The McCormack model for gas mixtures: Plane Couette flow

R. D. M. Garcia
HSH Scientific Computing, Rua Carlos de Campos, 286, São José dos Campos, SP 12242-540, Brazil
C. E. Siewert
Mathematics Department, North Carolina State University, Raleigh, North Carolina 27695-8205

(Received 20 April 2004; accepted 3 November 2004; published online 4 February 2005)

An analytical version of the discrete-ordinates method is used to establish a concise and particularly accurate solution to the problem of plane Couette flow for a binary gas mixture described by the McCormack kinetic model. The solution yields, for the general (specular-diffuse) case of Maxwell boundary conditions for each of the two species, the velocity, heat-flow, and shear-stress profiles for both types of particles, as well as the particle-flow and heat-flow rates associated with each of the two species of gas particles. Highly accurate numerical results are reported for the case of a helium-argon mixture confined between molybdenum and tantalum plates. The algorithm is considered especially easy to use, and the developed (FORTRAN) code requires typically less than a second on a 2.2 GHz Pentium 4 machine to compute all quantities of interest with at least five figures of accuracy. © 2005 American Institute of Physics. [DOI: 10.1063/1.1845911]

I. INTRODUCTION

The flow of a rarefied gas between two infinite plates that are moving in parallel and opposite directions is a classical problem in rarefied gas dynamics known as plane Couette flow. Under the assumption that the plate velocities are small compared to the reference Maxwellian speed \((2kT_0/m)^{1/2}\), where \(k\) is the Boltzmann constant, \(T_0\) is the (unperturbed) gas temperature, and \(m\) is the mass of a gas particle, the problem can be adequately modeled by the linearized Boltzmann equation.

There are numerous works dedicated to the study of linearized plane Couette flow of a single gas. A list of all these works would be too lengthy to report here, and thus we refer the reader to the books of Cercignani,1–3 Williams,4 and Ferziger and Kaper,5 as well as the review papers by Sharirov and Selezniev6 and Williams,7 for general background material and a discussion of previous works on the single-gas case. In regard to gas mixtures, however, the literature on this problem is scarce. We have found only three works8–10 on linearized plane Couette flow for gas mixtures, two of which9,10 are related to the present work as they are also based on the discrete-ordinates method. The work in Ref. 9 relies on space discretization and iteration, while Ref. 10 uses the same analytical discrete-ordinates (ADO) method that we use here. These works8–10 have addressed the special case of purely diffuse boundary conditions and are based on the relatively limited Hamel model,11 and so here we develop a concise and accurate ADO solution for plane Couette flow of a binary gas mixture described by the physically more consistent McCormack model.12 In addition, we consider general (specular-diffuse) Maxwell boundary conditions with a free choice of the accommodation coefficient for each species at each confining plate.

II. FORMULATION

In this work we base our analysis of a binary gas mixture on the McCormack model as introduced in an important paper12 published in 1973. While we use this model as defined in Ref. 12, we employ a notation that is appropriate to the analysis and computations we report here. The ADO method13 has been used in two recent works14,15 to solve a collection of basic flow problems, defined for binary gas mixtures in terms of the McCormack model, for semi-infinite media14 (Kramers’ problem and the half-space problem of thermal creep) and plane channels15 (Poiseuille flow, thermal-creep flow, and flow driven by density gradients). Other recent works based on the McCormack model for binary gas mixtures report ADO solutions for the temperature-jump problem16 and the heat-transfer problem in a plane channel.17 Our solution of the Couette flow problem for a gas mixture described by the McCormack model follows directly from the general analysis reported in Refs. 14 and 15, and so our presentation here is brief.

We consider that the required functions \(h_a(x,v)\) for the two types of particles (\(a=1,2\)) denote perturbations from Maxwellian distributions for each species, i.e.,

\[
f_a(x,v) = f_{a,0}(v)[1 + h_a(x,v)],
\]

where

\[
f_{a,0}(v) = n_a(\lambda_a/\pi)^{3/2}e^{\lambda_a v^2}, \quad \lambda_a = m_a/(2kT_0). \tag{2}
\]

Here \(m_a\) and \(n_a\) denote, respectively, the particle mass and the equilibrium density of the \(a\)th species, \(x\) is the spatial variable (measured, for example, in centimeters), \(v\), with components \(v_x, v_y, v_z\), and magnitude \(v\), is the particle velocity, and \(T_0\) is the reference temperature. It follows from McCormack’s work12 that the perturbations satisfy the coupled equations, for \(a=1,2,\)
\[ c_\alpha \frac{\partial}{\partial \tau} h_\alpha(x, \tau) + \omega_\alpha \gamma_\alpha h_\alpha(x, \tau) = \omega_\alpha \gamma_\alpha L_\alpha[h_1, h_2](x, \tau), \]

