ADO method. Following beginning work with the BGK model, we extended the ADO method in order to solve many of the basic problems in rarefied-gas dynamics that were defined in terms of the variable collision frequency model (CLF model) of Cercignani [11] and Loyalka and Ferziger [12]. Having seen that the ADO method is a convenient computational method for solving problems based on the CLF model and seeking improved results for physical quantities of interest, we now go back and make use of some early work of Shapiro and Corngold [13] and Loyalka and Ferziger [12] in order to define explicitly two extended model equations based on approximated forms of the linearized Boltzmann equation (LBE). While Refs. [2,12,13] have discussed, in general terms, the use of degenerate kernels for use in particle transport theory, we believe the use we make here of exact solutions of the homogeneous and of the inhomogeneous LBE provides a systematic basis for approximating the scattering kernel in the LBE. It is for this reason that the two models (the CES model and the CEBS model) are developed in detail.

This work starts with the LBE for rigid-sphere interactions, as discussed by Pekeris and Alterman [14], and so, while the model equations developed may readily be extended to other interaction laws, the basis of the work must be taken in the light of the LBE and rigid-sphere collisions. Although modern and intensive numerical methods based on finite-difference techniques and the numerical evaluation of multi-dimensional integrals can be used, as can the Monte Carlo method, to solve practical problems based on the LBE, our goal here is to explore a class of model equations that can be solved (essentially) analytically to yield results good enough for selected engineering applications. It is for this reason that we provide a systematic derivation of the models and report the final forms in sufficient detail that researchers seeking to develop numerical algorithms to solve practical problems will have a clearly defined starting point. We note here that while we have found success with our ADO method, the kernel of the integral operator of the LBE is not continuous [15] in the relevant variables, and for this reason we avoid the use of a global quadrature method for evaluating such integrals.

To start we follow the papers of Pekeris and Alterman [14] and Loyalka and Hickey [16] and consider the LBE written as

$$c\mu\frac{\partial}{\partial x}h(x,\boldsymbol{c}) = \sigma_0^2 n_0 \pi^{1/2} L\{h\}(x,\boldsymbol{c}), \tag{1}$$

where $c(2kT_0/m)^{1/2}$ is the magnitude of a particle velocity, x is the spatial variable (measured in cm) and $h(x, \boldsymbol{c})$ defines the perturbation from the equilibrium distribution

$$f_0(c) = n_0[m/(2\pi kT_0)]^{3/2}\mathrm{e}^{-c^2}. \tag{2}$$

Here n_0 is the (constant) density of gas particles, each of mass m, k is the Boltzmann constant and T_0 is a (constant) reference temperature. To be clear, we note while $h(x, \boldsymbol{c})$ defines the focus of our attention, the actual distribution function $f(x, \boldsymbol{c})$ in this formulation is expressed as

$$f(x, \boldsymbol{c}) = f_0(c)[1 + h(x, \boldsymbol{c})]. \tag{3}$$

In regard to Eq. (1), we continue to follow Refs. [14,16], and so we state that σ_0 is the collision diameter of the gas particles (in the rigid-sphere approximation) and that the collision process is described by

$$L\{h\}(x, \boldsymbol{c}) = -v(c)h(x, \boldsymbol{c}) + \int_0^\infty \int_{-1}^1 \int_0^{2\pi} \mathrm{e}^{-c'^2} h(x, \boldsymbol{c}')K(\boldsymbol{c}', \boldsymbol{c})c'^2 \,\mathrm{d}\chi' \,\mathrm{d}\mu' \,\mathrm{d}c', \tag{4}$$

where we use spherical coordinates $(c, \arccos\mu, \chi)$ to define the (dimensionless) velocity vector, where $v(c)$ is the "collision frequency" and where $K(\boldsymbol{c}', \boldsymbol{c})$ is the scattering kernel. It is clear that to proceed we require definitions of the scattering kernel $K(\boldsymbol{c}', \boldsymbol{c})$ and the collision frequency $v(c)$. In their work, Pekeris and Alterman [14] used an expansion in terms of Legendre polynomials (as functions of the scattering angle between "before" and "after" directions) to describe the scattering process. We use the spherical-harmonics addition theorem and write the scattering kernel of Pekeris and Alterman [14] as

$$K(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi}\sum_{n=0}^{\infty}\sum_{m=0}^{n}(2n+1)(2-\delta_{0,m})P_n^m(\mu')P_n^m(\mu)k_n(c', c)\cos m(\chi' - \chi). \tag{5}$$

Here the *normalized* Legendre functions

$$P_n^m(\mu) = \left[\frac{(n-m)!}{(n+m)!}\right]^{1/2}(1-\mu^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}\mu^m}P_n(\mu), \quad n \geqslant m, \tag{6}$$

where $P_n(\mu)$ denotes the usual Legendre polynomial, are such that

$$\int_{-1}^1 P_n^m(\mu)P_{n'}^m(\mu)\,\mathrm{d}\mu = \left(\frac{2}{2n+1}\right)\delta_{n,n'}. \tag{7}$$

