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Concise and accurate solutions to half-space binary-gas flow problems defined by the McCormack model and specular-diffuse wall conditions

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Abstract

An analytical version of the discrete-ordinates method (the ADO method) is used to establish concise and particularly accurate solutions to the viscous-slip and the half-space thermal-creep problems for a binary gas mixture. The kinetic equations used to describe the flow are based on the McCormack model for mixtures. In addition to a computation of the viscous-slip and thermal-slip coefficients, for the case of Maxwell boundary conditions for each of the two species, the velocity, heat-flow and shear-stress profiles are established for both types of particles. Numerical results are reported for three binary mixtures (Ne–Ar, He–Ar and He–Xe) with various molar concentrations. The complete solution requires only a (matrix) eigenvalue/eigenvector routine and the solution of a system of linear algebraic equations, and thus the algorithm is considered especially easy to use. The developed (FORTRAN) code requires typically less than 0.1 seconds on a 1.2 GHz Pentium-based PC to solve both problems.

1. Introduction

The study of slip phenomena in gas flows over plane boundaries is of major importance in gas dynamics, especially when the flow is in the transition or in the slip regimes [1,2]. In the transition regime the application of the Boltzmann equation (BE) or of kinetic model equations is necessary to describe the thermal creep and the mechanocaloric effects. In addition, in the slip regime the determination of the appropriate slip boundary conditions to be coupled with the hydrodynamic continuum equations should be obtained from the solution of kinetic type equations (BE or suitable models). The fundamental theoretical significance and the great practical importance of the slip coefficients easily justify the interest in this area of research. Most work in this regard has been focused on the case of a single gas [3–6]; however, the case of gas mixtures has also received some significant attention [7–12]. Efforts are now being made [13–18] to extend early work on gas mixtures in order to solve complicated binary gas problems in an efficient and accurate manner. This is achieved by adapting well-developed techniques for single-component gases to gas mixtures. The renewed interest in these problems is justified by the basic need of a thorough understanding of micro and mesoscale transport phenomena in mixtures due to an increasing number of technological applications [19,20].

One of the major difficulties in dealing with gas mixtures is the large number of parameters (concentration ratios, molecular masses and diameters, gas-surface accommodation coefficients, intermolecular laws and forces), which are involved in the

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calculations. Some of these parameters are deduced from modeling, while others are obtained from experimental data. Thus it is important to develop methodologies able to handle all these parameters with a modest computational effort. To deal with this kind of problem Ivchenko, Loyalka and Tompson [16,17] have developed general and convenient expressions for the slip coefficients of various binary gases. These authors compared their results with experimental work [21,22] and concluded that there was good agreement when the theoretical results are obtained through a second-order Chapman-Enskog approximation. Sharipov and Kalempa [14,15] have recently reported solutions of the velocity-slip and thermal-slip problems for three different gas mixtures based on the McCormack model equation [23]. Sharipov and Kalempa implemented the discrete-velocity method to solve the coupled equations, and they reported that they found good agreement with results [16,17] deduced from the Boltzmann equation. We consider that Sharipov and Kalempa [13–15] have demonstrated the merits of the McCormack kinetic model for describing binary gas flows.

During the last few years, an analytical version of the discrete-ordinates (ADO) method has been developed [24] and established as a simple, efficient and highly accurate methodology for solving problems in rarefied gas dynamics. A large number of a single-gas flow and thermal problems has been solved in a unified manner [25–27], while the method has also been used to solve [28,29] problems for mixtures described by the Hamel model [30]. In the present work the ADO method is used to solve the half-space viscous-slip (or the Kramers') and thermal-slip (or the half-space thermal-creep) binary-gas flow problems defined by the McCormack model, with specular-diffuse boundary conditions. Our objective here is to provide concise and accurate solutions (to the considered problems) that define what we consider to be a high standard of accuracy. In addition to defining good numerical results, these new solutions are valid for wall conditions described by a general specular-diffuse scattering law, and the solutions can be implemented at a computational cost much less, we believe, than the cost of evaluating basic quantities of interest with strictly numerical solutions. Finally, we note that our numerical results are reported on a species-specific basis so that various ways (that could depend on a specific application) of defining the velocity, heat-flow and shear-stress profiles for the binary mixture can be used. While we report, in this work, the viscous-slip and thermal-slip coefficients, we also establish velocity, heat-flow and shear-stress profiles.

