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Couette flow of a binary gas mixture

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The linearized binary model described by Hamel [Phys. Fluids 8, 418 (1964)] is used to obtain a set of kinetic equations and boundary conditions for the Couette flow problem. The derived set of two coupled integrodifferential equations is solved by iteration implementing standard discretization techniques. Highly accurate numerical results are presented for the mass velocity distribution and the total shear stress of the binary gas system.

I. INTRODUCTION

The flow of a gas mixture close to a plane or a cylindrical boundary is of basic interest in the field of rarefied gas dynamics. Complete solutions of such boundary value problems can give us the magnitude of the velocity slip or the temperature jump leading to appropriate boundary conditions for the hydrodynamic equations and in general provide insightful information on the behavior of gas mixtures. Over the past years a fairly complete treatment of the slip problems for a single component gas has been given.[1] The corresponding problems for gas mixtures have received less attention. The efforts in this direction are concentrated on the solution of the linearized Boltzmann equation and its model equations, including the ones proposed by Serovich,[2] Morse,[3] and Hamel.[4] As pointed out by Lang and Loyalka,[5] kinetic models for a gas mixture do not always include the detailed effects of intermolecular forces in a satisfying way. For that reason the solution should be based on the linearized Boltzmann equation itself. Following this principle accurate numerical results have been presented for various half-space kinetic theory problems.[5–7] In spite of this fact, there have recently appeared several analytical and numerical studies on the two-surface problem of evaporation and condensation for a vapor gas mixture[8,9] and on the Poiseuille flow problem for a binary gas mixture,[10] which are based on a modeled linearized Boltzmann equation. It should be noted that although all these results are valid only within the model approximations, they still provide considerable insight into the phenomena.

In this paper we develop a complete solution of the classical Couette flow problem for a two-gas mixture based on a linearized version of the kinetic model equations proposed by Hamel[4] in conjunction with diffuse boundary conditions. The resulting set of two coupled linear integrodifferential equations is solved numerically using standard discretization techniques and an iteration scheme that is unconditionally stable. The discretization of the velocity variable simply consists of evaluating the kinetic vector equation at discrete velocities. The discrete velocity method has been developed and used successfully in rarefied gas dynamics to study one- and two-dimensional monoatomic and diatomic gas flow problems.[11,12] The discretization in space is performed according to the ordinary diamond-difference scheme.[13]

The organization of this paper is as follows. In the next section the kinetic equations and the boundary conditions for the Couette flow problem are developed. In Sec. III the implemented numerical scheme is described and in Sec. IV extensive numerical results are presented. Finally Sec. V contains conclusions and a few general remarks.

II. KINETIC EQUATIONS AND BOUNDARY CONDITIONS

The linearized form of the model equation proposed by Hamel,[4] describing the stationary state of a binary gas mixture, gas A and gas B, can be written as[14]

$$\begin{aligned}\boldsymbol{\xi}_i\cdot\nabla h_i = {} & (n_i k_{il} + n_j k_{ij}) \\ & \times\left[-h_i + \rho_i + 2\mathbf{c}_i\cdot\mathbf{v}_i + t_i(c_i^2 - \tfrac{3}{2})\right] \\ & + n_j k_{ij}\,\mu_j\left[-2\mathbf{c}_i\cdot\mathbf{v}_i + 2\mathbf{c}_i\cdot\mathbf{v}_j(m_i/m_j)^{1/2}\right. \\ & \left. + 2\mu_i(t_j - t_i)(c_i^2 - \tfrac{3}{2})\right], \end{aligned} \tag{1}$$

where $i = \mathrm{A,B}$, $j = \mathrm{A,B}$, $i \neq j$, k_{il} and k_{ij} represent collisional parameters, m_i is the molecular mass, k is the Boltzmann constant, and $\mu_i = m_i/(m_i + m_j)$. The vector $h_i(\mathbf{x},\boldsymbol{\xi}_i)$ is a measure of the perturbation of the distribution function $f_i(\mathbf{x},\boldsymbol{\xi}_i)$ from an absolute Maxwellian,

$$f_i(\mathbf{x},\boldsymbol{\xi}_i) = \Phi_{0_i}[1 + h_i(\mathbf{x},\boldsymbol{\xi}_i)], \tag{2}$$