The basic elements $k_n(c', c)$ in the expansion of the scattering kernel are, in principle, available from the paper of Pekeris and Alterman [14] where explicit expressions are given for $n = 1$ and 2. For future use, we list these components, as well as the cases $n = 0$ and 3 taken from Loyalka and Hickey [16]. Noting that, in general, $k_n(c', c) = k_n(c, c')$, we make two corrections to the listing in Ref. [16], follow the style of Loyalka and Hickey [16] and write for $c' < c$

$$-(1/2)c'ck_0(c', c) = (2/3)c'^3 + 2c'c^2 - 4P(c'), \tag{8a}$$

$$-(1/2)c'^2c^2k_1(c', c) = (2/15)c'^5 - 4c' - (2/3)c'^3c^2 - 4(c'^2 - 1)P(c'), \tag{8b}$$

$$-(1/2)c'^3c^3k_2(c', c) = a_2(c', c) + b_2(c', c)P(c') \tag{8c}$$

and

$$-(1/2)c'^4c^4k_3(c',c) = a_3(c',c) + b_3(c',c)P(c') \tag{8d}$$

where

$$a_2(c',c) = (2/35)c'^7 - 3c'^3 + 18c' - [(2/15)c'^5 - 3c']c^2, \tag{9a}$$

$$b_2(c',c) = -6c'^4 + 15c'^2 - 18 + [2c'^2 - 3]c^2, \tag{9b}$$

$$a_3(c',c) = (2/63)c'^9 - 5c'^5 + 20c'^3 - 150c' - [(2/35)c'^7 - c'^3 + 30c']c^2 \tag{9c}$$

and

$$b_3(c',c) = -10c'^6 + 45c'^4 - 120c'^2 + 150 + [6c'^4 - 21c'^2 + 30]c^2. \tag{9d}$$

Here

$$P(c) = \mathrm{e}^{c^2}\int_0^c \mathrm{e}^{-x^2}\,\mathrm{d}x. \tag{10}$$

At this point we introduce a mean-free path l (which, for the moment, we leave arbitrary) and use the dimensionless variable $\tau = x/l$ to rewrite Eq. (1) as

$$c\mu\frac{\partial}{\partial\tau}h(\tau,\boldsymbol{c}) = \varepsilon L\{h\}(\tau,\boldsymbol{c}), \tag{11}$$

where the operator L is defined by Eq. (4) and

$$\varepsilon = \sigma_0^2 n_0 \pi^{1/2} l. \tag{12}$$

While it might be convenient to have introduced the idea of a mean-free path, we must keep in mind that this quantity cannot, at this point, be considered known since in reality it is a function of the actual solution we seek. Some workers choose to use a mean-free path based on viscosity for flow problems and a mean-free path based on thermal conductivity for heat-flow problems. In either case, the use of an appropriate mean-free path is especially important when working with model equations such as the CLF model we discuss later in this work.

2. Some solutions

In order to conserve mass, momentum and energy, the kernel $K(\boldsymbol{c}',\boldsymbol{c})$ used in Eq. (4) must be such that

$$\nu(c)\boldsymbol{S}(c,\mu,\chi) = \int_0^\infty\int_{-1}^1\int_0^{2\pi} \mathrm{e}^{-c'^2}\boldsymbol{S}(c',\mu',\chi')K(\boldsymbol{c}',\boldsymbol{c})c'^2\,\mathrm{d}\chi'\,\mathrm{d}\mu'\,\mathrm{d}c', \tag{13}$$

where

$$\boldsymbol{S}(c,\mu,\chi) = \begin{bmatrix} 1 \\ c\mu \\ c(1-\mu^2)^{1/2}\cos\chi \\ c(1-\mu^2)^{1/2}\sin\chi \\ c^2 \end{bmatrix}. \tag{14}$$

Taking note of Eq. (5), we find that Eq. (13) yields only the three conditions

$$\nu(c) = \int_0^\infty e^{-c'^2} k_0(c', c) c'^2 \, dc', \tag{15a}$$

$$\nu(c)c = \int_0^\infty e^{-c'^2} k_1(c', c) c'^3 \, dc' \tag{15b}$$

and

$$\nu(c)c^2 = \int_0^\infty e^{-c'^2} k_0(c', c) c'^4 \, dc'. \tag{15c}$$

Using Eqs. (8a) and (8b), we can confirm Eqs. (15b) and (15c) once we have used Eqs. (8a) and (15a) to find the collision frequency:

$$\nu(c) = \frac{2c^2 + 1}{c} \int_0^c e^{-x^2} \, dx + e^{-c^2}. \tag{16}$$

There are examples [17] in linear transport theory which suggest that, when there is a "discrete" solution that is independent of the spatial variable, we are able to find a second solution that is linear in the spatial variable. While there are not five solutions of Eq. (11) that are linear in the spatial variable, Cercignani [18] has reported three such solutions. The components of $\boldsymbol{S}(c, \mu, \chi)$ as listed in Eq. (14) are normally [1,2] referred to as the collisional invariants. To be clear, we let

$$h_1(\tau, \boldsymbol{c}) = 1, \tag{17a}$$

$$h_2(\tau, \boldsymbol{c}) = c\mu, \tag{17b}$$

$$h_3(\tau, \boldsymbol{c}) = c(1 - \mu^2)^{1/2} \cos \chi, \tag{17c}$$

$$h_4(\tau, \boldsymbol{c}) = c(1 - \mu^2)^{1/2} \sin \chi \tag{17d}$$

and

$$h_5(\tau, \boldsymbol{c}) = c^2 - 5/2 \tag{17e}$$

denote the exact solutions of Eq. (11) that are independent of the spatial variable. Note that instead of using c^2 as the fifth solution, we have elected to use a convenient linear combination of the first and fifth components of $\boldsymbol{S}(c, \mu, \chi)$ to define $h_5(\tau, \boldsymbol{c})$. To list the solutions of Eq. (11) that are linear in the spatial variable we first introduce the notation we use to discuss a class of integral equations that is basic to this work, viz.

