The McCormack model for gas mixtures: Heat transfer in a plane channel

R. D. M. Garcia
HSH Scientific Computing, Rua Carlos de Campos, 286, São José dos Campos, São Paulo 12242-540, Brazil

C. E. Siewert
Mathematics Department, North Carolina State University, Raleigh, North Carolina 27695-8205

(Received 22 March 2004; accepted 19 May 2004; published online 2 August 2004)

An analytical version of the discrete-ordinates method (the ADO method) is used to establish a concise and particularly accurate solution to the heat-transfer problem in a plane channel 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 density and temperature profiles for both types of particles, as well as the overall heat flow associated with each of the two species of gas particles. Numerical results are reported for two binary mixtures (Ne–Ar and He–Xe). 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. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1773711]

I. INTRODUCTION

The heat-transfer problem within the context of rarefied gas dynamics has been studied in terms of linear theory for a single-species gas based on the BGK model (see, for example, a work by Thomas, Chang, and Siewert,[1] and the references quoted therein) and, in more recent years, on the linearized Boltzmann equation for rigid-sphere interactions.[2,3] Very recently, this problem has also been studied in terms of the nonlinear Boltzmann equation for a mixture of two gases.[4]

In this work, we develop a concise and accurate solution for a mixture of two gases described by the McCormack kinetic model.[5] We do not discuss here many relevant works on this subject, but we refer instead to the books of Cercignani,[6,7] Williams,[8] and Ferziger and Kaper,[9] as well as review papers by Sharipov and Seleznev[10] and Williams,[11] for general background material.

II. A FORMULATION OF THE PROBLEM IN TERMS OF THE McCORMACK MODEL

In this work we base our analysis of a binary gas mixture on the McCormack model as introduced in an important paper[5] published in 1973. While we use this model as defined previously,[5] we employ an explicit notation that is appropriate to the analysis and computations we report here. We note that we have used an analytical discrete-ordinates (ADO) method[12] in two recent works[13,14] to solve a collection of basic flow problems, defined for mixtures in terms of the McCormack model, for semi-infinite media (Kramers' problem and the half-space problem of thermal creep) and plane channels (Poiseuille flow, thermal-creep flow, and flow driven by density gradients). A third work[15] reports a solution of the temperature-jump problem for a binary-gas mixture described by the McCormack model, and so some of our introductory material here is repeated from other works.[13–15] We consider that the required functions $h_\alpha(x,\mathbf{v})$ for the two types of particles ($\alpha=1$ and 2) denote perturbations from Maxwellian distributions for each species, i.e.,

$$f_\alpha(x,\mathbf{v}) = f_{\alpha,0}(v)[1 + h_\alpha(x,\mathbf{v})], \tag{1}$$

where

$$f_{\alpha,0}(v) = n_\alpha(\lambda_\alpha/\pi)^{3/2}e^{-\lambda_\alpha v^2}, \quad \lambda_\alpha = m_\alpha/(2kT_0). \tag{2}$$

Here k is the Boltzmann constant, m_α and n_α are the mass and the equilibrium density of the αth species, x is the spatial variable (measured, for example, in centimeters), $\mathbf{v}$, with components v_x, v_y, v_z and magnitude v, is the particle velocity, and T_0 is a reference temperature. It follows from McCormack's work[5] that the perturbations satisfy (for the case of spatial variations only in the x direction) the coupled equations

$$c_x\frac{\partial}{\partial x}h_\alpha(x,\mathbf{c}) + \omega_\alpha\gamma_\alpha h_\alpha(x,\mathbf{c}) = \omega_\alpha\gamma_\alpha\mathcal{L}_\alpha\{h_1,h_2\}(x,\mathbf{c}), \tag{3}$$

$$\alpha = 1,2,$$

where $\mathbf{c}$, with components c_x, c_y, c_z and magnitude c, is a dimensionless velocity variable,

$$\omega_\alpha = [m_\alpha/(2kT_0)]^{1/2} \tag{4}$$

and the collision frequencies γ_α are to be defined. Here we write the integral operators as

$$\mathcal{L}_\alpha\{h_1,h_2\}(x,\mathbf{c}) = \frac{1}{\pi^{3/2}}\sum_{\beta=1}^{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \times e^{-c'^2}h_\beta(x,\mathbf{c}')K_{\beta,\alpha}(\mathbf{c}',\mathbf{c})dc_x'dc_y'dc_z', \tag{5}$$

where the kernels $K_{\beta,\alpha}(\mathbf{c}',\mathbf{c})$ are listed explicitly in Appendix A of this paper. We note that in obtaining Eq. (3) from the form given by McCormack,[5] we have introduced the dimensionless velocity $\mathbf{c}$ differently in the two equations, i.e., for the case $\alpha=1$ we used the transformation $\mathbf{c}=\omega_1\mathbf{v}$, whereas for the case $\alpha=2$ we used the transformation $\mathbf{c}=\omega_2\mathbf{v}$. As we wish to work with a dimensionless spatial variable, we introduce

$$\tau = x/l_0, \tag{6}$$

where

$$l_0 = \frac{\mu v_0}{P_0} \tag{7}$$

is the mean-free path (based on viscosity) introduced by Sharipov and Kalempa.[16] Here

$$v_0 = (2kT_0/m)^{1/2}, \tag{8}$$

where

$$m = \frac{n_1 m_1 + n_2 m_2}{n_1 + n_2}. \tag{9}$$

Continuing, we express the viscosity of the mixture in terms of the partial pressures P_α and the collision frequencies γ_α as[16]

$$\mu = P_1/\gamma_1 + P_2/\gamma_2, \tag{10}$$

where

$$\frac{P_\alpha}{P_0} = \frac{n_\alpha}{n_1 + n_2}, \tag{11}$$

$$\gamma_1 = [\Psi_1\Psi_2 - \nu_{1,2}^{(4)}\nu_{2,1}^{(4)}][\Psi_2 + \nu_{1,2}^{(4)}]^{-1} \tag{12}$$

and

$$\gamma_2 = [\Psi_1\Psi_2 - \nu_{1,2}^{(4)}\nu_{2,1}^{(4)}][\Psi_1 + \nu_{2,1}^{(4)}]^{-1}. \tag{13}$$

Here

$$\Psi_1 = \nu_{1,1}^{(3)} + \nu_{1,2}^{(3)} - \nu_{1,1}^{(4)} \tag{14}$$

and

$$\Psi_2 = \nu_{2,2}^{(3)} + \nu_{2,1}^{(3)} - \nu_{2,2}^{(4)}, \tag{15}$$

and we note that the parameters $\nu_{i,j}^{(3)}$ and $\nu_{i,j}^{(4)}$ are given explicitly by Eqs. (A27) and (A28) of Appendix A.

Finally, to compact our notation we introduce

$$\sigma_\alpha = \gamma_\alpha \omega_\alpha l_0 \tag{16}$$

or, more explicitly,

$$\sigma_\alpha = \gamma_\alpha \frac{n_1/\gamma_1 + n_2/\gamma_2}{n_1 + n_2}(m_\alpha/m)^{1/2}, \tag{17}$$

and so we rewrite Eq. (3) in terms of the τ variable as

$$c_x \frac{\partial}{\partial \tau} h_\alpha(\tau,\mathbf{c}) + \sigma_\alpha h_\alpha(\tau,\mathbf{c}) = \sigma_\alpha \mathcal{L}_\alpha\{h_1,h_2\}(\tau,\mathbf{c}). \tag{18}$$