2. 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 [23] published in 1973. While we use this model as defined in [23], we use an explicit notation that is appropriate to the analysis and computations we report here. We consider that the required functions $h_\alpha(x, \boldsymbol{v})$ for the two type of particles ($\alpha = 1$ and 2) denote perturbations from Maxwellian distributions for each species, i.e.,

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

where

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

Here k is the Boltzmann constant, m_α and n_α are the mass and the equilibrium density of the α-th species, x is the spatial variable (measured, for example, in cm), $\boldsymbol{v}$, 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 [23] that the perturbations satisfy (for the case of variations in only one spatial variable) the coupled equations

$$c_x \frac{\partial}{\partial x} h_\alpha(x, \boldsymbol{c}) + \omega_\alpha \gamma_\alpha h_\alpha(x, \boldsymbol{c}) = \omega_\alpha \gamma_\alpha \mathcal{L}_\alpha\{h_1, h_2\}(x, \boldsymbol{c}), \quad \alpha = 1, 2, \tag{3}$$

where the vector $\boldsymbol{c}$, with components $c_x,\ c_y,\ c_z$ and magnitude c, is a dimensionless variable,

$$\omega_\alpha = \left[\frac{m_\alpha}{2kT_0}\right]^{1/2}, \tag{4}$$

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

$$\mathcal{L}_\alpha\{h_1, h_2\}(x, \boldsymbol{c}) = \frac{1}{\pi^{3/2}} \sum_{\beta=1}^{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-c'^2} h_\beta(x, \boldsymbol{c}') K_{\beta,\alpha}(\boldsymbol{c}', \boldsymbol{c})\, \mathrm{d}c'_x\, \mathrm{d}c'_y\, \mathrm{d}c'_z, \tag{5}$$

where the kernels $K_{\beta,\alpha}(\boldsymbol{c}', \boldsymbol{c})$ are listed explicitly in Appendix A of this paper. We note that in obtaining Eq. (3) from the form given by McCormack [23], we have introduced the dimensionless vector $\boldsymbol{c}$ differently in the two equations, i.e., for the case $\alpha = 1$ we used the transformation $\boldsymbol{c} = \omega_1 \boldsymbol{v}$, whereas for the case $\alpha = 2$ we used the transformation $\boldsymbol{c} = \omega_2 \boldsymbol{v}$. It can be noted that

by changing the independent variable $\boldsymbol{v}$ differently in the two balance equations, we arrive at the convenient form displayed in Eq. (3). As we wish to work with a dimensionless spatial variable, we introduce

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

where

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

is the mean-free path (based on viscosity) introduced by Sharipov and Kalempa [14]. Here, following [14], we write

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

where

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

Continuing to follow [14], we express the viscosity of the mixture in terms of the partial pressures P_α and the collision frequencies γ_α as

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

where

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

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

and

$$\gamma_2 = \left[\Psi_1\Psi_2 - \nu_{1,2}^{(4)}\nu_{2,1}^{(4)}\right]\left[\Psi_1 + \nu_{2,1}^{(4)}\right]^{-1}. \tag{12b}$$

Here definitions given in Appendix A have been used,

$$\Psi_1 = \nu_{1,1}^{(3)} + \nu_{1,2}^{(3)} - \nu_{1,1}^{(4)} \tag{13a}$$

and

$$\Psi_2 = \nu_{2,2}^{(3)} + \nu_{2,1}^{(3)} - \nu_{2,2}^{(4)}. \tag{13b}$$

Finally, to compact our notation we introduce

$$\sigma_\alpha = \gamma_\alpha \omega_\alpha l_0 \tag{14}$$

or, more explicitly,

$$\sigma_\alpha = \gamma_\alpha \frac{n_1/\gamma_1 + n_2/\gamma_2}{n_1 + n_2}\left(\frac{m_\alpha}{m}\right)^{1/2}, \tag{15}$$