$$\mathscr{L}_n\{f\}(c) = r(c), \quad c \in [0, \infty), \tag{18}$$

with $r(c)$ considered given, and with

$$\mathscr{L}_n\{f\}(c) = \nu(c)f(c) - \int_0^\infty e^{-x^2} f(x) k_n(x, c) x^2 \, dx. \tag{19}$$

While it is clear that Eq. (5) defines the scattering kernel for the LBE, we note that the components $k_n(c'c)$ of this scattering kernel, as used in Eq. (5), are the functions required in the integral equations defined in Eq. (18). We see also that, in contrast to the integration over velocity space that is required in the Boltzmann equation, we have in Eq. (18) a one-dimensional integral. Finally, we observe that Eq. (18) is not in the form of a classical Fredholm equation (because of the improper integral), but with some changes of variables the equation can clearly be redefined on a finite interval even though this process can introduce singularities into the kernel function [19].

Looking now to Refs. [14,16], we see that the Chapman–Enskog integral equations relevant to viscosity and heat conduction can be written, in our notation, respectively, as

$$\mathscr{L}_2\{c^2 b\}(c) = c^2 \tag{20}$$

and

$$\mathscr{L}_1\{ca\}(c) = c(c^2 - 5/2) \tag{21}$$

for $c \in [0, \infty)$. We note that the functions $a(c)$ and $b(c)$ are the same as the functions $a(p)$ and $b(p)$ used by Pekeris and Alterman [14]. We see also that we can rewrite our Eqs. (15) as

$$\mathscr{L}_0\{1\}(c) = 0, \tag{22a}$$

$$\mathscr{L}_1\{c\}(c) = 0 \tag{22b}$$

and

$$\mathscr{L}_0\{c^2\}(c) = 0 \tag{22c}$$

for $c \in [0, \infty)$. Noting Eqs. (21) and (22b), we conclude that an arbitrary constant can be added to any function $a(c)$ that satisfies Eq. (21), and so this function is generally normalized by imposing the condition [3]

$$\int_0^\infty \mathrm{e}^{-c^2} a(c) c^4 \, \mathrm{d}c = 0. \tag{23}$$

Making use of the manifestations of the Fredholm alternative [19] and the fact that Eqs. (22) show that there are solutions of homogeneous versions of the integral equations

$$\mathscr{L}_n\{f\}(c) = r(c), \quad c \in [0, \infty), \tag{24}$$

for the cases of $n = 0$ and 1, we can list solvability conditions for these two cases, viz.

$$\int_0^\infty \mathrm{e}^{-c^2} \begin{bmatrix} 1 \\ c^2 \end{bmatrix} r(c) c^2 \, \mathrm{d}c = \mathbf{0}, \quad n = 0 \tag{25a}$$

and

$$\int_0^\infty \mathrm{e}^{-c^2} r(c) c^3 \, \mathrm{d}c = 0, \quad n = 1. \tag{25b}$$

It can be seen from the forms of the kernels required in Eqs. (20) and (21) that these integral equations can provide a challenge to workers seeking numerical results for the functions $a(c)$ and $b(c)$, and so Pekeris and Alterman [14] reduced these two integral equations to ordinary 4th-order differential equations from which they obtained numerical results for the required functions $a(c)$ and $b(c)$. More recently, additional numerical results (based directly on the integral equations) for these important functions have been reported [16,20,21].

Having defined, by way of Eqs. (20), (21) and (23), the Chapman–Enskog functions $a(c)$ and $b(c)$, we have found three solutions of Eq. (11) that are linear in τ. We report these solutions as

$$h_3^*(\tau, \boldsymbol{c}) = c(1-\mu^2)^{1/2}\cos\chi[\varepsilon\tau - \mu c b(c)], \tag{26a}$$

$$h_4^*(\tau, \boldsymbol{c}) = c(1-\mu^2)^{1/2}\sin\chi[\varepsilon\tau - \mu c b(c)] \tag{26b}$$

and

$$h_5^*(\tau, \boldsymbol{c}) = (c^2 - 5/2)\varepsilon\tau - \mu c a(c). \tag{26c}$$

While Cercignani [18] has expressed his three solutions that are linear in the spatial variable in a different and less explicit way, those three solutions are linear combinations of our Eqs. (26). Having listed in Eqs. (17) and (26) eight linearly independent solutions of Eq. (11), we proceed now to use these eight solutions to define a synthetic kernel $F(\boldsymbol{c}', \boldsymbol{c})$ we can use to approximate the exact kernel $K(\boldsymbol{c}', \boldsymbol{c})$ that is listed as Eq. (5).