In this work we consider the heat-transfer problem in a plane channel, and so we seek solutions of Eqs. (18) that are valid for all $\tau\in(-a,a)$, and we use Maxwell boundary conditions at the walls. If we denote the temperatures of the walls located at $\tau=-a$ and $\tau=a$ by T_{w1} and T_{w2}, respectively, we can follow a recent review paper by Williams[11] and linearize the boundary conditions about T_0 to find

$$h_\alpha(-a,c_x,c_y,c_z) - (1-a_\alpha)h_\alpha(-a,-c_x,c_y,c_z) - a_\alpha \mathcal{I}_-\{h_\alpha\}(-a) = a_\alpha \delta(c^2-2) \tag{19a}$$

and

$$h_\alpha(a,-c_x,c_y,c_z) - (1-b_\alpha)h_\alpha(a,c_x,c_y,c_z) - b_\alpha \mathcal{I}_+\{h_\alpha\}(a) = -b_\alpha \delta(c^2-2) \tag{19b}$$

for $c_x>0$ and all c_y and c_z. Here we have chosen T_0 to be the average of T_{w1} and T_{w2}, and so we have written

$$T_{w1} = T_0(1+\delta) \tag{20a}$$

and

$$T_{w2} = T_0(1-\delta), \tag{20b}$$

where δ is the parameter we use to specify the deviations of the wall temperatures relative to the reference temperature T_0. We use $\{a_1,a_2\}$ and $\{b_1,b_2\}$ to denote the accommodation coefficients basic to the walls located at $\tau=\mp a$, and we have used

$$\mathcal{I}_\mp\{h_\alpha\}(\tau) = \frac{2}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty} \times e^{-c'^2} h_\alpha(\tau,\mp c_x',c_y',c_z') c_x' dc_x' dc_y' dc_z' \tag{21}$$

to denote the diffuse terms in Eqs. (19). Note that

$$h_\alpha(\tau,\mathbf{c}) \Leftrightarrow h_\alpha(\tau,c_x,c_y,c_z).$$

If we sought to compute the complete distribution functions $h_\alpha(\tau,\mathbf{c})$, then we would have to work explicitly with Eqs. (18) and (19); however, since we seek primarily the density and temperature perturbations

$$N_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-c^2} h_\alpha(\tau,\mathbf{c}) dc_x dc_y dc_z \tag{22}$$

and

$$T_\alpha(\tau) = \frac{2}{3\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \times e^{-c^2} h_\alpha(\tau,\mathbf{c})(c^2-3/2) dc_x dc_y dc_z, \tag{23}$$

we can work only with certain moments (integrals) of Eqs. (18) and (19). To this end, we first multiply Eq. (18) by

$$\phi_1(c_y,c_z) = (1/\pi)e^{-(c_y^2+c_z^2)} \tag{24}$$

and integrate over all c_y and all c_z. We then repeat this procedure using

$$\phi_2(c_y,c_z) = (1/\pi)e^{-(c_y^2+c_z^2)}(c_y^2+c_z^2-1). \tag{25}$$

Defining

$$g_{2\alpha-1}(\tau,c_x) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_1(c_y,c_z) h_\alpha(\tau,\mathbf{c}) dc_y dc_z \tag{26}$$

and

$$g_{2\alpha}(\tau,c_x)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi_2(c_y,c_z)h_\alpha(\tau,\mathbf{c})dc_ydc_z, \tag{27}$$

we find from these projections four coupled balance equations which we write (in matrix notation) as

$$\xi\frac{\partial}{\partial\tau}\mathbf{G}(\tau,\xi)+\mathbf{\Sigma}\mathbf{G}(\tau,\xi)=\mathbf{\Sigma}\int_{-\infty}^{\infty}\psi(\xi')\mathbf{K}(\xi',\xi)\mathbf{G}(\tau,\xi')d\xi', \tag{28}$$

where the components of $\mathbf{G}(\tau,\xi)$ are $g_\alpha(\tau,\xi), \alpha=1,2,3,4$, where we now use ξ in place of c_x and where

$$\mathbf{\Sigma}=\text{diag}\{\sigma_1,\sigma_1,\sigma_2,\sigma_2\} \tag{29}$$

and

$$\psi(\xi)=\pi^{-1/2}e^{-\xi^2}. \tag{30}$$

In addition, the elements $k_{i,j}(\xi',\xi)$ of the kernel $\mathbf{K}(\xi',\xi)$ are as listed in Appendix B of this work. To find the boundary conditions relevant to Eq. (28) we project Eqs. (19a) and (19b) against $\phi_1(c_y,c_z)$ and $\phi_2(c_y,c_z)$ to find

$$\mathbf{G}(-a,\xi)-\mathbf{S}_1\mathbf{G}(-a,-\xi)-2\mathbf{D}_1\int_0^{\infty}e^{-\xi'^2}\mathbf{G}(-a,-\xi')\xi'd\xi'$$
$$=\delta\mathbf{\Delta}_1\mathbf{R}(\xi) \tag{31a}$$

and

$$\mathbf{G}(a,-\xi)-\mathbf{S}_2\mathbf{G}(a,\xi)-2\mathbf{D}_2\int_0^{\infty}e^{-\xi'^2}\mathbf{G}(a,\xi')\xi'd\xi'$$
$$=-\delta\mathbf{\Delta}_2\mathbf{R}(\xi) \tag{31b}$$

for $\xi>0$. Here

$$\mathbf{S}_1=\text{diag}\{1-a_1,1-a_1,1-a_2,1-a_2\}, \tag{32a}$$

$$\mathbf{S}_2=\text{diag}\{1-b_1,1-b_1,1-b_2,1-b_2\}, \tag{32b}$$

$$\mathbf{D}_1=\text{diag}\{a_1,0,a_2,0\}, \tag{33a}$$

and

$$\mathbf{D}_2=\text{diag}\{b_1,0,b_2,0\}. \tag{33b}$$

In addition

$$\mathbf{\Delta}_1=\text{diag}\{a_1,a_1,a_2,a_2\}, \tag{34a}$$

$$\mathbf{\Delta}_2=\text{diag}\{b_1,b_1,b_2,b_2\}, \tag{34b}$$

and

$$\mathbf{R}(\xi)=\begin{bmatrix}\xi^2-1\\1\\\xi^2-1\\1\end{bmatrix}. \tag{35}$$

So, if we can solve Eq. (28), subject to Eqs. (31), we can use Eqs. (22) and (23) and Eqs. (26) and (27) and compute the density and temperature perturbations we seek from

$$N_\alpha(\tau)=\int_{-\infty}^{\infty}\psi(\xi)g_{2\alpha-1}(\tau,\xi)d\xi \tag{36}$$

and

$$T_\alpha(\tau)=\frac{2}{3}\int_{-\infty}^{\infty}\psi(\xi)[(\xi^2-1/2)g_{2\alpha-1}(\tau,\xi)+g_{2\alpha}(\tau,\xi)]d\xi. \tag{37}$$

III. THE SOLUTION OF THE HEAT-TRANSFER PROBLEM

In an earlier work[15] the ADO method was used to solve the temperature-jump problem as defined by the McCormack model for mixtures. In that work[15] the elementary solutions of a discrete-ordinates version of our Eq. (28) were established and reported in detail. In order to avoid much repetition, we do not repeat a development of these elementary solutions here, but a brief review of these solutions is given in Appendix C. And so we express our solution to the "**G** problem" as

$$\mathbf{G}(\tau,\pm\xi_i)=\mathbf{G}_*(\tau,\pm\xi_i)+\sum_{j=4}^{4N}[A_j\mathbf{\Phi}(\nu_j,\pm\xi_i)e^{-(a+\tau)/\nu_j}$$
$$+B_j\mathbf{\Phi}(\nu_j,\mp\xi_i)e^{-(a-\tau)/\nu_j}], \tag{38}$$

where

$$\mathbf{G}_*(\tau,\xi)=A_1\mathbf{G}_1+A_2\mathbf{G}_2+A_3\mathbf{G}_3(\xi)+B_1\mathbf{G}_4(\xi)$$
$$+B_2\mathbf{G}_5(\tau,\xi)+B_3\mathbf{G}_6(\tau,\xi), \tag{39}$$

and where the constants $\{A_j,B_j\}$ are to be determined so that the result given by Eq. (38) will satisfy discrete-ordinates versions of the boundary conditions, which we write here as

$$\mathbf{G}(-a,\xi_i)-\mathbf{S}_1\mathbf{G}(-a,-\xi_i)$$
$$-2\pi^{1/2}\mathbf{D}_1\sum_{k=1}^{N}w_k\xi_k\psi(\xi_k)\mathbf{G}(-a,-\xi_k)=\delta\mathbf{\Delta}_1\mathbf{R}(\xi_i) \tag{40a}$$