(3)

where \( c, c_x, c_y, c_z \) and magnitude \( c \) is a dimensionless velocity variable, \( \omega_\alpha = \lambda_\alpha^{1/2} \) and \( \gamma_\alpha \) denotes the collision frequency for the \( \alpha \)th species. Here we write the integral operators as

\[ L_\alpha[h_1, h_2](x, \tau) = \frac{1}{\pi^{3/2}} \sum_{\beta=1}^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\tau^2} h_\beta(x, \tau') \times K_{\beta, \alpha}(c', c) dc' dc' dc', \]

(4)

where the kernels \( K_{\beta, \alpha}(c', c) \) are listed explicitly in Refs. 14 and 15. As shown in detail in these works, a dimensionless spatial variable \( \tau \) defined in terms of a viscosity-based mean-free path \( l_0 \) originally introduced by Sharipov and Kalempa, can be used to restate the problem in a more convenient way. Thus, following Refs. 14 and 15, we rewrite Eq. (3) as

\[ c_\alpha \frac{\partial}{\partial \tau} h_\alpha(\tau, c) + \sigma_\alpha h_\alpha(\tau, c) = \sigma_\alpha L_\alpha[h_1, h_2](\tau, c), \]

(5)

where \( \sigma_\alpha = \gamma_\alpha \omega_\alpha l_0 \) or, more explicitly,

\[ \sigma_\alpha = \gamma_\alpha (m_1/m_1 + n_2/\gamma_2) / (n_1 + n_2) \right] (m_\alpha/m)^{1/2}. \]

(6)

Here the mass average is defined as

\[ m = (n_1 m_1 + n_2 m_2) / (n_1 + n_2). \]

(7)

In this work, we consider the problem of plane Couette flow between plates that are located at \( \tau = -a \) and \( \tau = a \) and that are moving with specified velocities in the \( z \) direction, and so we seek solutions of Eq. (5) that are valid for all \( \tau \in (-a, a) \) and that satisfy the Maxwell boundary conditions

\[ h_\alpha(-a, c_x, c_y, c_z) - (1 - a) h_\alpha(-a, -c_x, c_y, c_z) - a \mathcal{I}_-h_\alpha(-a) = 2 a \gamma_\alpha \omega_\alpha u_0 c_z, \]

(8a)

and

\[ h_\alpha(a, -c_x, c_y, c_z) - (1 - b) h_\alpha(a, c_x, c_y, c_z) - b \mathcal{I}_+h_\alpha(a) = 2 b \gamma_\alpha \omega_\alpha u_0 c_z, \]

(8b)

for \( c_z > 0 \) and all \( c_x \) and \( c_y \). Note that \( h_\alpha(\tau, c) \) \( \Rightarrow h_\alpha(\tau, c_x, c_y, c_z) \) and that we use \( a_1 \) and \( a_2 \) to denote the two accommodation coefficients basic to the plate located at \( \tau = -a \) and \( b_1 \) and \( b_2 \) to denote the two accommodation coefficients for the plate located at \( \tau = a \). In addition, \( \gamma_\alpha = (m_\alpha/m)^{1/2} \), and we have used

\[ \mathcal{I}_\pm h_\alpha(\tau) = \frac{1}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\tau^2} h_\alpha(\tau, c_x, c_y, c_z) \times c_x dc_x dc_y dc_z \]

(9)

to denote the diffuse terms in Eqs. (8). In writing Eqs. (8) we have used \( \omega_\alpha (2 k T_0 / m)^{1/2} \) to express the wall velocities in dimensionless units. In other words, \( u_{\alpha,0} \) and \( u_{\alpha,2} \) are the velocities (in the \( z \) direction) given to the two confining plates.

If we sought to compute the complete distribution functions \( h_\alpha(\tau, c) \), then we would have to work explicitly with Eqs. (5) and (8); however, since we seek here only the velocity profiles, the heat-flow profiles and the shear-stress profiles,

\[ u_\alpha(\tau) = \frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\tau^2} h_\alpha(\tau, c) c_x dc_x dc_y dc_z, \]

(10)

\[ q_\alpha(\tau) = \frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\tau^2} h_\alpha(\tau, c) (c^2 - 5/2) c_x dc_x dc_y dc_z, \]

(11)

and

\[ p_\alpha(\tau) = \frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\tau^2} h_\alpha(\tau, c) c_z c_x dc_x dc_y dc_z, \]