for $|h_i| \ll 1$, where

$$\Phi_{0_i} = n_0(m_i/2\pi kT_0)^{3/2}\exp[-m_i(\boldsymbol{\xi}_i - \mathbf{V}_0)^2/2kT_0] \tag{3}$$

and n_0, $\mathbf{V}_0$, and T_0 are equilibrium values of density, velocity, and temperature, respectively. The perturbations ρ_i in density, $\mathbf{v}_i$ in velocity, and t_i in temperature are defined by

$$\rho_i = (n_i - n_0)/n_0, \tag{4a}$$

$$\mathbf{v}_i = (\mathbf{V}_i - \mathbf{V}_0)/(m_i/2kT_0)^{-1/2}, \tag{4b}$$

$$t_i = (T_i - T_0)/T_0, \tag{4c}$$

with

$$n_i = \int f_i\, d^3\boldsymbol{\xi}, \tag{5a}$$

$$V_i = \frac{1}{n_i}\int \boldsymbol{\xi}_i f_i\, d^3\boldsymbol{\xi}, \tag{5b}$$

and

$$T_i = \frac{1}{3kn_i}\int (\boldsymbol{\xi}_i - \mathbf{V}_i)^2 m_i f_i\, d^3\boldsymbol{\xi}, \tag{5c}$$

while the shifted variable $\mathbf{c}_i$ in Eq. (1) is expressed as

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$$\mathbf{c}_i = (\boldsymbol{\xi}_i - \mathbf{V}_0)(m_i/2kT_0)^{1/2}. \tag{6}$$

Restricting the study to the Couette flow problem we consider the flow of a binary gas mixture, enclosed between two parallel plates at $x = 0$ and $x = d$, caused by the steady motion of the upper and lower plate in the z direction, with velocity $U/2$ and $-U/2$, respectively. The temperature T is supposed to be constant for both the plates and the distribution function f_i depends only on x and $\boldsymbol{\xi}_i$. The particles are emitted from the walls with a Maxwellian having drift velocity $\pm U/2$. The basic hypothesis $U \ll 1$ allows the Boltzmann equation to be linearized,[15] according to Eq. (2), where Φ_{0_i} is the absolute equilibrium Maxwellian with $\mathbf{V}_0 = 0$ and $h(x,\boldsymbol{\xi}_i)$ is the unknown perturbation of the distribution function. By assuming purely diffuse reflection at the surfaces, the boundary conditions take the following form when linearized:

$$h_i(0,\boldsymbol{\xi}_i) = -(m_i/2kT_0)U\xi_{z_i}, \quad \xi_{x_i} > 0, \tag{7}$$

and

$$h_i(d,\boldsymbol{\xi}_i) = (m_i/2kT_0)U\xi_{z_i}, \quad \xi_{x_i} < 0. \tag{8}$$

Further let us write

$$h_i(x,\boldsymbol{\xi}_i) = (m_i/2kT_0)U\xi_{z_i}Y_i(x,\xi_{x_i}). \tag{9}$$

Substitute this *Ansatz* into Eq. (2) and introduce the resulting equation into Eqs. (5) to obtain, after some manipulation, the perturbed quantities

$$\rho_i = v_{x_i} = v_{y_i} = t_i = 0 \tag{10a}$$

and

$$v_{z_i} = \left(\frac{m_i}{2kT_0}\right)\frac{U}{2\sqrt{\pi}}\int_{-\infty}^{\infty} Y_i(x,\xi_{x_i}) \times \exp\left(-\frac{m_i}{2kT_0}\xi_{x_i}^2\right)d\xi_{x_i}. \tag{10b}$$

Substituting Eqs. (9) and (10) into Eq. (1), $Y_i(x,\mu)$ satisfies the following coupled integrodifferential equations:

$$\mu\frac{\partial Y_i}{\partial x} + \beta_1 Y_i(x,\mu) = \frac{\beta_i - \alpha_i}{\sqrt{\pi}}\int_{-\infty}^{\infty} Y_i(x,s)e^{-s^2}\,ds + \frac{\alpha_i}{\sqrt{\pi}}\int_{-\infty}^{\infty} Y_j(x,s)e^{-s^2}\,ds, \tag{11}$$