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

$$c_x \frac{\partial}{\partial \tau} h_\alpha(\tau, \boldsymbol{c}) + \sigma_\alpha h_\alpha(\tau, \boldsymbol{c}) = \sigma_\alpha \mathcal{L}_\alpha\{h_1, h_2\}(\tau, \boldsymbol{c}). \tag{16}$$

In this work we consider the viscous-slip and thermal-slip problems, and so we will seek solutions of Eqs. (16) that are valid for all $\tau > 0$, and we use Maxwell boundary conditions at the wall, viz.,

$$h_\alpha(0, c_x, c_y, c_z) = (1 - a_\alpha) h_\alpha(0, -c_x, c_y, c_z) + a_\alpha \mathcal{I}\{h_\alpha\}(0), \tag{17}$$

for $c_x > 0$ and all c_y and c_z. Note that

$$h_\alpha(\tau, \boldsymbol{c}) \Leftrightarrow h_\alpha(\tau, c_x, c_y, c_z) \tag{18}$$

and that we use a_1 and a_2 to denote the two accommodation coefficients. In addition, we have used

$$\mathcal{I}\{h_\alpha\}(\tau) = \frac{2}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \mathrm{e}^{-c'^2} h_\alpha(\tau, -c'_x, c'_y, c'_z) c'_x \,\mathrm{d}c'_x \,\mathrm{d}c'_y \,\mathrm{d}c'_z \tag{19}$$

to denote the diffuse term in Eq. (17). In this work, we consider half-space problems, and so we must, in addition to the boundary condition listed as Eq. (17), specify some conditions on the desired solutions as τ tends to infinity. This point will be addressed later in this work when the two specific problems of interest are discussed in detail.

Here we seek to compute the velocity profiles

$$u_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2} h_\alpha(\tau, \boldsymbol{c}) c_z \,\mathrm{d}c_x \,\mathrm{d}c_y \,\mathrm{d}c_z, \tag{20a}$$

the shear-stress profiles

$$p_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2} h_\alpha(\tau, \boldsymbol{c}) c_x c_z \,\mathrm{d}c_x \,\mathrm{d}c_y \,\mathrm{d}c_z \tag{20b}$$

and the heat-flow profiles

$$q_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2} h_\alpha(\tau, \boldsymbol{c})(c^2 - 5/2) c_z \,\mathrm{d}c_x \,\mathrm{d}c_y \,\mathrm{d}c_z, \tag{20c}$$

and so we can obtain these quantities from "moments" of Eq. (16). To this end, we first multiply Eq. (16) by

$$\phi_1(c_y, c_z) = \frac{1}{\pi}\,\mathrm{e}^{-(c_y^2 + c_z^2)} c_z \tag{21}$$

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

$$\phi_2(c_y, c_z) = \frac{1}{\pi}\,\mathrm{e}^{-(c_y^2 + c_z^2)}\big(c_y^2 + c_z^2 - 2\big) c_z. \tag{22}$$

Defining

$$g_{2\alpha-1}(\tau, c_x) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_1(c_y, c_z) h_\alpha(\tau, \boldsymbol{c}) \,\mathrm{d}c_y \,\mathrm{d}c_z \tag{23a}$$

and

$$g_{2\alpha}(\tau, c_x) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_2(c_y, c_z) h_\alpha(\tau, \boldsymbol{c}) \,\mathrm{d}c_y \,\mathrm{d}c_z, \tag{23b}$$

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

$$\xi \frac{\partial}{\partial \tau}\boldsymbol{G}(\tau, \xi) + \boldsymbol{\Sigma}\boldsymbol{G}(\tau, \xi) = \boldsymbol{\Sigma}\int_{-\infty}^{\infty} \psi(\xi')\boldsymbol{K}(\xi', \xi)\boldsymbol{G}(\tau, \xi') \,\mathrm{d}\xi', \tag{24}$$

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

$$\boldsymbol{\Sigma} = \mathrm{diag}\{\sigma_1, \sigma_1, \sigma_2, \sigma_2\} \tag{25}$$

and

$$\psi(\xi) = \pi^{-1/2}\,\mathrm{e}^{-\xi^2}. \tag{26}$$

In addition, the components $k_{i,j}(\xi', \xi)$ of the kernel $\boldsymbol{K}(\xi', \xi)$ are as listed in Appendix B of this work.