(12)

we can work only with certain moments of Eqs. (5) and (8). Continuing to follow Refs. 14 and 15, we first multiply Eq. (5) by

\[ \phi_1(c_x, c_z) = (1/\pi) e^{-c_x^2/c_z^2} c_z, \]

(13)

and integrate the resulting equation over all \( c_x \) and all \( c_z \). We then repeat this procedure using

\[ \phi_2(c_x, c_z) = (1/\pi) e^{-c_x^2/c_z^2} (c_x^2 + c_z^2 - 2) c_z \]

(14)

and define, for \( \alpha = 1 \) and 2,

\[ g_{2\alpha-1}(\tau, c_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_1(c_x, c_z) h_\alpha(\tau, c) dc_x dc_z \]

(15a)

and

\[ g_{2\alpha}(\tau, c_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_2(c_x, c_z) h_\alpha(\tau, c) dc_x dc_z \]

(15b)

to find from these projections four coupled balance equations that we can write in matrix notation as

\[ \xi \frac{\partial}{\partial \tau} G(\tau, \xi) + \Sigma G(\tau, \xi) = \int_{-\infty}^{\infty} \psi(\xi') K(\xi, \xi') G(\tau, \xi') d\xi'. \]

(16)

Here the components of \( G(\tau, \xi) \) are \( g_{\alpha}(\tau, \xi) \), for \( \alpha = 1, 2, 3, \) and 4, and we now use \( \xi \) in place of \( c_z \). In addition, we define

\[ \Sigma = \text{diag}(\sigma_1, \sigma_1, \sigma_2, \sigma_2) \]

(17)

and

\[ \psi(\xi) = \pi^{-1/2} e^{-\xi^2}, \]

(18)

and we note that the elements of the kernel \( K(\xi', \xi) \) are given explicitly in Refs. 14 and 15. To deduce the boundary conditions relevant to Eq. (16), we project Eqs. (8) against \( \phi_1(c_x, c_z) \) and \( \phi_2(c_x, c_z) \) to find

\[ G(-a, \xi) - S_1 G(-a, -\xi) = u_{\alpha,0} \right] (a_1 r_1 0 a_2 z_2 0)^T \]

(19a)

and...
\[ \mathbf{G}(a, \xi) - \mathbf{S}_j \mathbf{G}(a, \xi) = u_w \gamma [b_1 r_1, 0, b_2 r_2, 0]^T \]  

(19b)

for \( \xi > 0 \). Here, \( T \) denotes the transpose operation.

\[ \mathbf{S}_1 = \text{diag}(1-a_1, 1-a_1, 1-a_2, 1-a_2) \]  

(20a)

and

\[ \mathbf{S}_2 = \text{diag}(1-b_1, 1-b_1, 1-b_2, 1-b_2). \]  

(20b)

To close this section we note that the McCormack model (for rigid-sphere interactions) requires only the ratio of the two particle masses \( m_1/m_2 \), the ratio of the number densities \( n_1/n_2 \), and the ratio of the particle diameters \( d_1/d_2 \). Once these parameters are specified we seek to find the profiles listed in Eqs. (10)–(12) for selected values of the half-distance between plates \( a \) measured in mean-free paths, the two plate velocities \( u_{w,1} \) and \( u_{w,2} \), and the four accommodation coefficients \( a_1, a_2, b_1, b_2 \). Using Eqs. (13)–(15), we find we can write these profiles as

\[ u_r(a) = \int_{-\infty}^{\infty} \psi(\xi)g_{2a-1}(\tau, \xi) d\xi, \]  

(21)

where \( s = (m_2/m_1)^{1/2} \). Finally, the constants \( A_1, B_1, \{A_j, B_j\} \)

**III. AN ANALYTICAL DISCRETE-ORDINATES SOLUTION**

A general ADO solution to Eq. (16) has been fully developed and documented in Ref. 14, and so we omit the details of the derivation in this presentation. To start, we split the integral in Eq. (16) into two half-range integrals—one over \((0, \infty)\) and the other over \((-\infty, 0)\)—and then we change \( \xi \) to \(-\xi\) in the latter. Doing this, we only have to deal with one half-range integration interval, \((0, \infty)\). Next, using a Gaussian quadrature set of order \( N \) with nodes \( \{\xi_i\} \) and weights \( \{w_i\} \) to approximate integrals over \((0, \infty)\), we can follow Ref. 14 and express our approximate solution for \( \mathbf{G}(\tau, \xi) \) at the discrete ordinates \( \pm \xi_i, i = 1, 2, \ldots, N \), as

\[ \mathbf{G}(\tau, \pm \xi_i) = A_1 \mathbf{G}_+ + B_1 \mathbf{G}_-(\tau, \pm \xi_i) \]

\[ + \sum_{j=2}^{4N} [A_j \Phi(\nu_j, \pm \xi_i) + B_j \Phi(\nu_j, \mp \xi_i)] e^{-(\alpha_j^+(\nu_j))}, \]  