$i = \mathrm{A,B}$, $j = \mathrm{A,B}$, $i \neq j$, where

$$\beta_i = (m_i/2kT_0)^{1/2}(n_i k_{ii} + n_j k_{ij}) \tag{12a}$$

and

$$\alpha_i = (m_i/2kT_0)^{1/2} n_j k_{ij}\,\mu_j, \tag{12b}$$

with $\mu = \xi_{x_i}(m_i/2kT_0)^{1/2}$. Thus the Couette flow problem for a binary gas mixture has been reduced to the problem of solving Eq. (11) subject to the boundary conditions

$$Y_i(0,\mu) = -1, \quad \mu > 0, \tag{13a}$$

and

$$Y_i(d,\mu) = 1, \quad \mu < 0, \tag{13b}$$

with the new function $Y_i(x,\mu)$, $i = \mathrm{A,B}$, to be the basic unknown.

For each species the normalized macroscopic velocity may be expressed as

$$V_{z_i} = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} Y_i(x,s)e^{-s^2}\,ds \tag{14}$$

while the shear stress is defined by

$$\sigma_i(x) = m_i\iiint \xi_{x_i}(\xi_{z_i} - V_{z_i})f_i\,d^3\boldsymbol{\xi}_i. \tag{15}$$

It is easy to show that the ratio of this stress to its value in the free molecular limit, after linearization has taken place, can be expressed as

$$\tau_i(x) = -\int_{-\infty}^{\infty} Y_i(x,s)se^{-s^2}\,ds. \tag{16}$$

The physically significant quantities of the mixture are the hydrodynamic velocity

$$u(x) = [m_\mathrm{A}n_\mathrm{A}V_\mathrm{A}(x) + m_\mathrm{B}n_\mathrm{B}V_\mathrm{B}(x)]/[m_\mathrm{A}n_\mathrm{A} + m_\mathrm{B}n_\mathrm{B}], \tag{17}$$

and the normal total stress

$$\tau = -[m_\mathrm{A}^{1/2}n_\mathrm{A}\tau_\mathrm{A}(x) + m_\mathrm{B}^{1/2}n_\mathrm{B}\tau_\mathrm{B}(x)]/[m_\mathrm{A}^{1/2}n_\mathrm{A} + m_\mathrm{B}^{1/2}n_\mathrm{B}]. \tag{18}$$

To obtain numerical results for the normalized mass velocity and stress, we need to study the vector equation (11), which is a system of two linear integrodifferential equations for $Y_i(x,\mu)$ associated with the boundary conditions (13).

III. FORMULATION OF THE NUMERICAL SCHEME

Equation (11) may be solved by an iteration scheme described by the equations

$$\mu\frac{\partial Y_i^{l+1}}{\partial x} + \beta_i Y_i^{l+1}(x,\mu) = (\beta_i - \alpha_i)\Phi_i^l(x) + \alpha_i\Phi_j^l(x) \tag{19}$$

and

$$\Phi_i^{l+1}(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} Y_i^{l+1}(x,s)e^{-s^2}\,ds, \tag{20}$$

where l denotes the iteration index, with a starting guess $\Phi_i^0(x) = 0$. For an infinite medium the convergence rate of this iteration map is shown by the following Fourier analysis to be always less or equal to one. Let

$$\psi_i^{l+1}(x,\mu) = Y_i^{l+1}(x,\mu) - Y_i^l(x,\mu) \tag{21a}$$

and

$$\varphi_i^{l+1}(x) = \Phi_i^{l+1}(x) - \Phi_i^l(x) \tag{21b}$$

and subtract Eqs. (19) and (20) for successive values of l to find the following equations:

$$\mu\frac{\partial\psi_i^{l+1}}{\partial x} + \beta_i\psi_i^{l+1}(x,\mu) = (\beta_i - \alpha_i)\varphi_i^l(x) + \alpha_i\varphi_j^l(x) \tag{22a}$$

and

$$\varphi_i^{l+1}(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \psi_i^{l+1}(x,s)e^{-s^2}\,ds. \tag{22b}$$