3. A synthetic kernel

Even if we truncate the expansion of the scattering kernel given as Eq. (5) after only a few terms, the problem of solving the resulting approximation of the LBE is still difficult from a numerical point of view. The numerical difficulty comes about basically because the components $k_n(c', c)$ required in Eq. (5) have derivatives (even for small values of n) that are discontinuous at $c' = c$. It is for this reason, keeping in mind that we intend to implement our work numerically, that we seek to approximate the true kernel by physically meaningful approximations that can be more easily incorporated into a numerical algorithm. In this regard, we note that the variable collision (CLF) model of Cercignani [11] and Loyalka and Ferziger [22] has been used in two recent works [8,9] in order to try to improve basic results available from the classical BGK model [10]. We now extend the variant of the variable collision frequency model used in Refs. [8,9] by replacing the exact components $k_n(c', c)$ of a truncated form of the scattering kernel $K(\boldsymbol{c}', \boldsymbol{c})$ with a more general synthetic approximation. And so to begin, we truncate Eq. (5) and write the synthetic scattering kernel as

$$F(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi}\sum_{n=0}^{N}\sum_{m=0}^{n}(2n+1)(2-\delta_{0,m})P_n^m(\mu')P_n^m(\mu)f_n(c', c)\cos m(\chi' - \chi), \tag{27}$$

where, instead of using $k_n(c', c)$ as in Eq. (5), we intend to use synthetic approximations $f_n(c', c)$ which we express, initially for $N = 2$, as

$$f_0(c', c) = A_0(c')A_0(c) + B_0(c')B_0(c), \tag{28a}$$

$$f_1(c', c) = A_1(c')A_1(c) + B_1(c')B_1(c) \tag{28b}$$

and

$$f_2(c', c) = A_2(c')A_2(c), \tag{28c}$$

where the functions $\{A_n(x), B_n(x)\}$ are to be determined. Continuing, we now write our approximated balance equation as

$$c\mu\frac{\partial}{\partial\tau}h(\tau, \boldsymbol{c}) = \varepsilon L^*\{h\}(\tau, \boldsymbol{c}), \tag{29}$$

where

$$L^*\{h\}(\tau, \boldsymbol{c}) = -\nu(c)h(\tau, \boldsymbol{c}) + \int_0^\infty \int_{-1}^1 \int_0^{2\pi} \mathrm{e}^{-c'^2} h(\tau, \boldsymbol{c}')F(\boldsymbol{c}', \boldsymbol{c})c'^2 \,\mathrm{d}\chi' \,\mathrm{d}\mu' \,\mathrm{d}c'. \tag{30}$$

Here $F(\boldsymbol{c}', \boldsymbol{c})$ is given by Eq. (27) with $N = 2$.

At this point we define the conditions we wish to use to define the components $f_n(c', c)$, $n=0,1,2$, of the $F(\boldsymbol{c}', \boldsymbol{c})$. We simply insist that the five exact solutions listed as Eqs. (17) and the three exact solutions listed as Eqs. (26) be also solutions to Eq. (29). And so upon substituting Eqs. (17) into Eq. (29) we find three conditions:

$$\int_0^\infty \mathrm{e}^{-c'^2} f_0(c', c)c'^2 \,\mathrm{d}c' = \nu(c), \tag{31a}$$

$$\int_0^\infty \mathrm{e}^{-c'^2} f_0(c', c)c'^4 \,\mathrm{d}c' = \nu(c)c^2 \tag{31b}$$

and

$$\int_0^\infty \mathrm{e}^{-c'^2} f_1(c', c)c'^3 \,\mathrm{d}c' = \nu(c)c. \tag{31c}$$

Now substituting the three solutions listed as Eqs. (26) into Eq. (29), we find two additional conditions, viz.

$$\int_0^\infty \mathrm{e}^{-c'^2} a(c')f_1(c', c)c'^3 \,\mathrm{d}c' = \nu(c)ca(c) - c(c^2 - 5/2) \tag{31d}$$

and

$$\int_0^\infty \mathrm{e}^{-c'^2} b(c')f_2(c', c)c'^4 \,\mathrm{d}c' = \nu(c)c^2 b(c) - c^2. \tag{31e}$$

To reiterate, we consider here that the only unknowns in Eqs. (31) are the components $f_n(c', c)$, $n = 0, 1, 2$, that we seek to define our approximate scattering kernel $F(\boldsymbol{c}', \boldsymbol{c})$ for $N = 2$. We can substitute the forms given by Eqs. (28) into Eqs. (31) to find the required approximating components. For $f_0(c, c)$ we find

$$f_0(c', c) = \nu(c')\nu(c)[\varpi_{01} + \varpi_{02}(c'^2 - \omega)(c^2 - \omega)], \tag{32}$$

where

$$\varpi_{01} = \frac{1}{\nu_2}, \tag{33a}$$

$$\varpi_{02} = \frac{\nu_2}{\nu_2\nu_6 - \nu_4^2} \tag{33b}$$

and

$$\omega = \frac{\nu_4}{\nu_2} \tag{33c}$$

with

$$\nu_n = \int_0^\infty \mathrm{e}^{-c^2} \nu(c)c^n \,\mathrm{d}c. \tag{34}$$

For $f_1(c,c)$ we find

$$f_1(c',c) = \varpi_{11} c' \nu(c') c \nu(c) + \varpi_{12} \Delta_1(c') \Delta_1(c), \tag{35}$$