(24)

where the separation constants \( \{\nu_j\} \) and the elementary solutions \( \{\Phi(\nu_j, \pm \xi_i)\} \) are determined \(^{14} \) from the solution of an eigensystem of order \( 4N \). Since one of the eigenvalues of that eigensystem approaches zero as \( N \) is increased, the corresponding elementary solutions are replaced with the exact solutions

\[ \mathbf{G}_+ = \begin{bmatrix} 1 \\ 0 \\ s \\ 0 \end{bmatrix} \]  

(25a)

and

\[ \mathbf{G}_-(\tau, \xi) = \begin{bmatrix} \sigma_1 \tau - \xi \\ 0 \\ s\sigma_1 (\tau - \xi/\sigma_2) \end{bmatrix}, \]  

(25b)
IV. NUMERICAL RESULTS

In order to demonstrate that our ADO solution for the problem of plane Couette flow yields highly accurate results with modest computational effort, we report detailed numerical results for a specific case based on the McCormack model for rigid-sphere interactions in a mixture of He and Ar and plates made of different materials (Mo for the plate located at \( \tau=-a \) and Ta for the plate located at \( \tau=a \)). Thus, the gas parameters are

\[
m_1 = 4.0026, \quad m_2 = 39.948, \quad d_2/d_1 = 1.665, \quad c_1 = 0.3,
\]

where \( c_n = n_n / n \), with \( n = n_1 + n_2 \), whereas the plate parameters are

\[
a_1 = 0.20, \quad a_2 = 0.67, \quad b_1 = 0.46, \quad b_2 = 0.78,
\]

\[
u_{n,1} = 1.0, \quad \nu_{n,2} = -1.0, \quad a = 1.5.
\]

We note that the accommodation coefficients used in our calculation are the accommodation coefficients for tangential momentum, which we consider a natural choice for this problem. Specifically, we are using here the results of measurements performed by Lord\(^{19}\) for He and Ar particles reflecting from Mo and Ta surfaces.

We report in Table I our converged numerical results for the velocity, heat-flow, and shear-stress profiles. We note that these results were generated with a quadrature scheme based on the transformation \( v(\xi) = e^{-\xi} \) to map \( \xi \in [0, \infty) \) onto \( v \in [0, 1] \) and a linear mapping of the Gauss–Legendre scheme onto the interval \([0, 1]\). In regard to numerical linear algebra, we have used the EISPACK package\(^{20}\) to solve the eigensystem that determines the separation constants and the elementary solutions, and LINPACK\(^{21}\) to solve the linear system for the 8N unknowns \( A_1, B_1, A_j, B_j \).

To establish some confidence in our results, we have observed numerical stability in all entries of Table I, as the order of the quadrature \( N \) was varied between 40 and 100, in increments of 20. Moreover, as a measure of the correctness of our computational implementation, we have verified that the tabulated shear-stress profiles satisfy the identity

\[
c_1 p_1(\tau) + c_2 p_2(\tau) = p,
\]

where the constant \( p \) is what we call total shear stress. We note that Eq. (32) can be formally deduced by taking zero-order moments [with \( \phi(\xi) \) as the weighting function] of the first and third rows of Eq. (16), combining the resulting equations and integrating over space.

In addition to the velocity, heat-flow, and shear-stress profiles, we have computed in this work the particle-flow and heat-flow rates per unit area, defined for each species \( (\alpha=1, 2) \) as

\[
U_{\alpha} = \frac{1}{2a} \int_{-a}^{a} u_{\alpha}(\tau) d\tau
\]

and

\[
Q_{\alpha} = \frac{1}{2a} \int_{-a}^{a} q_{\alpha}(\tau) d\tau.
\]

Thus, we have used the discrete-ordinates approximations

\[
U = A_1 \left[ \frac{1}{s} + \frac{1}{2a} \sum_{j=2}^{4N} \nu_j X(\nu_j)(A_j + B_j)[1 - e^{-2a\nu_j}] \right]
\]

and

\[
Q = \frac{1}{2a} \sum_{j=2}^{4N} \nu_j Y(\nu_j)(A_j + B_j)[1 - e^{-2a\nu_j}],
\]

where the vectors \( \mathbf{U} \) and \( \mathbf{Q} \) have, respectively, \( U_{\alpha} \) and \( Q_{\alpha} \) for \( \alpha=1 \) and 2 as components, to compute the particle-flow and heat-flow rates shown in Table II for several values of the half-distance between plates \( a \).