and

$$\mathbf{G}(a,-\xi_i)-\mathbf{S}_2\mathbf{G}(a,\xi_i)-2\pi^{1/2}\mathbf{D}_2\sum_{k=1}^{N}w_k\xi_k\psi(\xi_k)\mathbf{G}(a,\xi_k)$$
$$=-\delta\mathbf{\Delta}_2\mathbf{R}(\xi_i) \tag{40b}$$

for $i=1,2,\ldots,N$. Here, as mentioned in Appendix C, $\{w_k,\xi_k\}$ are the N weights and nodes used to evaluate integrals over the interval $[0,\infty)$. We can now enter the solution listed as Eq. (38) into Eqs. (40) to define a system of linear algebraic equations for the constants $\{A_j,B_j\}$. However, there is a complication. It can be shown that both $\mathbf{G}_1$ and $\mathbf{G}_2$ satisfy homogeneous versions of the boundary conditions listed as Eqs. (31), and so the constants A_1 and A_2 cannot be determined from these boundary conditions. It follows that the boundary conditions listed as Eqs. (31) are not sufficient to define a unique solution to the considered heat-transfer problem. This issue was encountered and discussed in earlier work, and so we follow previous papers[3,17] and impose the additional conditions

$$\int_{-a}^{a} N_\beta(\tau)d\tau = 0, \quad \beta = 1,2. \tag{41}$$

To be clear about Eq. (41), we note that the number density for particles of type α is given by

$$n_\alpha(x) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_{\alpha,0}(v)[1 + h_\alpha(x,\mathbf{v})]dv_x dv_y dv_z, \tag{42a}$$

where $f_{\alpha,0}(v)$ is given by Eq. (2). Making use of our dimensionless variables and Eq. (22), we can rewrite Eq. (42a) as

$$n_\alpha(\tau) = n_\alpha[1 + N_\alpha(\tau)]. \tag{42b}$$

Now, since the total number of particles of type α in the channel (per unit cross sectional area) is given by $2an_\alpha$, it follows that

$$\int_{-a}^{a} n_\alpha(\tau)d\tau = 2an_\alpha, \tag{42c}$$

and so, using Eq. (42b) in the left-hand side of Eq. (42c), we find the justification for Eq. (41).

We see now that if we augment the linear system obtained when Eq. (38) is substituted into Eqs. (40) with the two conditions listed as Eq. (41), we find a system of $8N+2$ equations for the $8N$ unknowns. However, considering that this augmented system has rank $8N$, we seek unique solutions for the constants $\{A_j, B_j\}$. And so, considering that we have solved the mentioned system of linear equations, we can evaluate Eqs. (36) and (37) to obtain the desired density and temperature profiles, viz.,

$$\mathbf{N}(\tau) = \begin{bmatrix} A_1 - B_2\tau \\ A_2 - B_3\tau \end{bmatrix} + \sum_{j=4}^{4N} \mathbf{X}(\nu_j)[A_j e^{-(a+\tau)/\nu_j} + B_j e^{-(a-\tau)/\nu_j}] \tag{43}$$

and

$$\mathbf{T}(\tau) = [A_3 + (c_1B_2 + c_2B_3)\tau]\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{2}{3}\sum_{j=4}^{4N} \mathbf{Y}(\nu_j)[A_j e^{-(a+\tau)/\nu_j} + B_j e^{-(a-\tau)/\nu_j}], \tag{44}$$

where $c_1 = n_1/n$, $c_2 = n_2/n$, with $n = n_1 + n_2$,

$$\mathbf{X}(\nu_j) = \sum_{k=1}^{N} w_k \psi(\xi_k)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}[\mathbf{\Phi}(\nu_j,\xi_k) + \mathbf{\Phi}(\nu_j,-\xi_k)] \tag{45}$$

and

$$\mathbf{Y}(\nu_j) = \sum_{k=1}^{N} w_k \psi(\xi_k)\begin{bmatrix} \xi_k^2 - 1/2 & 1 & 0 & 0 \\ 0 & 0 & \xi_k^2 - 1/2 & 1 \end{bmatrix} \times [\mathbf{\Phi}(\nu_j,\xi_k) + \mathbf{\Phi}(\nu_j,-\xi_k)]. \tag{46}$$

Note that in Eq. (43) we have used $N_1(\tau)$ and $N_2(\tau)$ to define the components of $\mathbf{N}(\tau)$, and similarly the components of $\mathbf{T}(\tau)$ in Eq. (44) are $T_1(\tau)$ and $T_2(\tau)$.

In addition to the density and temperature perturbations, we consider that the flow and the heat flow (in the x direction) are also of interest. These quantities are defined for each of the two species by

$$U_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-c^2} h_\alpha(\tau,\mathbf{c})c_x dc_x dc_y dc_z \tag{47}$$

and

$$Q_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-c^2} h_\alpha(\tau,\mathbf{c}) \times (c^2 - 5/2)c_x dc_x dc_y dc_z \tag{48}$$

for $\alpha = 1,2$. Noting Eqs. (24)–(27), we can rewrite Eqs. (47) and (48) as

$$U_\alpha(\tau) = \int_{-\infty}^{\infty} \psi(\xi) g_{2\alpha-1}(\tau,\xi)\xi d\xi \tag{49}$$

and

$$Q_\alpha(\tau) = \int_{-\infty}^{\infty} \psi(\xi)[(\xi^2 - 3/2)g_{2\alpha-1}(\tau,\xi) + g_{2\alpha}(\tau,\xi)]\xi d\xi. \tag{50}$$

Upon multiplying Eq. (28) by $\psi(\xi)$ and integrating over all ξ we can conclude that both $U_1(\tau)$ and $U_2(\tau)$ are constants, and we can then use either of Eqs. (31) to show that $U_1(\tau) = 0$ and that $U_2(\tau) = 0$.

In regard to the heat flow associated with each of the two species, we have taken moments of Eq. (28) to find, after some elementary algebra, the expression

$$\varphi_1 Q_1(\tau) + \varphi_2 Q_2(\tau) = Q_0, \tag{51}$$

where Q_0 is a constant and where

$$\varphi_1 = \frac{c_1}{c_1 + rc_2} \tag{52a}$$

and

$$\varphi_2 = \frac{rc_2}{c_1 + rc_2}, \tag{52b}$$

with $r = (m_1/m_2)^{1/2}$. If we define the two components of $\mathbf{Q}(\tau)$ to be $Q_1(\tau)$ and $Q_2(\tau)$, then we can use Eqs. (38) and (50) to find

$$\mathbf{Q}(\tau) = \mathbf{Q}_* + \sum_{j=4}^{4N} \mathbf{Z}(\nu_j)[A_j e^{-(a+\tau)/\nu_j} - B_j e^{-(a-\tau)/\nu_j}], \tag{53}$$

where

$$\mathbf{Z}(\nu_j) = \sum_{k=1}^{N} w_k \xi_k \psi(\xi_k)\begin{bmatrix} \xi_k^2 - 3/2 & 1 & 0 & 0 \\ 0 & 0 & \xi_k^2 - 3/2 & 1 \end{bmatrix} \times [\mathbf{\Phi}(\nu_j,\xi_k) - \mathbf{\Phi}(\nu_j,-\xi_k)]. \tag{54}$$

In addition, we can use the vectors $\mathbf{U}_\beta$ and $\mathbf{V}_\beta$ defined in Appendix C in order to write

TABLE I. The density, temperature, and heat-flow profiles for the Ne–Ar mixture.