where

$$\Delta_1(c) = \nu(c)[a_* c - c a(c)] + c(c^2 - 5/2). \tag{36}$$

In addition,

$$\varpi_{11} = \frac{1}{\nu_4}, \tag{37a}$$

$$\varpi_{12} = [a_1 - a_2 - a_* a_3]^{-1} \tag{37b}$$

and

$$a_* = a_3/\nu_4 \tag{37c}$$

where

$$a_1 = \int_0^\infty e^{-c^2} \nu(c) a^2(c) c^4 \, dc, \tag{38a}$$

$$a_2 = \int_0^\infty e^{-c^2} a(c) c^6 \, dc \tag{38b}$$

and

$$a_3 = \int_0^\infty e^{-c^2} \nu(c) a(c) c^4 \, dc. \tag{38c}$$

Finally, for $f_2(c,c)$ we find

$$f_2(c',c) = \varpi_2 [c'^2 - \nu(c') c'^2 b(c')][c^2 - \nu(c) c^2 b(c)], \tag{39}$$

where

$$\varpi_2 = \frac{1}{\nu_*} \tag{40}$$

with

$$\nu_* = \int_0^\infty e^{-c^2} b(c)[\nu(c) c^2 b(c) - c^2] c^4 \, dc. \tag{41}$$

At this point our model of the LBE is completely defined, viz.

$$c\mu \frac{\partial}{\partial \tau} h(\tau, \boldsymbol{c}) = \varepsilon L^*\{h\}(\tau, \boldsymbol{c}), \tag{42}$$

where

$$L^*\{h\}(\tau, \boldsymbol{c}) = -\nu(c) h(\tau, \boldsymbol{c}) + \int_0^\infty \int_{-1}^1 \int_0^{2\pi} e^{-c'^2} h(\tau, \boldsymbol{c}') F(\boldsymbol{c}', \boldsymbol{c}) c'^2 \, d\chi' \, d\mu' \, dc'. \tag{43}$$

Here

$$F(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi} \nu(c') \nu(c) [\varpi_{01} + 3\varpi_{11} (\boldsymbol{c}' \cdot \boldsymbol{c}) + \varpi_{02} (c'^2 - \omega)(c^2 - \omega)] + M(\boldsymbol{c}', \boldsymbol{c}) + N(\boldsymbol{c}', \boldsymbol{c}), \tag{44}$$

where

$$M(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi} 3\varpi_{12}[(\boldsymbol{c}' \cdot \boldsymbol{c})/(c'c)]\Delta_1(c')\Delta_1(c) \tag{45a}$$

and

$$N(\boldsymbol{c}', \boldsymbol{c}) = \frac{5}{4\pi}\varpi_2 \Delta_2(c')\Delta_2(c) \sum_{m=0}^{2} (2 - \delta_{0,m}) P_2^m(\mu') P_2^m(\mu) \cos m(\chi' - \chi) \tag{45b}$$

with

$$\Delta_1(c) = \nu(c)[a_* c - ca(c)] + c(c^2 - 5/2), \tag{46a}$$

$$\Delta_2(c) = c^2 - \nu(c)c^2 b(c) \tag{46b}$$

and (in a consistent notation)

$$\boldsymbol{c}' \cdot \boldsymbol{c} = c'c \sum_{m=0}^{1} (2 - \delta_{0,m}) P_1^m(\mu') P_1^m(\mu) \cos m(\chi' - \chi). \tag{47}$$

We note that $M(\boldsymbol{c}', \boldsymbol{c})$ and $N(\boldsymbol{c}', \boldsymbol{c})$ in Eq. (44) are the terms resulting from the use of the Chapman–Enskog functions $a(c)$ and $b(c)$ and the conditions listed as Eqs. (31d) and (31e). To have a simple way to refer to this model that we considered to derive much of its character from the Chapman–Enskog integral equations relevant to viscosity and heat conduction and synthetic approximations, we refer to this model as the CES model. Although we have used here a different and more explicit procedure to derive this model, the resulting kernel satisfies some conditions suggested by Loyalka and Ferziger [12].

4. Mean-free paths

To have our final results in terms of the real spatial variable x (in cm), what we use for a mean-free path l is not important, if the molecular diameter σ_0 and the density n_0 are known. However, since these physical quantities may not be known some workers choose to work in terms of a specific mean-free path. We can mention two convenient choices. For the Poiseuille-flow problem, Loyalka and Hickey [16] use

$$l = l_p = (\mu_*/p_0)(2kT_0/m)^{1/2}, \tag{48}$$

where μ_* is the mean viscosity and $p_0 = n_0 kT_0$ is the pressure. And so since Pekeris and Alterman [14] give (for rigid-sphere collisions)

$$\mu_* = \frac{8(2mkT_0)^{1/2}}{15\pi\sigma_0^2} \int_0^\infty e^{-c^2} b(c) c^6 \, dc, \tag{49}$$

where $b(c)$ is defined by

$$\nu(c)c^2 b(c) - \int_0^\infty e^{-c'^2} b(c') k_2(c', c) c'^4 \, dc' = c^2, \tag{50}$$

we can use Eq. (12) to find, for this case,

$$\varepsilon = \varepsilon_p = \frac{16}{15}\pi^{-1/2}\int_0^\infty e^{-c^2} b(c)c^6\,dc. \tag{51}$$