So, if we can solve Eq. (24) we can compute the quantities of interest from

$$u_\alpha(\tau) = \int_{-\infty}^{\infty} \psi(\xi) g_{2\alpha-1}(\tau,\xi)\,\mathrm{d}\xi, \tag{27a}$$

$$p_\alpha(\tau) = \int_{-\infty}^{\infty} \psi(\xi) g_{2\alpha-1}(\tau,\xi)\xi\,\mathrm{d}\xi \tag{27b}$$

and

$$q_\alpha(\tau) = \int_{-\infty}^{\infty} \psi(\xi)\left[\left(\xi^2 - \frac{1}{2}\right) g_{2\alpha-1}(\tau,\xi) + g_{2\alpha}(\tau,\xi)\right]\mathrm{d}\xi. \tag{27c}$$

To complete this section, we project Eq. (17) against $\phi_1(c_y, c_z)$ and $\phi_2(c_y, c_z)$ to find the boundary condition

$$\boldsymbol{G}(0,\xi) - \boldsymbol{S}\boldsymbol{G}(0,-\xi) = \boldsymbol{0}, \quad \xi \in (0,\infty), \tag{28}$$

subject to which we must solve Eq. (24). Here

$$\boldsymbol{S} = \mathrm{diag}\{1-a_1, 1-a_1, 1-a_2, 1-a_2\}. \tag{29}$$

In addition to the boundary condition listed as Eq. (28), a condition, for each of the two considered problems, on $\boldsymbol{G}(\tau,\xi)$ as τ tends to infinity must also be specified. This will be done later in this work.

3. The elementary solutions

As we intend to find a particular solution if an inhomogeneous source term $\boldsymbol{S}(\xi)$ is added to Eq. (24), we now proceed to establish (in terms of the ADO method) the elementary solutions of

$$\xi\frac{\partial}{\partial\tau}\boldsymbol{G}(\tau,\xi) + \boldsymbol{\Sigma}\boldsymbol{G}(\tau,\xi) = \boldsymbol{\Sigma}\int_{-\infty}^{\infty} \psi(\xi')\boldsymbol{K}(\xi',\xi)\boldsymbol{G}(\tau,\xi')\,\mathrm{d}\xi'. \tag{30}$$

We seek solutions of Eq. (30) of the form

$$\boldsymbol{G}(\tau,\xi) = \boldsymbol{\Phi}(\nu,\xi)\,\mathrm{e}^{-\tau/\nu}, \tag{31}$$

where the separation constants ν and the elementary solutions $\boldsymbol{\Phi}(\nu,\xi)$ are to be determined. Substituting Eq. (31) into Eq. (30), we find

$$(\nu\boldsymbol{\Sigma} - \xi\boldsymbol{I})\boldsymbol{\Phi}(\nu,\xi) = \nu\boldsymbol{\Sigma}\int_0^{\infty} \psi(\xi')\big[\boldsymbol{K}(\xi',\xi)\boldsymbol{\Phi}(\nu,\xi') + \boldsymbol{K}(-\xi',\xi)\boldsymbol{\Phi}(\nu,-\xi')\big]\mathrm{d}\xi' \tag{32a}$$

and

$$(\nu\boldsymbol{\Sigma} + \xi\boldsymbol{I})\boldsymbol{\Phi}(\nu,-\xi) = \nu\boldsymbol{\Sigma}\int_0^{\infty} \psi(\xi')\big[\boldsymbol{K}(\xi',-\xi)\boldsymbol{\Phi}(\nu,\xi') + \boldsymbol{K}(-\xi',-\xi)\boldsymbol{\Phi}(\nu,-\xi')\big]\mathrm{d}\xi' \tag{32b}$$