η	$N_1(-a+2\eta a)$	$N_2(-a+2\eta a)$	$-T_1(-a+2\eta a)$	$-T_2(-a+2\eta a)$	$Q_1(-a+2\eta a)$	$Q_2(-a+2\eta a)$
0.0	−1.928 34(−1)	−3.786 48(−1)	1.558 83(−1)	−1.788 26(−2)	1.556 84(−1)	3.000 03(−1)
0.1	−1.382 11(−1)	−2.499 54(−1)	2.217 73(−1)	1.224 38(−1)	1.759 82(−1)	2.809 65(−1)
0.2	−1.017 18(−1)	−1.736 91(−1)	2.687 27(−1)	2.019 07(−1)	1.889 32(−1)	2.688 20(−1)
0.3	−6.773 44(−2)	−1.092 19(−1)	3.126 25(−1)	2.668 76(−1)	1.977 53(−1)	2.605 46(−1)
0.4	−3.449 50(−2)	−5.021 64(−2)	3.554 42(−1)	3.250 87(−1)	2.037 31(−1)	2.549 39(−1)
0.5	−1.369 82(−3)	6.060 81(−3)	3.979 72(−1)	3.799 58(−1)	2.075 36(−1)	2.513 70(−1)
0.6	3.202 95(−2)	6.131 34(−2)	4.407 54(−1)	4.336 28(−1)	2.095 18(−1)	2.495 11(−1)
0.7	6.613 32(−2)	1.170 24(−1)	4.843 79(−1)	4.879 66(−1)	2.098 05(−1)	2.492 42(−1)
0.8	1.017 10(−1)	1.751 10(−1)	5.298 20(−1)	5.453 81(−1)	2.083 16(−1)	2.506 39(−1)
0.9	1.408 02(−1)	2.395 10(−1)	5.794 53(−1)	6.107 22(−1)	2.046 81(−1)	2.540 48(−1)
1.0	1.989 17(−1)	3.344 52(−1)	6.496 60(−1)	7.117 47(−1)	1.977 70(−1)	2.605 31(−1)

$$\mathbf{Q}_* = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}(B_2\mathbf{U}_1 + B_3\mathbf{U}_2) + \frac{3}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \times(B_2\mathbf{V}_1 + B_3\mathbf{V}_2). \quad (55)$$

To conclude this section, we note that the case of a single-species gas can be achieved here as any one of three limiting cases defined as

$$c_1 = 0 \text{ or } c_2 = 0 \text{ or } m_1 = m_2 \text{ and } d_1 = d_2.$$

In each of the limiting cases, the resulting value of Q_0 is the constant heat flow for the single-gas case.

IV. NUMERICAL RESULTS

In order to demonstrate that our ADO solution for the considered heat-transfer problem can yield accurate results with a relatively modest computational effort, we report detailed numerical results for two test cases.

The first test case consists of a Ne–Ar mixture and the second of a He–Xe mixture. We note that only the mass ratio m_1/m_2, the diameter ratio d_1/d_2, and the density ratio n_1/n_2 are needed to define the McCormack model for rigid-sphere interactions. In particular, noting the convenient choice of mean-free path made in Sec. II and the ratios of parameters that result, it is easy to see that the constant factor $(\pi k T_0/32)^{1/2}$ in Eq. (A35) of Appendix A need not be specified. And so we use $m_1=20.183$, $m_2=39.948$, and $d_2/d_1=1.406$ in our first test case, and $m_1=4.0026$, $m_2=131.30$, and $d_2/d_1=2.226$ in our second test case. We use $n_1/(n_1+n_2)=0.4$ for both test cases.

The remaining input data are taken to be the same for both test cases. Thus, we consider a channel with half width $a=1.5$, and we assign the accommodation coefficients $a_1=0.2$ and $a_2=0.4$ to the wall at $\tau=-a$ and $b_1=0.6$ and $b_2=0.8$ to the wall at $\tau=a$, where the subscripts identify the type of particle. We use here $\delta=1.0$.

We report in Tables I and II our converged numerical results for the density, temperature, and heat-flow profiles. We have verified that the tabulated heat-flow profiles satisfy the identity expressed by Eq. (51). In addition, we note that all numerical results were generated with a quadrature scheme defined upon using the transformation $v(\xi)=e^{-\xi}$ to map $\xi\in[0,\infty)$ onto $v\in[0,1]$ and then mapping the Gauss–Legendre scheme linearly onto the interval $[0,1]$. To establish confidence in the accuracy of our results, we have observed numerical stability in all entries of the tables, as the order of the quadrature N was varied between 40 and 100, in increments of 20.

In regard to numerical linear algebra, we have used subroutines from the EISPACK collection[18] to find the required eigenvalues and eigenvectors, and we used subroutines from

TABLE II. The density, temperature, and heat-flow profiles for the He–Xe mixture.

η	$N_1(-a+2\eta a)$	$N_2(-a+2\eta a)$	$-T_1(-a+2\eta a)$	$-T_2(-a+2\eta a)$	$Q_1(-a+2\eta a)$	$Q_2(-a+2\eta a)$
0.0	−1.622 36(−1)	−3.796 89(−1)	2.358 93(−1)	2.352 84(−3)	1.629 29(−1)	3.080 15(−1)
0.1	−1.104 16(−1)	−2.582 55(−1)	3.029 85(−1)	1.307 98(−1)	1.654 49(−1)	2.983 96(−1)
0.2	−7.849 92(−2)	−1.814 04(−1)	3.482 92(−1)	2.083 81(−1)	1.674 36(−1)	2.908 08(−1)
0.3	−5.073 22(−2)	−1.146 69(−1)	3.887 38(−1)	2.735 39(−1)	1.690 64(−1)	2.845 90(−1)
0.4	−2.471 08(−2)	−5.279 33(−2)	4.270 89(−1)	3.326 29(−1)	1.704 04(−1)	2.794 76(−1)
0.5	5.928 23(−4)	6.481 57(−3)	4.645 76(−1)	3.884 78(−1)	1.714 94(−1)	2.753 12(−1)
0.6	2.583 32(−2)	6.455 66(−2)	5.020 01(−1)	4.428 76(−1)	1.723 59(−1)	2.720 09(−1)
0.7	5.162 83(−2)	1.226 57(−1)	5.401 30(−1)	4.973 90(−1)	1.730 11(−1)	2.695 19(−1)
0.8	7.886 21(−2)	1.823 68(−1)	5.800 33(−1)	5.540 09(−1)	1.734 53(−1)	2.678 34(−1)
0.9	1.094 91(−1)	2.469 63(−1)	6.239 94(−1)	6.166 82(−1)	1.736 70(−1)	2.670 05(−1)
1.0	1.558 04(−1)	3.367 25(−1)	6.853 92(−1)	7.079 49(−1)	1.736 05(−1)	2.672 54(−1)

TABLE III. Comparison of results for a normalized heat flow ($-q_1^*$).

		$m_1/m_2=2$ and $d_1/d_2=1$		$m_1/m_2=4$ and $d_1/d_2=2$	
n_1/n_2	Kn	NLBE (Ref. 4)	This work	NLBE (Ref. 4)	This work
1.0(1)	1.0(−1)	0.184	0.181	0.207	0.202
1.0(1)	1.0	0.509	0.519	0.547	0.557
1.0(1)	1.0(1)	0.656	0.683	0.693	0.721
1.0	1.0(−1)	0.209	0.205	0.370	0.358
1.0	1.0	0.589	0.599	0.814	0.830
1.0	1.0(1)	0.763	0.794	0.966	1.006
1.0(−1)	1.0(−1)	0.245	0.241	0.659	0.653
1.0(−1)	1.0	0.677	0.689	1.124	1.159
1.0(−1)	1.0(1)	0.871	0.906	1.244	1.298

the LINPACK package[19] to find a least-squares solution (via QR decomposition) for the augmented system of $8N+2$ linear algebraic equations and $8N$ unknowns $\{A_j, B_j\}$ mentioned in Sec. III. We should mention that we have also followed the alternative route of combining some equations to transform the overdetermined system obtained when Eq. (38) is used in Eqs. (40) into a square system for all unknowns, except A_1 and A_2. This system was solved by Gaussian elimination and then A_1 and A_2 were determined using Eq. (41). We have concluded that both approaches yielded essentially the same results.

As a (not very severe) test of our results, we have found agreement for the case of a single-species gas with S-model[10] 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 were reported earlier.[3] As noted,[15] the McCormack model (as used in this work) reduces, for the special case of a single gas, to the S model, not the BGK model.