For the temperature-jump problem, Loyalka and Ferziger [22] use

$$l = l_t = [4\lambda_*/(5n_0k)][m/(2kT_0)]^{1/2}, \tag{52}$$

where λ_* is the heat-conduction coefficient, which Pekeris and Alterman [14] express (for rigid-sphere collisions) as

$$\lambda_* = \frac{4k(2kT_0/m)^{1/2}}{3\pi\sigma_0^2}\int_0^\infty e^{-c^2} a(c)c^6\,dc, \tag{53}$$

where

$$\nu(c)ca(c) - \int_0^\infty e^{-c'^2} a(c')k_1(c',c)c'^3\,dc' = c(c^2 - 5/2) \tag{54a}$$

with

$$\int_0^\infty e^{-c^2} a(c)c^4\,dc = 0. \tag{54b}$$

In this way we find

$$\varepsilon = \varepsilon_t = \frac{16}{15}\pi^{-1/2}\int_0^\infty e^{-c^2} a(c)c^6\,dc. \tag{55}$$

In regard to numerical work, we note that Hermite cubic splines have been used [21] to solve the Chapman–Enskog integral equations for viscosity and heat conduction, our Eqs. (20), (21) and (23), and Eqs. (51) and (55) have been evaluated to yield

$$\varepsilon_p = 0.449027806\ldots \tag{56a}$$

and

$$\varepsilon_t = 0.679630049\ldots\ . \tag{56b}$$

Noting that the Prandtl number normally used in kinetic theory written as

$$Pr = \frac{5}{2}\frac{\mu_* k}{m\lambda_*} \tag{57}$$

can be expressed as

$$Pr = \varepsilon_p/\varepsilon_t \tag{58}$$

and so using Eqs. (56) in Eq. (58), we find the result

$$Pr = 0.660694457\ldots\ , \tag{59}$$

which we believe to be correct (for the LBE and rigid-sphere collisions) to all digits given.

5. The CLF model

If we wish to use the CES model worked out in detail in Section 3 of this paper, we must first solve the Chapman–Enskog integral equations for viscosity and heat conduction to obtain the functions $a(c)$ and $b(c)$. On the other hand, we can obtain a lower-order model just by approximating these two functions. If we go back to Eqs. (50) and (54a) and ignore the integral terms we obtain what we consider to be first estimates of $a(c)$ and $b(c)$. We label these estimates $a_0(c)$ and $b_0(c)$ and write

$$a_0(c) = \nu^{-1}(c)(c^2 - 5/2) + \hat{a} \tag{60a}$$

and

$$b_0(c) = \nu^{-1}(c), \tag{60b}$$

where we have included in Eq. (60a) a constant $\hat{a}$ since we know $a(c)$ is determined from Eq. (54a) only to within an additive constant. Now applying the normalization condition listed as Eq. (23) to $a_0(c)$, we find

$$\hat{a} = -(8/3)\pi^{-1/2} \int_0^\infty e^{-c^2} \nu^{-1}(c)(c^2 - 5/2)c^4 \, dc. \tag{61}$$

If we use $a_0(c)$ and $b_0(c)$, in place of the correct solutions $a(c)$ and $b(c)$, we find that Eq. (44) reduces to

$$F(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi} \nu(c')\nu(c)[\varpi_{01} + 3\varpi_{11}(\boldsymbol{c}' \cdot \boldsymbol{c}) + \varpi_{02}(c'^2 - \omega)(c^2 - \omega)] \tag{62}$$

and so using Eq. (62) with Eqs. (42) and (43) and considering that the collision frequency is arbitrary, not fixed by Eq. (16), we then have what we [8,9] refer to as the CLF model (variable collision frequency model) or the generalized BGK model [3].

Returning now to the issue of mean-free paths, or alternatively corresponding choices for the ε defined by Eq. (12), we note that within the context of the CLF model, we can use Eqs. (60) and (61) in Eqs. (51) and (55) to find the approximate results

$$\varepsilon_{p,0} = \frac{16}{15}\pi^{-1/2} \int_0^\infty e^{-c^2} \nu^{-1}(c)c^6 \, dc \tag{63}$$

and

$$\varepsilon_{t,0} = \frac{16}{15}\pi^{-1/2} \int_0^\infty e^{-c^2} \nu^{-1}(c)(c^2 - 5/2)^2 c^4 \, dc. \tag{64}$$

Eqs. (63) and (64), yield, respectively, for the BGK case [$\nu(c) = 1$], the Williams case [$\nu(c) = c$] and the rigid-sphere case [$\nu(c)$ as given by Eq. (16)], the following:

$$\varepsilon_{p,0} = 1, \tag{65a}$$

$$\varepsilon_{p,0} = 0.601802222\ldots \tag{65b}$$

and

$$\varepsilon_{p,0} = 0.278804053\ldots \tag{65c}$$

along with

$$\varepsilon_{t,0} = 1, \tag{66a}$$

$$\varepsilon_{t,0} = 0.677027500\ldots \tag{66b}$$

and

$$\varepsilon_{t,0} = 0.275334588\ldots\ . \tag{66c}$$

We can see that using, for the three variants of the CLF model mentioned above, the approximate values $\varepsilon_{p,0}$ and $\varepsilon_{t,0}$ in Eq. (58) yields poor results for the Prandtl number.