from which we conclude, since

$$\boldsymbol{K}(\xi',-\xi) = \boldsymbol{K}(-\xi',\xi), \tag{33}$$

that

$$\boldsymbol{\Phi}(\nu,\xi) = \boldsymbol{\Phi}(-\nu,-\xi). \tag{34}$$

Now, adding and subtracting Eqs. (32), one from the other, we find that

$$\frac{1}{\xi^2}\left[\boldsymbol{\Sigma}^2\boldsymbol{V}(\nu,\xi) - \int_0^{\infty} \psi(\xi')\boldsymbol{\mathcal{K}}(\xi',\xi)\boldsymbol{V}(\nu,\xi')\,\mathrm{d}\xi'\right] = \lambda\boldsymbol{V}(\nu,\xi) \tag{35a}$$

and

$$\boldsymbol{U}(\nu,\xi)=\frac{\nu}{\xi}\boldsymbol{\Sigma}\left[\boldsymbol{V}(\nu,\xi)-\int_0^\infty \psi(\xi')\boldsymbol{K}_-(\xi',\xi)\boldsymbol{V}(\nu,\xi')\,\mathrm{d}\xi'\right], \tag{35b}$$

where

$$\boldsymbol{U}(\nu,\xi)=\boldsymbol{\Phi}(\nu,\xi)+\boldsymbol{\Phi}(\nu,-\xi) \tag{36a}$$

and

$$\boldsymbol{V}(\nu,\xi)=\boldsymbol{\Phi}(\nu,\xi)-\boldsymbol{\Phi}(\nu,-\xi). \tag{36b}$$

Here

$$\lambda=\frac{1}{\nu^2}, \tag{37}$$

$$\boldsymbol{K}_+(\xi',\xi)=\boldsymbol{K}(\xi',\xi)+\boldsymbol{K}(-\xi',\xi), \tag{38a}$$

$$\boldsymbol{K}_-(\xi',\xi)=\boldsymbol{K}(\xi',\xi)-\boldsymbol{K}(-\xi',\xi) \tag{38b}$$

and

$$\boldsymbol{\mathcal{K}}(\xi',\xi)=\frac{\xi}{\xi'}\boldsymbol{\Sigma}\boldsymbol{K}_+(\xi',\xi)\boldsymbol{\Sigma}+\boldsymbol{\Sigma}^2\boldsymbol{K}_-(\xi',\xi)-\int_0^\infty \psi(\xi'')\frac{\xi}{\xi''}\boldsymbol{\Sigma}\boldsymbol{K}_+(\xi'',\xi)\boldsymbol{\Sigma}\boldsymbol{K}_-(\xi',\xi'')\,\mathrm{d}\xi''. \tag{39}$$

We now introduce a "half-range" quadrature scheme (with weights and nodes, w_k and ξ_k) and rewrite Eqs. (35) evaluated at the quadrature points as

$$\frac{1}{\xi_i^2}\left[\boldsymbol{\Sigma}^2\boldsymbol{V}(\nu_j,\xi_i)-\sum_{k=1}^{N} w_k\psi(\xi_k)\boldsymbol{\mathcal{K}}(\xi_k,\xi_i)\boldsymbol{V}(\nu_j,\xi_k)\right]=\lambda_j\boldsymbol{V}(\nu_j,\xi_i) \tag{40}$$

and

$$\boldsymbol{U}(\nu_j,\xi_i)=\frac{\nu_j}{\xi_i}\boldsymbol{\Sigma}\left[\boldsymbol{V}(\nu_j,\xi_i)-\sum_{k=1}^{N} w_k\psi(\xi_k)\boldsymbol{K}_-(\xi_k,\xi_i)\boldsymbol{V}(\nu_j,\xi_k)\right], \tag{41}$$

for $i=1,2,\ldots,N$. Eq. (40) defines our eigenvalue problem, to which we have added the subscript j to label the eigenvalues and eigenvectors. Once this eigenvalue problem is solved, we have the elementary solutions from

$$\boldsymbol{\Phi}(\nu_j,\xi_i)=\frac{1}{2}\big[\boldsymbol{U}(\nu_j,\xi_i)+\boldsymbol{V}(\nu_j,\xi_i)\big] \tag{42a}$$

and

$$\boldsymbol{\Phi}(\nu_j,-\xi_i)=\frac{1}{2}\big[\boldsymbol{U}(\nu_j,\xi_i)-\boldsymbol{V}(\nu_j,\xi_i)\big]. \tag{42b}$$