Finally, we note that we have also used our code to compute the normalized heat flow reported by Kosuge, Aoki, and Takata[4] for the problem of a binary mixture of rigid-sphere gases confined between two diffusely reflecting parallel plates with different temperatures. These authors employed an iterative finite-difference technique to solve the two coupled nonlinear Boltzmann equations that describe the problem and reported numerical results in tabular form for a normalized heat flow defined as

$$q_1^* = [2p_0(2kT_{w1}/m_1)^{1/2}]^{-1}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[m_1 f_1(x,\mathbf{v}) + m_2 f_2(x,\mathbf{v})]v^2 v_x dv_x dv_y dv_z, \tag{56}$$

where, except for the pressure $p_0=k(n_1+n_2)T_{w1}$, all symbols have been defined in our work. We have found that q_1^* can be expressed in terms of our constant Q_0 introduced in Eq. (51) as

$$q_1^* = (1+\delta)^{-3/2}(c_1 + rc_2)Q_0, \tag{57}$$

and so we report in Table III our numerical results for q_1^*, along with those based on the nonlinear Boltzmann equation (NLBE) for rigid-sphere interactions reported by Kosuge, Aoki, and Takata.[4] Since our mean-free path is defined in a way different from that of Kosuge, Aoki, and Takata,[4] the equivalent channel width in our formulation is computed from

$$2a = l_0^*/(l_0\mathrm{Kn}), \tag{58}$$

where l_0 is the mean-free path given by Eq. (7) and l_0^* and Kn are, respectively, the mean-free path and the Knudsen number used by Kosuge, Aoki, and Takata.[4] We note also that to compute our entries in Table III, we have put all our accommodation coefficients equal to unity, and we have used $\delta=-1/3$. We see from Table III that, as might be expected, the McCormack model appears to yield better results (for the heat flow) for small Knudsen numbers (large channel widths).

V. CONCLUDING REMARKS

To conclude this work, we note that we believe that our solution to the considered heat-transfer problem is especially concise and easy to use. In our formulation we have utilized at each wall a general form of the Maxwell boundary condition, and we have reported what we believe to be highly accurate (within the context of the kinetic model used) results for the density, temperature, and heat-flow profiles for two test cases. It should be noted that our complete, species-specific results for the density, temperature, and heat-flow perturbations are continuous in the τ variable and thus are valid anywhere in the gas.

In this work we have considered only the case of rigid-sphere interactions, but the solutions can be used for other scattering laws, such as the one defined by the Lennard-Jones potential, simply by using appropriate definitions of the Ω integrals[9,20] mentioned in Appendix A. It can be noted here that the McCormack model has the attractive feature that it preserves the basic physical laws prescribed by the Boltzmann equation, while at the same time this kinetic model does not require the heavy numerical work that is associated with the full Boltzmann equation. The work of McCormack[5] also is considered important in the one-species limit since by a specific choice of γ, a free parameter in the model, we are able to obtain either the S model[10] or the explicit $N=5$ model reported by Gross and Jackson in their famous work.[21] And because the McCormack model, even in the one-species limit, allows some choice of the collision frequency γ, other kinetic models are also contained in McCormack's formulation. Having said that, we recall that in this work we have used Eqs. (12) and (13) to define the collision frequencies for a two-species gas.

Finally, in regard to computational requirements, we note that since our solutions require 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 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.

ACKNOWLEDGMENT

The authors take this opportunity to thank J. R. Thomas, Jr. for helpful discussions regarding this work.

APPENDIX A: BASIC ELEMENTS OF THE DEFINING EQUATIONS

Here we list some basic results that are required to define certain elements of the main text of this paper. First of all, in regard to Eq. (5), we note that

$$K_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) = K^{(1)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) + K^{(2)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) + K^{(3)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) + K^{(4)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}),\ \ \alpha,\beta = 1,2, \tag{A1}$$

where

$$K^{(1)}_{1,1}(\mathbf{c}',\mathbf{c}) = 1 + \{2[1-\eta^{(1)}_{1,2}] - \eta^{(2)}_{1,2}(c'^2-5/2)\}\mathbf{c}'\cdot\mathbf{c}, \tag{A2}$$

$$K^{(2)}_{1,1}(\mathbf{c}',\mathbf{c}) = (2/3)[1-2r*\eta^{(1)}_{1,2}](c'^2-3/2)(c^2-3/2), \tag{A3}$$

$$K^{(3)}_{1,1}(\mathbf{c}',\mathbf{c}) = 2\varpi_1[(\mathbf{c}'\cdot\mathbf{c})^2-(1/3)c'^2c^2], \tag{A4}$$

$$K^{(4)}_{1,1}(\mathbf{c}',\mathbf{c}) = [(4/5)\beta_1(c'^2-5/2) - \eta^{(2)}_{1,2}](c^2-5/2)\mathbf{c}'\cdot\mathbf{c}, \tag{A5}$$

$$K^{(1)}_{2,1}(\mathbf{c}',\mathbf{c}) = r\{2\eta^{(1)}_{1,2} + \eta^{(2)}_{1,2}[r^2(c'^2-5/2)+c^2-5/2]\}\mathbf{c}'\cdot\mathbf{c}, \tag{A6}$$

$$K^{(2)}_{2,1}(\mathbf{c}',\mathbf{c}) = (4/3)r*\eta^{(1)}_{1,2}(c'^2-3/2)(c^2-3/2), \tag{A7}$$

$$K^{(3)}_{2,1}(\mathbf{c}',\mathbf{c}) = 2\eta^{(4)}_{1,2}[(\mathbf{c}'\cdot\mathbf{c})^2-(1/3)c'^2c^2], \tag{A8}$$

$$K^{(4)}_{2,1}(\mathbf{c}',\mathbf{c}) = (4/5)\eta^{(6)}_{1,2}(c'^2-5/2)(c^2-5/2)\mathbf{c}'\cdot\mathbf{c}, \tag{A9}$$

$$K^{(1)}_{2,2}(\mathbf{c}',\mathbf{c}) = 1 + \{2[1-\eta^{(1)}_{2,1}] - \eta^{(2)}_{2,1}(c'^2-5/2)\}\mathbf{c}'\cdot\mathbf{c}, \tag{A10}$$

$$K^{(2)}_{2,2}(\mathbf{c}',\mathbf{c}) = (2/3)[1-2s*\eta^{(1)}_{2,1}](c'^2-3/2)(c^2-3/2), \tag{A11}$$

$$K^{(3)}_{2,2}(\mathbf{c}',\mathbf{c}) = 2\varpi_2[(\mathbf{c}'\cdot\mathbf{c})^2-(1/3)c'^2c^2], \tag{A12}$$

$$K^{(4)}_{2,2}(\mathbf{c}',\mathbf{c}) = [(4/5)\beta_2(c'^2-5/2) - \eta^{(2)}_{2,1}](c^2-5/2)\mathbf{c}'\cdot\mathbf{c}, \tag{A13}$$

$$K^{(1)}_{1,2}(\mathbf{c}',\mathbf{c}) = s\{2\eta^{(1)}_{2,1} + \eta^{(2)}_{2,1}[s^2(c'^2-5/2)+c^2-5/2]\}\mathbf{c}'\cdot\mathbf{c}, \tag{A14}$$

$$K^{(2)}_{1,2}(\mathbf{c}',\mathbf{c}) = (4/3)s*\eta^{(1)}_{2,1}(c'^2-3/2)(c^2-3/2), \tag{A15}$$

$$K^{(3)}_{1,2}(\mathbf{c}',\mathbf{c}) = 2\eta^{(4)}_{2,1}[(\mathbf{c}'\cdot\mathbf{c})^2-(1/3)c'^2c^2], \tag{A16}$$

and

$$K^{(4)}_{1,2}(\mathbf{c}',\mathbf{c}) = (4/5)\eta^{(6)}_{2,1}(c'^2-5/2)(c^2-5/2)\mathbf{c}'\cdot\mathbf{c}. \tag{A17}$$