6. An additional model equation

In defining what we have called the CES model of the linearized Boltzmann equation, we established five conditions on the synthetic kernel $F(\boldsymbol{c}', \boldsymbol{c})$ by insisting that the known solutions of the homogeneous LBE listed as Eqs. (17) and (26) be also solutions of the model equation. As we have no more known solutions we require other conditions if we wish to have a more general model equation. Since the classical problems of Poiseuille flow and thermal-creep flow in a plane channel are normally defined in terms of an inhomogeneous version of the LBE, we intend to define our new model equation by insisting that the particular solution required for the LBE be also a particular solution of the inhomogeneous model equation. We therefore add driving terms to Eq. (11) and consider flow in a plane-parallel channel, $\tau \in [-a, a]$, to be defined by

$$c(1-\mu^2)^{1/2}\cos\chi[k_1 + k_2(c^2 - 5/2)] + c\mu\frac{\partial}{\partial\tau}h(\tau, \boldsymbol{c}) = \varepsilon L\{h\}(\tau, \boldsymbol{c}). \tag{67}$$

Here we have the Cartesian components of velocity defined as

$$c_x = c\mu, \tag{68a}$$

$$c_y = c(1-\mu^2)^{1/2}\sin\chi \tag{68b}$$

and

$$c_z = c(1-\mu^2)^{1/2}\cos\chi \tag{68c}$$

and so the driving terms in Eq. (67) correspond to flow in the z direction due to a pressure gradient (Poiseuille flow: $k_1 = 1$ and $k_2 = 0$) and due to a temperature gradient (thermal-creep flow: $k_1 = 0$ and $k_2 = 1$). For this class of flow problems, we consider that the information we seek can be expressed in terms of the velocity profile

$$u(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} \mathrm{e}^{-c^2}h(\tau, \boldsymbol{c})(1-\mu^2)^{1/2}c^3\cos\chi\,\mathrm{d}\chi\,\mathrm{d}\mu\,\mathrm{d}c \tag{69}$$

and the heat-flow profile

$$q(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} \mathrm{e}^{-c^2}h(\tau, \boldsymbol{c})(1-\mu^2)^{1/2}(c^2-5/2)c^3\cos\chi\,\mathrm{d}\chi\,\mathrm{d}\mu\,\mathrm{d}c, \tag{70}$$

which we can write as

$$u(\tau) = \frac{1}{\pi^{1/2}} \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} g(\tau, c, \mu)(1-\mu^2)^{1/2} c^3 \, \mathrm{d}\mu \, \mathrm{d}c \tag{71}$$

and

$$q(\tau) = \frac{1}{\pi^{1/2}} \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} g(\tau, c, \mu)(1-\mu^2)^{1/2} (c^2 - 5/2) c^3 \, \mathrm{d}\mu \, \mathrm{d}c, \tag{72}$$

where we have defined

$$g(\tau, c, \mu) = \frac{1}{\pi} \int_0^{2\pi} h(\tau, \boldsymbol{c}) \cos \chi \, \mathrm{d}\chi. \tag{73}$$

Since the velocity and heat-flow profiles have been expressed in terms of an azimuthal moment of $h(\tau, \boldsymbol{c})$, we multiply Eq. (67) by $\cos \chi$, integrate over χ and let

$$g(\tau, c, \mu) = (1-\mu^2)^{1/2} \psi(\tau, c, \mu) \tag{74}$$

to find

$$c[k_1 + k_2(c^2 - 5/2)] + c\mu \frac{\partial}{\partial \tau} \psi(\tau, c, \mu) = \varepsilon L_1\{\psi\}(\tau, c, \mu), \tag{75}$$

where

$$L_1\{\psi\}(\tau, c, \mu) = -\nu(c)\psi(\tau, c, \mu) + \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c'^2} \psi(\tau, c'\mu') k(c', \mu' : c, \mu) c'^2 \, \mathrm{d}\mu' \, \mathrm{d}c' \tag{76}$$

with

$$k(c', \mu' : c, \mu) = (1-\mu'^2) \sum_{n=1}^\infty \Pi_n(\mu') \Pi_n(\mu) k_n(c', c). \tag{77}$$

Here the component functions $k_n(c', c)$ are the same as used in Eq. (5) and the polynomials

$$\Pi_n(\mu) = \left[\frac{2n+1}{2n(n+1)} \right]^{1/2} \frac{\mathrm{d}}{\mathrm{d}\mu} P_n(\mu), \quad n \geqslant 1, \tag{78}$$

are such that

$$\int_{-1}^1 (1-\mu^2) \Pi_n(\mu) \Pi_{n'}(\mu) \, \mathrm{d}\mu = \delta_{n,n'}. \tag{79}$$