Assuming for simplicity $\alpha_i = \alpha_j$ and $\beta_i = \beta_j$ and introducing the *Ansätze*

$$\psi_i^{l+1}(x,\mu) = g(\mu)e^{i\lambda x}, \tag{23a}$$

$$\varphi_i^{l}(x) = e^{i\lambda x}, \tag{23b}$$

and

$$\varphi_i^{l+1}(x) = \omega\varphi_i^{l}(x) \tag{23c}$$

into Eqs. (22a) and (22b), we obtain

$$\omega = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-s^2}}{1 + (\lambda s/\beta_i)^2}\, ds. \tag{24}$$

Here α is the eigenvalue corresponding to the Fourier frequency λ and the spectral radius (largest eigenvalue) $\rho = \sup_\lambda |\omega|$ represents the slowest possible reduction in the error from one iteration to the next. The maximum value of $|\omega|$, which occurs for $\lambda = 0$, is $\omega = 1$. However for a finite system, the flat $\lambda = 0$ mode, with the corresponding eigenfunction $g(\mu) = 1$, cannot be present and thus the method described by Eqs. (19) and (20) converges absolutely ($\rho < 1$).

To implement the proposed method on a digital computer, we treat the space and velocity variables through a number of discretization techniques. The discrete velocity approximation consists of requiring Eq. (19) to hold only for a number of discrete velocities μ_m and then applying a compatible quadrature approximation to the integral terms. The discrete velocity equations may be written as

$$\mu_m \frac{\partial Y_{i,m}^{l+1}}{\partial x} + \beta_i Y_{i,m}^{l+1}(x) = (\beta_i - \alpha_i)\Phi_i^l(x) + \alpha_i \Phi_j^l(x), \tag{25}$$

where $Y(x,\mu_m)$ is denoted by $Y_{i,m}(x)$. We choose the points $\{\mu_m\}$ to be the zeros of the Hermite polynomials of degree $2M$ and the Gauss–Hermite quadrature formulas

$$\Phi_i(x) = \frac{1}{\sqrt{\pi}} \sum_{m=1}^{2M} Y_{i,m}(x) w_m, \tag{26}$$

where the w_m are the weights associated with the μ integration, are taken to operate on an even number of velocities that are symmetric about $\mu = 0$.

To discretize the spatial variable we use the so-called diamond-difference scheme.[13] We define a spatial grid with K mesh points and the associated diamond-differenced discrete-velocity equations are

$$\begin{aligned}(\mu_m/h)(Y_{i,m,k+1}^{l+1} - Y_{i,m,k}^{l+1}) &+ (\beta_i/2)(Y_{i,m,k+1}^{l+1} + Y_{i,m,k}^{l+1}) \\ &= [(\beta_i - \alpha_i)/2](\Phi_{i,k+1}^{l} + \Phi_{i,k}^{l}) \\ &\quad + (\alpha_i/2)(\Phi_{j,k+1}^{l} + \Phi_{j,k}^{l})\end{aligned} \tag{27}$$

and

$$\Phi_{i,k} = \frac{1}{\sqrt{\pi}} \sum_{m=1}^{2M} Y_{i,m,k} w_m, \tag{28}$$

with $h = x_{k+1} - x_k$. The cases $\mu_m > 0$ and $\mu_m < 0$ are considered separately in order to construct marching schemes that follow the direction of the particle travel. To illustrate the sweep through the mesh, we first march upward and calculate successively $Y_{i,m,2}$, $Y_{i,m,3}$,..., $Y_{i,m,K}$ for $\mu_m > 0$, with $Y_{i,m,1}$ known from the boundary condition. Since $Y_{i,m,K}$ is known for $\mu_m < 0$ from the second boundary condition we then march from $x = d$ to $x = 0$. These sweeps through the mesh are executed for all discrete velocity pairs $(-\mu_m, \mu_m)$. The sweeping algorithm described above is very effective mainly because we obtain one iteration matrix that is lower triangular. We complete our discussion on the numerical scheme by introducing the quadrature approximations

$$V_{i,k} = \Phi_{i,k} \tag{29}$$

and

$$\tau_{i,k} = -\sum_{m=1}^{2M} Y_{i,m,k}\, \mu_m w_m \tag{30}$$

for the relative velocity and the normalized shear stress, respectively, in terms of the unknown function $Y_{i,m,k}$.

TABLE I. Normalized shear stress in the "single" gas Couette flow problem.