Here we used

$$r = (m_1/m_2)^{1/2} \tag{A18a}$$

and

$$s = (m_2/m_1)^{1/2}, \tag{A18b}$$

along with

$$r* = r^2/(1+r^2) \tag{A19a}$$

and

$$s* = s^2/(1+s^2). \tag{A19b}$$

In addition,

$$\varpi_1 = 1 + \eta^{(4)}_{1,1} - \eta^{(3)}_{1,1} - \eta^{(3)}_{1,2}, \tag{A20}$$

$$\varpi_2 = 1 + \eta^{(4)}_{2,2} - \eta^{(3)}_{2,2} - \eta^{(3)}_{2,1}, \tag{A21}$$

$$\beta_1 = 1 + \eta^{(6)}_{1,1} - \eta^{(5)}_{1,1} - \eta^{(5)}_{1,2}, \tag{A22}$$

and

$$\beta_2 = 1 + \eta^{(6)}_{2,2} - \eta^{(5)}_{2,2} - \eta^{(5)}_{2,1}, \tag{A23}$$

where

$$\eta^{(k)}_{i,j} = \nu^{(k)}_{i,j}/\gamma_i. \tag{A24}$$

Following McCormack,[5] we write

$$\nu^{(1)}_{\alpha,\beta} = \frac{16}{3}\frac{m_{\alpha,\beta}}{m_\alpha}n_\beta\Omega^{11}_{\alpha,\beta}, \tag{A25}$$

$$\nu^{(2)}_{\alpha,\beta} = \frac{64}{15}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^2 n_\beta\left(\Omega^{12}_{\alpha,\beta} - \frac{5}{2}\Omega^{11}_{\alpha,\beta}\right), \tag{A26}$$

$$\nu^{(3)}_{\alpha,\beta} = \frac{16}{5}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^2 \frac{m_\alpha}{m_\beta}n_\beta\left(\frac{10}{3}\Omega^{11}_{\alpha,\beta} + \frac{m_\beta}{m_\alpha}\Omega^{22}_{\alpha,\beta}\right), \tag{A27}$$

$$\nu^{(4)}_{\alpha,\beta} = \frac{16}{5}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^2 \frac{m_\alpha}{m_\beta}n_\beta\left(\frac{10}{3}\Omega^{11}_{\alpha,\beta} - \Omega^{22}_{\alpha,\beta}\right), \tag{A28}$$

$$\nu^{(5)}_{\alpha,\beta} = \frac{64}{15}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^3 \frac{m_\alpha}{m_\beta}n_\beta\Gamma^{(5)}_{\alpha,\beta}, \tag{A29}$$

and

$$\nu_{\alpha,\beta}^{(6)} = \frac{64}{15}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^3\left(\frac{m_\alpha}{m_\beta}\right)^{3/2} n_\beta \Gamma_{\alpha,\beta}^{(6)}, \tag{A30}$$

with

$$\Gamma_{\alpha,\beta}^{(5)} = \Omega_{\alpha,\beta}^{22} + \left(\frac{15m_\alpha}{4m_\beta} + \frac{25m_\beta}{8m_\alpha}\right)\Omega_{\alpha,\beta}^{11} - \left(\frac{m_\beta}{2m_\alpha}\right)(5\Omega_{\alpha,\beta}^{12} - \Omega_{\alpha,\beta}^{13}), \tag{A31}$$

and, after a correction by Pan and Storvick,[22]

$$\Gamma_{\alpha,\beta}^{(6)} = -\Omega_{\alpha,\beta}^{22} + \tfrac{55}{8}\Omega_{\alpha,\beta}^{11} - \tfrac{5}{2}\Omega_{\alpha,\beta}^{12} + \tfrac{1}{2}\Omega_{\alpha,\beta}^{13}. \tag{A32}$$

In addition,

$$m_{\alpha,\beta} = m_\alpha m_\beta/(m_\alpha + m_\beta) \tag{A33}$$

and the Ω functions are the Chapman–Cowling integrals[9,20] which for the case of rigid-sphere interactions take the simple forms

$$\Omega_{\alpha,\beta}^{12} = 3\Omega_{\alpha,\beta}^{11}, \tag{A34a}$$

$$\Omega_{\alpha,\beta}^{13} = 12\Omega_{\alpha,\beta}^{11}, \tag{A34b}$$

and

$$\Omega_{\alpha,\beta}^{22} = 2\Omega_{\alpha,\beta}^{11}, \tag{A34c}$$

with

$$\Omega_{\alpha,\beta}^{11} = \frac{1}{4}\left(\frac{\pi k T_0}{2m_{\alpha,\beta}}\right)^{1/2}(d_\alpha + d_\beta)^2. \tag{A35}$$

Here, as noted in the main text of this work, k is the Boltzmann constant, T_0 is a reference temperature, and d_1 and d_2 are the diameters of the two types of particles.

APPENDIX B: THE BASIC KERNELS FOR TEMPERATURE-DENSITY PROBLEMS

We express the elements of the kernel $\mathbf{K}(\xi',\xi)$ required in Eq. (28) as follows:

$$k_{1,1}(\xi',\xi) = 1 + f_{1,1}(\xi',\xi)\xi'\xi + (2/3)[1 - 2r*\eta_{1,2}^{(1)} + 2\varpi_1]\times(\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B1}$$

$$k_{1,2}(\xi',\xi) = [(4/5)\beta_1(\xi^2 - 3/2) - \eta_{1,2}^{(2)}]\xi'\xi + (2/3)[1 - 2r*\eta_{1,2}^{(1)} - \varpi_1](\xi^2 - 1/2), \tag{B2}$$

$$k_{1,3}(\xi',\xi) = f_{1,3}(\xi',\xi)\xi'\xi + (4/3)[r*\eta_{1,2}^{(1)} + \eta_{1,2}^{(4)}]\times(\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B3}$$

$$k_{1,4}(\xi',\xi) = [r^3\eta_{1,2}^{(2)} + (4/5)\eta_{1,2}^{(6)}(\xi^2 - 3/2)]\xi'\xi + (2/3)\times[2r*\eta_{1,2}^{(1)} - \eta_{1,2}^{(4)}](\xi^2 - 1/2), \tag{B4}$$

$$k_{2,1}(\xi',\xi) = [(4/5)\beta_1(\xi'^2 - 3/2) - \eta_{1,2}^{(2)}]\xi'\xi + (2/3)[1 - 2r*\eta_{1,2}^{(1)} - \varpi_1](\xi'^2 - 1/2), \tag{B5}$$

$$k_{2,2}(\xi',\xi) = (2/3)[1 - 2r*\eta_{1,2}^{(1)}] + (1/3)\varpi_1 + (4/5)\beta_1\xi'\xi, \tag{B6}$$

$$k_{2,3}(\xi',\xi) = [r\eta_{1,2}^{(2)} + (4/5)\eta_{1,2}^{(6)}(\xi'^2 - 3/2)]\xi'\xi + (2/3)\times[2r*\eta_{1,2}^{(1)} - \eta_{1,2}^{(4)}](\xi'^2 - 1/2), \tag{B7}$$

$$k_{2,4}(\xi',\xi) = (4/5)\eta_{1,2}^{(6)}\xi'\xi + (1/3)[4r*\eta_{1,2}^{(1)} + \eta_{1,2}^{(4)}], \tag{B8}$$

$$k_{3,1}(\xi',\xi) = f_{3,1}(\xi',\xi)\xi'\xi + (4/3)[s*\eta_{2,1}^{(1)} + \eta_{2,1}^{(4)}]\times(\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B9}$$

$$k_{3,2}(\xi',\xi) = [s^3\eta_{2,1}^{(2)} + (4/5)\eta_{2,1}^{(6)}(\xi^2 - 3/2)]\xi'\xi + (2/3)\times[2s*\eta_{2,1}^{(1)} - \eta_{2,1}^{(4)}](\xi^2 - 1/2), \tag{B10}$$

$$k_{3,3}(\xi',\xi) = 1 + f_{3,3}(\xi',\xi)\xi'\xi + (2/3)[1 - 2s*\eta_{2,1}^{(1)} + 2\varpi_2]\times(\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B11}$$

$$k_{3,4}(\xi',\xi) = [(4/5)\beta_2(\xi^2 - 3/2) - \eta_{2,1}^{(2)}]\xi'\xi + (2/3)[1 - 2s*\eta_{2,1}^{(1)} - \varpi_2](\xi^2 - 1/2), \tag{B12}$$

$$k_{4,1}(\xi',\xi) = [s\eta_{2,1}^{(2)} + (4/5)\eta_{2,1}^{(6)}(\xi'^2 - 3/2)]\xi'\xi + (2/3)\times[2s*\eta_{2,1}^{(1)} - \eta_{2,1}^{(4)}](\xi'^2 - 1/2), \tag{B13}$$

$$k_{4,2}(\xi',\xi) = (4/5)\eta_{2,1}^{(6)}\xi'\xi + (1/3)[4s*\eta_{2,1}^{(1)} + \eta_{2,1}^{(4)}], \tag{B14}$$

$$k_{4,3}(\xi',\xi) = [(4/5)\beta_2(\xi'^2 - 3/2) - \eta_{2,1}^{(2)}]\xi'\xi + (2/3)[1 - 2s*\eta_{2,1}^{(1)} - \varpi_2](\xi'^2 - 1/2), \tag{B15}$$

and

$$k_{4,4}(\xi',\xi) = (2/3)[1 - 2s*\eta_{2,1}^{(1)}] + (1/3)\varpi_2 + (4/5)\beta_2\xi'\xi. \tag{B16}$$