Since Eq. (75) has an inhomogeneous driving term, we now wish to define particular solutions corresponding to the two special cases $k_1 = 1, k_2 = 0$ and $k_1 = 0, k_2 = 1$ that are appropriate, respectively, to Poiseuille flow and thermal-creep flow. We consider first the case of thermal creep, and proposing a particular solution that depends only on c, we find

$$\psi_{ps}(\tau, c, \mu) = -ca(c)/\varepsilon, \ \ k_1 = 0, \quad k_2 = 1, \tag{80}$$

where (still) $a(c)$ is defined by the Chapman–Enskog equation for heat conduction. Turning to the case of Poiseuille flow, we note that the driving term is itself a solution of the homogeneous equation, and so we can anticipate that some effort will be required to define a particular solution. We follow Simons [23], Williams [3] and Loyalka and Hickey [16] and propose, in our notation,

$$\psi_{ps}(\tau,c,\mu)=[A(c)\tau^2+D(c)]\Pi_1(\mu)+B(c)\tau\Pi_2(\mu)+E(c)\Pi_3(\mu) \tag{81}$$

which we substitute into Eq. (75), with $k_1=1, k_2=0$, to find

$$\psi_{ps}(\tau,c,\mu)=\{c(\varepsilon\tau)^2-2c^2b(c)\varepsilon\tau\mu+c^3d(c)/5+c^3e(c)(5\mu^2-1)/5\}/(\varepsilon\varepsilon_p). \tag{82}$$

Here (still) $b(c)$ is defined by the Chapman–Enskog equation for viscosity, $d(c)$ must satisfy

$$\mathscr{L}_1\{c^3d\}(c)=2c^3b(c)-5c\varepsilon_p \tag{83}$$

and $e(c)$ must be a solution of

$$\mathscr{L}_3\{c^3e\}(c)=2c^3b(c). \tag{84}$$

Here we continue to make use of the notation introduced in Eq. (19).

We note that because of the definition of ε_p, as given by Eq. (51), we are assured that the right-hand side of Eq. (83) satisfies the solvability condition listed as Eq. (25b). Finally, since a constant multiple of c can, because of Eq. (22b), always be added to $c^3d(c)$, we can use the normalization

$$\int_0^\infty \mathrm{e}^{-c^2}d(c)c^6\,\mathrm{d}c=0 \tag{85}$$

so that (for Poiseuille flow) the contribution to the velocity profile from the particular solution will come only from the first term in Eq. (82). We note that Loyalka and Hickey [16] refer to the functions we have called $d(c)$ and $e(c)$ as Burnett solutions. To distinguish between these two important functions, which have been discussed by Simons [23] and which were also evaluated numerically in Refs. [20,21], we refer to them as the first and second Burnett functions. Considering that the two Burnett functions are known, we find that we can extend our synthetic kernel to the case of $N=3$ by adding to the conditions listed as Eqs. (31) two new conditions, viz.

$$\int_0^\infty \mathrm{e}^{-c'^2}d(c')f_1(c',c)c'^5\,\mathrm{d}c'=\nu(c)c^3d(c)-2c^3b(c)+5c\varepsilon_p \tag{86a}$$

and

$$\int_0^\infty \mathrm{e}^{-c'^2}e(c')f_3(c',c)c'^5\,\mathrm{d}c'=\nu(c)c^3e(c)-2c^3b(c). \tag{86b}$$

It follows that we can now write

$$f_0(c',c)=A_0(c')A_0(c)+B_0(c')B_0(c), \tag{87a}$$

$$f_1(c',c)=A_1(c')A_1(c)+B_1(c')B_1(c)+C_1(c')C_1(c), \tag{87b}$$

$$f_2(c',c)=A_2(c')A_2(c) \tag{87c}$$

and

$$f_3(c',c)=A_3(c')A_3(c). \tag{87d}$$

Eqs. (31) and (86) are used to determine $f_n(c',c)$, $n=0,1,2,3$, so as to define our new synthetic kernel. Because we have now included the first and second Burnett functions, as well as the

Chapman–Enskog functions for viscosity and heat conduction, we refer to this new model based on a synthetic kernel as the CEBS model. This model, we recall, will have the eight exact solutions listed as Eqs. (17) and (26) as solutions of the homogeneous model equation, and it will also have the exact particular solutions for thermal creep and Poiseuille flow as particular solutions of the corresponding inhomogeneous model equation. Finally, since our CEBS model has one more term ($N=3$ rather than $N=2$) in the synthetic scattering kernel, we have hopes that the model will prove to be a good addition to the class of model equations already available for approximating the LBE.

7. Concluding remarks

In this work we have made consistent use of the idea of approximating the exact scattering kernel relevant to the linearized Boltzmann equation (LBE) for rigid-sphere interactions with a synthetic kernel that maintains some basic properties of the exact kernel. More specifically we insist that a model equation defined by an approximating synthetic kernel accept as solutions certain known solutions of the homogeneous LBE or the inhomogeneous LBE relevant to forced flow in a plane channel. By developing what we hope will prove to be improved model equations (what we call the CES model and the CEBS model) that are amenable to analytical and simple numerical methods of solution, we anticipate that numerical results for engineering applications will be made available without the need of extensive computation methods required when the LBE must be solved numerically. In addition to the two mentioned model equations, the variable collision frequency model (CLF model) or generalized BGK model is obtained as a special case, and expressions from approximations to the solutions of the Chapman–Enskog integral equations for viscosity and heat conduction are used to define mean-free paths that are consistent with the CLF model equation.

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