Note that the separation constants defined by

$$\nu_j=\pm\lambda_j^{-1/2} \tag{43}$$

occur in $\pm$ pairs. From this point, we take ν_j to be the positive root listed in Eq. (43). Once we have solved the eigenvalue problem defined by Eq. (40), we can write our general (discrete ordinates) solution to Eq. (30) as

$$\boldsymbol{G}(\tau,\pm\xi_i)=\sum_{j=1}^{4N}\big[A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\,\mathrm{e}^{-\tau/\nu_j}+B_j\boldsymbol{\Phi}(\nu_j,\mp\xi_i)\,\mathrm{e}^{\tau/\nu_j}\big], \tag{44}$$

for $i=1,2,\ldots,N$. Here the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the boundary conditions of a specific problem. Before proceeding to develop our solutions to the viscous-slip and the thermal-slip problems, we make one modification to Eq. (44). While we could use the solution as given by Eq. (44), we can also improve it. We have found that the eigenvalue problem yields one separation constant, say ν_1, that approximates the one expected unbounded separation constant. And so, instead of using what we see as an approximate solution that corresponds to ν_1 in Eq. (44), we replace the contribution

from ν_1 with the exact solution we would expect if the approximation parameter N were unbounded. In this way, we replace one (the least accurate) approximate solution with an exact solution that allows us to capture the correct asymptotic form,

$$\boldsymbol{G}(\tau,\pm\xi_i) = A\boldsymbol{G}_+ + B\boldsymbol{G}_-(\tau,\pm\xi_i) + \sum_{j=2}^{4N}\left[A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\,\mathrm{e}^{-\tau/\nu_j} + B_j\boldsymbol{\Phi}(\nu_j,\mp\xi_i)\,\mathrm{e}^{\tau/\nu_j}\right], \tag{45}$$

for $i = 1, 2, \ldots, N$. Here

$$\boldsymbol{G}_+ = \begin{bmatrix} 1 \\ 0 \\ s \\ 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{G}_-(\tau,\xi) = \begin{bmatrix} \sigma_1\tau - \xi \\ 0 \\ s\sigma_1(\tau - \xi/\sigma_2) \\ 0 \end{bmatrix} \tag{46a,b}$$

are two exact solutions of Eq. (30). In the work, we use

$$r = \left(\frac{m_1}{m_2}\right)^{1/2} \quad \text{and} \quad s = \left(\frac{m_2}{m_1}\right)^{1/2} \tag{47a,b}$$

in order to compact our notation.

4. The problems

Having developed our elementary solutions of Eq. (30), we are now ready to use them to solve the two specific problems basic to our current study. First, however, we note that while Eqs. (20) define the species-specific quantities $u_\alpha(\tau)$, $p_\alpha(\tau)$ and $q_\alpha(\tau)$, for $\alpha = 1, 2$, the way to define the basic elements for a binary gas mixture is not so clear. Here we follow other works [13–18] and define these basic elements as

$$u(\tau) = \varphi_{u,1}u_1(\tau) + \varphi_{u,2}u_2(\tau), \tag{48a}$$

$$p(\tau) = \varphi_{p,1}p_1(\tau) + \varphi_{p,2}p_2(\tau) \tag{48b}$$

and

$$q(\tau) = \varphi_{q,1}q_1(\tau) + \varphi_{q,2}q_2(\tau), \tag{48c}$$

where the "adaptation coefficients" $\varphi_{i,\alpha}$, $i = u, p, q$, $\alpha = 1, 2$, are to be specified. Since these factors have been defined in several ways in other works [13–18], and since the choice of these factors could conveniently be made differently for different applications of the theory, we develop our solution and report our numerical results without specifying these factors.