Here we have used

$$f_{1,1}(\xi',\xi) = 2[1 - \eta_{1,2}^{(1)}] - \eta_{1,2}^{(2)}(\xi'^2 + \xi^2 - 3) + (4/5)\beta_1(\xi'^2 - 3/2)(\xi^2 - 3/2), \tag{B17}$$

$$f_{1,3}(\xi',\xi) = 2r\eta_{1,2}^{(1)} + r\eta_{1,2}^{(2)}[r^2(\xi'^2 - 3/2) + \xi^2 - 3/2] + (4/5)\eta_{1,2}^{(6)}(\xi'^2 - 3/2)(\xi^2 - 3/2), \tag{B18}$$

$$f_{3,1}(\xi',\xi) = 2s\eta_{2,1}^{(1)} + s\eta_{2,1}^{(2)}[s^2(\xi'^2 - 3/2) + \xi^2 - 3/2] + (4/5)\eta_{2,1}^{(6)}(\xi'^2 - 3/2)(\xi^2 - 3/2), \tag{B19}$$

and

$$f_{3,3}(\xi',\xi) = 2[1 - \eta_{2,1}^{(1)}] - \eta_{2,1}^{(2)}(\xi'^2 + \xi^2 - 3) + (4/5)\beta_2(\xi'^2 - 3/2)(\xi^2 - 3/2). \tag{B20}$$

APPENDIX C: THE ELEMENTARY SOLUTIONS

While our complete work regarding the elementary solutions was reported earlier,[15] we give here a brief description of the way in which these solutions are defined. To start, we rewrite Eq. (28) as

$$\xi\frac{\partial}{\partial\tau}\mathbf{G}(\tau,\xi)+\mathbf{\Sigma}\mathbf{G}(\tau,\xi)=\mathbf{\Sigma}\int_0^\infty\psi(\xi')[\mathbf{K}(\xi',\xi)\mathbf{G}(\tau,\xi')+\mathbf{K}(-\xi',\xi)\mathbf{G}(\tau,-\xi')]d\xi', \quad \text{(C1)}$$

and we then look for solutions of Eq. (C1) of the form

$$\mathbf{G}(\tau,\xi)=\mathbf{\Phi}(\nu,\xi)e^{-\tau/\nu}. \quad \text{(C2)}$$

Substitution of Eq. (C2) into Eq. (C1) leads us, after we use the N weights and nodes $\{w_k,\xi_k\}$ to represent the integration process in Eq. (C1) and after we evaluate the resulting version of Eq. (C1) at $\{\pm\xi_i\}$, to the eigenvalue problem

$$(1/\xi_i^2)\left[\mathbf{\Sigma}^2\mathbf{V}(\nu_j,\xi_i)-\sum_{k=1}^N w_k\psi(\xi_k)\boldsymbol{\mathcal{K}}(\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)\right]=\lambda_j\mathbf{V}(\nu_j,\xi_i). \quad \text{(C3)}$$

Here

$$\boldsymbol{\mathcal{K}}(\xi',\xi)=(\xi/\xi')\mathbf{\Sigma}\mathbf{K}_+(\xi',\xi)\mathbf{\Sigma}+\mathbf{\Sigma}^2\mathbf{K}_-(\xi',\xi)-\int_0^\infty\psi(\xi'')\times(\xi/\xi'')\mathbf{\Sigma}\mathbf{K}_+(\xi'',\xi)\mathbf{\Sigma}\mathbf{K}_-(\xi',\xi'')d\xi'', \quad \text{(C4)}$$

where

$$\mathbf{K}_+(\xi',\xi)=\mathbf{K}(\xi',\xi)+\mathbf{K}(-\xi',\xi) \quad \text{(C5a)}$$

and

$$\mathbf{K}_-(\xi',\xi)=\mathbf{K}(\xi',\xi)-\mathbf{K}(-\xi',\xi) \quad \text{(C5b)}$$

and where the kernel $\mathbf{K}(\xi',\xi)$ is defined in Appendix B. Upon solving the resulting eigenvalue problem, we use the eigenvalues λ_j and the eigenvectors $\mathbf{V}(\nu_j,\xi_k)$ to establish the separation constants

$$\nu_j=\pm\lambda_j^{-1/2} \quad \text{(C6)}$$

and the vectors

$$\mathbf{U}(\nu_j,\xi_i)=(\nu_j/\xi_i)\mathbf{\Sigma}\left[\mathbf{V}(\nu_j,\xi_i)-\sum_{k=1}^N w_k\psi(\xi_k)\mathbf{K}_-(\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)\right]. \quad \text{(C7)}$$

We now can use

$$\mathbf{\Phi}(\nu_j,\xi_i)=(1/2)[\mathbf{U}(\nu_j,\xi_i)+\mathbf{V}(\nu_j,\xi_i)] \quad \text{(C8a)}$$

and

$$\mathbf{\Phi}(\nu_j,-\xi_i)=(1/2)[\mathbf{U}(\nu_j,\xi_i)-\mathbf{V}(\nu_j,\xi_i)] \quad \text{(C8b)}$$

to establish the discrete-ordinates elementary solutions. As noted,[15] there are three (plus/minus) pairs of separation constants that appear to become unbounded as the order of our quadrature scheme increases, and so we replace the corresponding discrete-ordinates elementary solutions with the six exact solutions

$$\mathbf{G}_1=\begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \quad \text{(C9a)}$$

$$\mathbf{G}_2=\begin{bmatrix}0\\0\\1\\0\end{bmatrix}, \quad \text{(C9b)}$$

$$\mathbf{G}_3(\xi)=\begin{bmatrix}\xi^2-1/2\\1\\\xi^2-1/2\\1\end{bmatrix}, \quad \text{(C9c)}$$

$$\mathbf{G}_4(\xi)=\begin{bmatrix}r\xi\\0\\\xi\\0\end{bmatrix}, \quad \text{(C9d)}$$

$$\mathbf{G}_5(\tau,\xi)=\tau\mathbf{H}_1(\xi)+\mathbf{F}_1(\xi) \quad \text{(C10a)}$$

and

$$\mathbf{G}_6(\tau,\xi)=\tau\mathbf{H}_2(\xi)+\mathbf{F}_2(\xi). \quad \text{(C10b)}$$