Distance between plates d	Present work $m_A/m_B = 1.0$ $n_A/n_B = 1.0$	Exact numerical results for a single gas[a]
0.1	0.929	0.926
1.0	0.602	0.601
2.0	0.444	0.444
3.0	0.354	0.354
4.0	0.294	0.294
5.0	0.252	0.252
7.0	0.196	0.196
10.0	0.147	0.147
20.0	0.0806	0.0804

[a] See Ref. 17.

IV. NUMERICAL RESULTS

The numerical evaluation of the problem, as it has been carried out, depends on the following parameters:

$$m_A/m_B,\ n_A/n_B,\ k_{AA}/k_{AB},\ k_{AA}/k_{BB},\ \hat{d}.$$

The first two parameters are the relative molecular mass and the relative number density of the A species with respect to

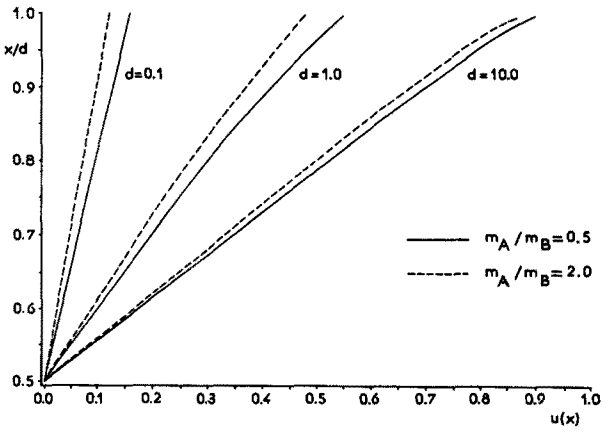

FIG. 1. Mean mass flow velocity profiles for $n_A/n_B = 1.0$.

the B species, k_{AA}, k_{BB}, k_{AB} ($k_{BA} = k_{AB}$)[4] are collisional parameters assumed to be constants and $\hat{d}$ is a number proportional to the Knudsen number, defined by $\hat{d} = \beta_A d$. All these coefficients have a qualitative effect on the physical quantities of interest of the Couette flow problem. However, for simplicity and clarity we restrict our results to the special case $k_{AA} = k_{AB} = k_{BB}$. By taking $\beta_A = 1$ the physical characteristics of the first gas are fixed and the new parameter $\hat{d}$ is now equal to the distance between the plates, measured in mean free paths. Thus the velocity and shear stress of the two component gas mixture depend only on d, m_A/m_B, and n_A/n_B. More numerical results may be obtained upon request.

In the case of a single gas we have the known result that the shear stress between the plates is constant.[16] In a similar fashion it has been shown that for a binary gas mixture in conjunction with the Couette flow problem, the shear stress of each component is a function of x while the total stress of the mixture remains constant.[6] This result is used successfully as a benchmark for testing the accuracy of the numerical results. All computations are based on a set of 64 discrete velocities and are converged to a pointwise relative criterion of 10^{-4} on the velocity. To judge the accuracy to expect from the numerical scheme in Table I, we compare our results for the single gas case, which is a limit situation of the present work to exact numerical results available in the literature.[17] The agreement is excellent and we believe that the numerical results obtained in the framework of the proposed method are accurate to at least two significant figures.

The velocities shown in Figs. 1 and 2 (the Couette flow problem is symmetrical about a point at $x = d/2$) for the inverse Knudsen number d, the relative molecular mass m_A/m_B, and the relative number density n_A/n_B taking the values in the sets {0.1, 1.0, 10.0}, {0.5, 2.0}, and {0.1, 10.0}, respectively, provide some information about the qualitative nature of the flow field. The plotted mean flow velocity of the mixture is associated with the velocities of the component gases according to Eq. (17). The velocity profiles shown in Fig. 1 indicate that the velocity slip at the boundaries becomes larger as the binary gas mixture becomes lighter. The distributions presented in Fig. 2 show that, keeping the molecular mass ratio constant, the magnitude of the velocity slip becomes larger as the concentration of the heavier component decreases. Overall it is evident that the molecular ratio is the dominant parameter affecting the shape of the velocity profiles that are also sensitive to the concentration ratio. Finally Table II contains results for the total shear stress equation (18) for a wide range of the Knudsen number ($\mathrm{Kn} = 1/d$) and for different sets of parameters.