4.1. The viscous-slip problem

The viscous-slip problem (also known as Kramers' problem) has no driving (inhomogeneous) term in Eq. (24), and so our solution can be constructed from Eq. (45). Since there is no explicit driving term for this problem, the solution is required to diverge as τ tends to infinity, but at the same time the bulk velocity of the mixture should satisfy

$$\lim_{\tau\to\infty}\frac{\mathrm{d}}{\mathrm{d}\tau}u(\tau) = k_p, \tag{49}$$

where k_p is a normalization constant that depends on the choice of adaptation factors to be used. The condition listed as Eq. (49) requires us to take $B_j = 0$ in Eq. (45), and in order to accommodate all choices of adaptation factors to be used, we first normalize our solution by taking

$$B = \frac{1}{\sigma_1}. \tag{50}$$

It follows that the constants A and A_j can be obtained from the system of linear algebraic equations we find when

$$\boldsymbol{G}(\tau,\pm\xi_i) = A\boldsymbol{G}_+ + \frac{1}{\sigma_1}\boldsymbol{G}_-(\tau,\pm\xi_i) + \sum_{j=2}^{4N}A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\,\mathrm{e}^{-\tau/\nu_j} \tag{51}$$

is substituted into a discrete-ordinates version of Eq. (28) evaluated at the N quadrature points ξ_i. Once these constants are established we can use Eqs. (27) and express our final results as

$$u_1(\tau) = A + \tau + \sum_{j=2}^{4N} A_j N_{u,1}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{52a}$$

$$u_2(\tau) = s(A + \tau) + \sum_{j=2}^{4N} A_j N_{u,2}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{52b}$$

$$p_1(\tau) = -\frac{1}{2} + \sum_{j=2}^{4N} A_j N_{p,1}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{52c}$$

$$p_2(\tau) = -\frac{1}{2}\frac{s\sigma_1}{\sigma_2} + \sum_{j=2}^{4N} A_j N_{p,2}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j} \tag{52d}$$

and

$$q_\alpha(\tau) = \sum_{j=2}^{4N} A_j N_{q,\alpha}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}. \tag{52e}$$

If we use $u_{\mathrm{asy}}(\tau)$ to denote the asymptotic part (the part that excludes the exponential factors) of $u(\tau)$ then

$$u_{1,\mathrm{asy}}(\tau) = A + \tau \tag{53a}$$

and

$$u_{2,\mathrm{asy}}(\tau) = s(A + \tau), \tag{53b}$$

where Eq. (47b) has been noted. And so using the definition

$$\zeta_P = \frac{u_{\mathrm{asy}}(0)}{u'_{\mathrm{asy}}(0)}, \tag{54}$$

we see that

$$\zeta_P = A \tag{55}$$

is the viscous slip coefficient for the bulk velocity of the mixture defined by Eq. (48a) for any choice of the adaptation factors. To complete Eqs. (52), we find

$$N_{u,\alpha}(\nu_j) = \boldsymbol{F}_\alpha^{\mathrm{T}} \sum_{k=1}^{N} w_k \psi(\xi_k) \big[\boldsymbol{\Phi}(\nu_j, \xi_k) + \boldsymbol{\Phi}(\nu_j, -\xi_k)\big], \tag{56a}$$

$$N_{p,\alpha}(\nu_j) = \boldsymbol{F}_\alpha^{\mathrm{T}} \sum_{k=1}^{N} w_k \psi(\xi_k) \xi_k \big[\boldsymbol{\Phi}(\nu_j, \xi_k) - \boldsymbol{\Phi}(\nu_j, -\xi_k)\big] \tag{56b}$$

and

$$N_{q,\alpha}(\nu_j) = \sum_{k=1}^{N} w_k \psi(\xi_k) \boldsymbol{F}_{q,\alpha}^{\mathrm{T}}(\xi_k) \big[\boldsymbol{\Phi}(\nu_j, \xi_k) + \boldsymbol{\Phi}(\nu_j, -\xi_k)\big], \tag{56c}$$

where we use the superscript T to denote the transpose operation and where

$$\boldsymbol{F}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{F}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \boldsymbol{F}_{q,1}(\xi) = \begin{bmatrix} \xi^2 - 1/2 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{F}_{q,2}(\xi) = \begin{bmatrix} 0 \\ 0 \\ \xi^2 - 1/2 \\ 1 \end{bmatrix}. \tag{57a–d}$$

While we have introduced the (arbitrary) normalization listed in Eq. (50), the bulk velocity

$$u(\tau) = k_P \frac{\varphi_{u,1} u_1(\tau) + \varphi_{u,2} u_2(\tau)}{\varphi_{u,1} + s\varphi_{u,2}} \tag{58}$$

will satisfy Eq. (49) for any choice of the adaptation factors.