Here

$$\mathbf{H}_1(\xi)=\begin{bmatrix}-1+c_1(\xi^2-1/2)\\c_1\\c_1(\xi^2-1/2)\\c_1\end{bmatrix} \quad \text{(C11a)}$$

and

$$\mathbf{H}_2(\xi)=\begin{bmatrix}c_2(\xi^2-1/2)\\c_2\\-1+c_2(\xi^2-1/2)\\c_2\end{bmatrix}, \quad \text{(C11b)}$$

with $c_1=n_1/n$ and $c_2=n_2/n$. In addition, and as discussed,[15] the vector-valued functions $\mathbf{F}_\beta(\xi)$ are solutions of the integral equations

$$\mathbf{F}_\beta(\xi)=-\xi\mathbf{\Sigma}^{-1}\mathbf{H}_\beta(\xi)+\int_{-\infty}^{\infty}\psi(\xi')\mathbf{K}(\xi',\xi)\mathbf{F}_\beta(\xi')d\xi' \quad \text{(C12)}$$

for $\beta=1,2$ and $\xi\in(-\infty,\infty)$. Previously[15] it was shown that $\mathbf{F}_\beta(\xi)$ could be expressed as

$$\mathbf{F}_\beta(\xi)=\xi\mathbf{U}_\beta+\xi(\xi^2-3/2)\mathbf{V}_\beta, \quad \text{(C13)}$$

where the constant vectors $\mathbf{U}_\beta$ and $\mathbf{V}_\beta$ are solutions of the (rank 8) linear systems defined by

$$(\mathbf{I}-\boldsymbol{\mathcal{A}})\mathbf{U}_1-\boldsymbol{\mathcal{C}}\mathbf{V}_1=[c_2/\sigma_1\ \ -c_1/\sigma_1\ \ -c_1/\sigma_2\ \ -c_1/\sigma_2]^T, \quad \text{(C14)}$$

$$(\mathbf{I}-\mathcal{D})\mathbf{V}_1-\mathcal{B}\mathbf{U}_1=[-c_1/\sigma_1\ 0\ -c_1/\sigma_2\ 0]^T, \tag{C15}$$

and

$$[0\ 0\ 1\ 0]\mathbf{U}_1=0, \tag{C16}$$

for $\beta=1$, and by

$$(\mathbf{I}-\mathcal{A})\mathbf{U}_2-\mathcal{C}\mathbf{V}_2=[-c_2/\sigma_1\ -c_2/\sigma_1\ c_1/\sigma_2\ -c_2/\sigma_2]^T, \tag{C17}$$

$$(\mathbf{I}-\mathcal{D})\mathbf{V}_2-\mathcal{B}\mathbf{U}_2=[-c_2/\sigma_1\ 0\ -c_2/\sigma_2\ 0]^T, \tag{C18}$$

and

$$[0\ 0\ 1\ 0]\mathbf{U}_2=0, \tag{C19}$$

for $\beta=2$. Here $\mathbf{I}$ is the identity matrix, and the superscript T is used to denote the transpose operation. In addition

$$\mathcal{A}=\begin{bmatrix} 1-\eta_{1,2}^{(1)} & -(1/2)\eta_{1,2}^{(2)} & r\eta_{1,2}^{(1)} & (r^3/2)\eta_{1,2}^{(2)} \\ -(1/2)\eta_{1,2}^{(2)} & (2/5)\beta_1 & (r/2)\eta_{1,2}^{(2)} & (2/5)\eta_{1,2}^{(6)} \\ s\eta_{2,1}^{(1)} & (s^3/2)\eta_{2,1}^{(2)} & 1-\eta_{2,1}^{(1)} & -(1/2)\eta_{2,1}^{(2)} \\ (s/2)\eta_{2,1}^{(2)} & (2/5)\eta_{2,1}^{(6)} & -(1/2)\eta_{2,1}^{(2)} & (2/5)\beta_2 \end{bmatrix}, \tag{C20}$$

$$\mathcal{B}=\begin{bmatrix} -(1/2)\eta_{1,2}^{(2)} & (2/5)\beta_1 & (r/2)\eta_{1,2}^{(2)} & (2/5)\eta_{1,2}^{(6)} \\ 0 & 0 & 0 & 0 \\ (s/2)\eta_{2,1}^{(2)} & (2/5)\eta_{2,1}^{(6)} & -(1/2)\eta_{2,1}^{(2)} & (2/5)\beta_2 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{C21}$$

$$\mathcal{C}=\begin{bmatrix} -(3/4)\eta_{1,2}^{(2)} & 0 & (3r^3/4)\eta_{1,2}^{(2)} & 0 \\ (3/5)\beta_1 & 0 & (3/5)\eta_{1,2}^{(6)} & 0 \\ (3s^3/4)\eta_{2,1}^{(2)} & 0 & -(3/4)\eta_{2,1}^{(2)} & 0 \\ (3/5)\eta_{2,1}^{(6)} & 0 & (3/5)\beta_2 & 0 \end{bmatrix}, \tag{C22}$$

and

$$\mathcal{D}=\begin{bmatrix} (3/5)\beta_1 & 0 & (3/5)\eta_{1,2}^{(6)} & 0 \\ 0 & 0 & 0 & 0 \\ (3/5)\eta_{2,1}^{(6)} & 0 & (3/5)\beta_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{C23}$$

[1] J. R. Thomas, Jr., T. S. Chang, and C. E. Siewert, "Heat transfer between parallel plates with arbitrary surface accommodation," Phys. Fluids **16**, 2116 (1973).

[2] T. Ohwada, K. Aoki, and Y. Sone, in *Rarefied Gas Dynamics: Theoretical and Computational Techniques*, edited by E. P. Muntz, D. P. Weaver, and D. H. Campbell (AIAA, Washington, 1989), p. 70.

[3] C. E. Siewert, "Heat transfer and evaporation/condensation problems based on the linearized Boltzmann equation," Eur. J. Mech. B/Fluids **22**, 391 (2003).

[4] S. Kosuge, K. Aoki, and S. Takata, in *Rarefied Gas Dynamics: 22nd International Symposium*, edited by T. J. Bartel and M. A. Gallis (AIP, Melville, 2001), p. 289.

[5] F. J. McCormack, "Construction of linearized kinetic models for gaseous mixtures and molecular gases," Phys. Fluids **16**, 2095 (1973).

[6] C. Cercignani, *Mathematical Methods in Kinetic Theory* (Plenum, New York, 1969).

[7] C. Cercignani, *Rarefied Gas Dynamics: From Basic Concepts to Actual Calculations* (Cambridge University Press, Cambridge, 2000).

[8] M. M. R. Williams, *Mathematical Methods in Particle Transport Theory* (Butterworth, London, 1971).

[9] J. H. Ferziger and H. G. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, 1972).

[10] F. Sharipov and V. Seleznev, "Data on internal rarefied gas flows," J. Phys. Chem. Ref. Data **27**, 657 (1998).

[11] M. M. R. Williams, "A review of the rarefied gas dynamics theory associated with some classical problems in flow and heat transfer," ZAMP **52**, 500 (2001).

[12] L. B. Barichello and C. E. Siewert, "A discrete-ordinates solution for a non-grey model with complete frequency redistribution," J. Quant. Spectrosc. Radiat. Transf. **62**, 665 (1999).

[13] C. E. Siewert and D. Valougeorgis, "Concise and accurate solutions to half-space binary-gas flow problems defined by the McCormack model and specular-diffuse wall conditions," Eur. J. Mech. B/Fluids (in press).

[14] C. E. Siewert and D. Valougeorgis, "The McCormack model: channel flow of a binary gas mixture driven by temperature, pressure and density gradients," Eur. J. Mech. B/Fluids **23**, 645 (2004).

[15] C. E. Siewert, "The McCormack model for gas mixtures: the temperature-jump problem," ZAMP (in press).

[16] F. Sharipov and D. Kalempa, "Velocity slip and temperature jump coefficients for gaseous mixtures. I. Viscous slip coefficient," Phys. Fluids **15**, 1800 (2003).

[17] C. E. Siewert, "A discrete-ordinates solution for heat transfer in a plane channel," J. Comput. Phys. **152**, 251 (1999).

[18] B. T. Smith, J. M. Boyle, J. J. Dongarra, B. S. Garbow, Y. Ikebe, V. C. Klema, and C. B. Moler, *Matrix Eigensystem Routines-EISPACK Guide* (Springer, Berlin, 1976).

[19] J. J. Dongarra, J. R. Bunch, C. B. Moler, and G. W. Stewart, *LINPACK Users' Guide* (SIAM, Philadelphia, 1979).

[20] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-uniform Gases* (Cambridge University Press, Cambridge, 1952).

[21] E. P. Gross and E. A. Jackson, "Kinetic models and the linearized Boltzmann equation," Phys. Fluids **2**, 432 (1959).

[22] S. Pan and T. S. Storvick, "Kinetic theory calculations of pressure effects of diffusion," J. Chem. Phys. **97**, 2671 (1992).