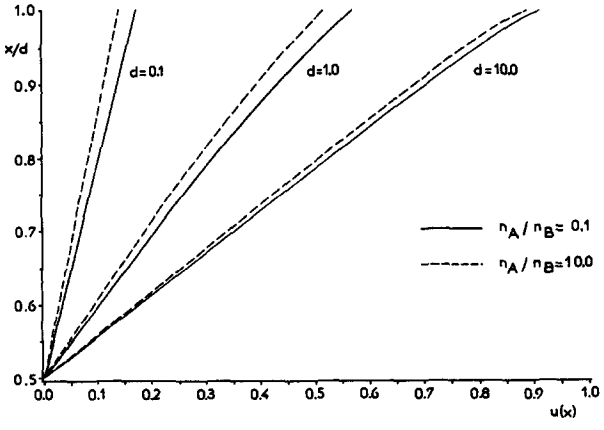

FIG. 2. Mean mass flow velocity profiles for $m_A/m_B = 0.5$.

TABLE II. Normalized total shear stress of the binary Couette flow problem.

Distance between plates d	m_A/m_B = 0.5, n_A/n_B = 0.1	m_A/m_B = 0.5, n_A/n_B = 10.0	m_A/m_B = 2.0, n_A/n_B = 0.1	m_A/m_B = 2.0, n_A/n_B = 10.0
0.1	0.905	0.927	0.948	0.931
0.5	0.679	0.732	0.789	0.744
1.0	0.529	0.529	0.666	0.607
2.0	0.372	0.435	0.514	0.449
3.0	0.288	0.345	0.421	0.359
4.0	0.235	0.287	0.358	0.299
5.0	0.199	0.245	0.311	0.257
7.0	0.152	0.191	0.247	0.200
10.0	0.112	0.143	0.189	0.151
20.0	0.060	0.078	0.106	0.082

V. CONCLUSIONS

We have derived the solution to a system of kinetic equations governing the fluid dynamic quantities of the Couette flow problem for a binary gas mixture. The numerical convergence of the method is excellent and the velocity profiles and the normalized shear stresses of the gas mixture have been computed very accurately with modest computational effort. To the author's knowledge these results have not been reported previously. The present analysis can be extended to investigate kinetic theory problems described by a set of four coupled equations such as parallel-plate heat transfer and evaporation in binary mixtures.

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[1]C. Cercignani, *Theory and Application of the Boltzmann Equation* (Elsevier, New York, 1975).
[2]L. Serovich, Phys. Fluids **5**, 908 (1962).
[3]T. F. Morse, Phys. Fluids **6**, 1420 (1963).
[4]B. B. Hamel, Phys. Fluids **8**, 418 (1964).
[5]H. Lang and S. K. Loyalka, Z. Naturforsch. Teil A **27**, 1307 (1972).
[6]S. K. Loyalka, Phys. Fluids **14**, 2599 (1971).
[7]S. K. Loyalka, Phys. Fluids **17**, 897 (1974).
[8]T. Soga, Phys. Fluids **25**, 1978 (1982).
[9]Y. Onishi, in *Rarefied Gas Dynamics*, edited by H. Ogushi (University of Tokyo Press, Tokyo, 1984), Vol. II, pp. 874–884.
[10]L. Carlomusto and L. M. deSocio, Z. Angew. Math. Phys. **29**, 206 (1978).
[11]D. P. Giddens, A. B. Huang, and V. Y. C. Young, Phys. Fluids **14**, 2645 (1970).
[12]A. B. Huang, P. F. Hwang, D. P. Giddens, and R. Srinivasan, Phys. Fluids **16**, 814 (1973).
[13]E. E. Lewis and W. F. Miller, Jr., *Computational Methods of Neutron Transport* (Wiley, New York, 1984).
[14]J. F. Cavalier and W. Greenberg, Phys. Fluids **27**, 1114 (1984).
[15]C. Cercignani, J. Math. Anal. Appl. **11**, 93 (1965).
[16]C. Cercignani, and C. D. Pagani, Phys. Fluids **9**, 1167 (1966).
[17]S. K. Loyalka, N. Petrellis, and T. S. Storvick, Z. Angew. Math. Phys. **30**, 514 (1979).