In a recent work\(^{22}\) the McCormack model was used to study the problem of Couette flow for a binary gas mixture in a plane channel for the special case of purely diffuse reflection at the walls. In that work\(^{22}\) two interaction laws were used: one based on the rigid-sphere model and the other on a “so-called” realistic potential. It is interesting to note that it is reported,\(^{22}\) in regard to the total shear stress, that the difference between the results for the two interaction potentials is very slight. On the other hand, we have found in this work that our results, all based on rigid-sphere interactions, can be
greatly affected by the accommodation coefficients used to define combinations of specular and diffuse reflection boundary conditions. For this reason, we use the results reported in Table III for the ratio between the total shear stress \( p \) defined in Eq. (32) and the free-molecular shear stress

\[
p_{\text{fm}} = \frac{1}{2\pi^2} (u_{n1} - u_{n2}) \left[ c_1 r_1 \frac{a_1 b_1}{a_1 + b_1 - a_1 b_1} + c_2 r_2 \frac{a_2 b_2}{a_2 + b_2 - a_2 b_2} \right]
\]

for the specified He–Ar mixture to illustrate just how important the use of a general (specular/diffuse) boundary condition is. In regard to the numerical results reported in Table 2 of Ref. 22 for the total shear stress, we were able to confirm the four-digit results listed there.

As a final check of our work, we note that we have found agreement for the case of a single-species gas, a limiting case in this work that can be realized by taking either \( c_1 = 0 \) or \( c_2 = 0 \) or \( m_1 = m_2 \) and \( d_1 = d_2 \), with S-model6 results obtained from a special case of the code written to establish the results based on the linearized Boltzmann equation (for rigid-sphere interactions) that are reported in Ref. 23. As noted,17 the McCormack model reduces, for the special case of a single-species gas and for the explicit choices of the collision frequencies \( \gamma_n \) used in this and other works,14–17 to the S model, not the BGK model.

V. CONCLUDING REMARKS

In conclusion, we note that we regard our solution to the considered problem of plane Couette flow for a binary gas mixture as especially concise and easy to use. We have utilized in our formulation a general form of the Maxwell boundary condition at each plate, and we have reported what we believe to be highly accurate species-specific results for the velocity, heat-flow, and shear-stress profiles for a typical case. It should be noted that our formulas are continuous in the \( \tau \) variable and thus are valid anywhere in the gas.

Since our solution requires only a matrix eigenvalue/eigenvector routine and a solver of linear algebraic equations, the algorithm is especially efficient, fast, and easy to implement. In fact, the developed (FORTRAN) code requires typically less than a second (on a 2.2 GHz mobile Pentium 4 machine) to yield all quantities of interest with what we believe to be five or six figures of accuracy.

Finally, we would like to mention the two reasons why, in our opinion, the ADO method that we have used in this work is so effective: (i) the half-range quadrature scheme allows a better treatment of the boundary conditions than a full-range scheme, and (ii) the eigenvalue problem is formulated in a particularly useful way.

\[\begin{align*}
\text{Tab. III. The ratio } p & / p_{\text{fm}} \text{ for a He–Ar mixture with various choices of the} \\
\text{accommodation coefficients and the half-distance between plates.} \\
\hline
a & -U_1 & -U_2 & -Q_1 & -Q_2 \\
\hline
0.001 & 1.67431(-1) & 1.38739(-1) & 6.34188(-5) & 4.19370(-5) \\
0.01 & 1.56694(-1) & 1.38303(-1) & 9.83920(-5) & 2.02099(-4) \\
0.1 & 1.14448(-1) & 1.33720(-1) & 7.40489(-4) & 7.92737(-4) \\
0.5 & 6.50888(-2) & 1.15167(-1) & 1.94200(-3) & 1.10928(-3) \\
1.0 & 4.59674(-2) & 9.86680(-2) & 1.77915(-3) & 8.11098(-4) \\
2.0 & 3.05386(-2) & 7.69956(-2) & 1.13538(-3) & 4.19033(-4) \\
5.0 & 1.60915(-2) & 6.46030(-2) & 3.44038(-4) & 1.11566(-4) \\
10.0 & 9.15607(-3) & 2.75642(-2) & 1.03530(-4) & 3.31495(-5) \\
20.0 & 4.93613(-3) & 1.52212(-2) & 2.83831(-5) & 9.08389(-6) \\
50.0 & 2.07437(-3) & 6.49003(-3) & 4.81817(-6) & 1.54203(-6) \\
\hline
\end{align*}\]