In regard to our numerical work, we report in a following section of this work, the viscous-slip coefficient ζ_P and the species-specific profiles $u_\alpha(\tau)$ and $q_\alpha(\tau)$ for selected sets of data. In this way results are available for any choice of the adaptation factors $\varphi_{i,\alpha}$. Having completed our solution to the viscous-slip problem, we look now at the second of the two problems solved in this work.

4.2. The half-space thermal creep problem

In regard to the case of thermal creep, the flow is caused by a constant temperature gradient in the direction (z: parallel to the wall) of the flow, and so it is helpful to linearize the particle velocity distribution functions about a local Maxwellian, rather than an absolute Maxwellian as was done in Eq. (1). We thus write

$$f_\alpha(\tau,\eta,\boldsymbol{c}) = f_{\alpha,0}(c)\left\{1+\eta\left[\left(c^2-\frac{3}{2}\right)K_\eta + R_\eta\right] + h_\alpha(\tau,\boldsymbol{c})\right\}, \tag{59}$$

where $\eta = z/l_0$, K_η and R_η are the (non-dimensional) temperature and density gradients in the η direction and

$$f_{\alpha,0}(c) = n_\alpha\left(\frac{\lambda_\alpha}{\pi}\right)^{3/2} \mathrm{e}^{-c^2}, \quad \lambda_\alpha = \frac{m_\alpha}{2kT_0}. \tag{60}$$

For the problem of thermal creep we take $R_\eta = -K_\eta$, and then let $k_T = K_\eta$ so that Eq. (59) becomes

$$f_\alpha(\tau,\eta,\boldsymbol{c}) = f_{\alpha,0}(c)\left[1+\eta\left(c^2-\frac{5}{2}\right)k_T + h_\alpha(\tau,\boldsymbol{c})\right]. \tag{61}$$

As a result of this linearizion, an inhomogeneous source

$$\boldsymbol{S}(\xi) = k_T\begin{bmatrix}(1/2)(\xi^2-1/2)\\ 1\\ (1/2)(\xi^2-1/2)\\ 1\end{bmatrix} \tag{62}$$

must now be added to Eq. (24) to yield

$$\boldsymbol{S}(\xi) + \xi\frac{\partial}{\partial\tau}\boldsymbol{G}(\tau,\xi) + \boldsymbol{\Sigma}\boldsymbol{G}(\tau,\xi) = \boldsymbol{\Sigma}\int_{-\infty}^{\infty}\psi(\xi')\boldsymbol{K}(\xi',\xi)\boldsymbol{G}(\tau,\xi')\,\mathrm{d}\xi'. \tag{63}$$

Since we have linearized about a local Maxwellian, we now require our solution to Eq. (63) to be bounded as τ tends to infinity, and so we write our (discrete ordinates) solution as

$$\boldsymbol{G}(\tau,\pm\xi_i) = \boldsymbol{G}_p(\tau,\pm\xi_i) + A\boldsymbol{G}_+ + \sum_{j=2}^{4N} A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\,\mathrm{e}^{-\tau/\nu_j}, \tag{64}$$

where $\boldsymbol{G}_p(\tau,\xi)$ is a particular solution that corresponds to the inhomogeneous driving term $\boldsymbol{S}(\xi)$. We impose the (arbitrary) normalization $k_T = 1$ and find that we can write

$$\boldsymbol{G}_p(\tau,\xi) = \begin{bmatrix}E(\xi^2-1/2-sw)\\ 2E\\ F(\xi^2-1/2-rw)\\ 2F\end{bmatrix}, \tag{65}$$

where we have again used Eqs. (47). After we note definitions given in Appendix A, we can write

$$w = \frac{5}{4}r\frac{\nu_{1,2}^{(2)}}{\nu_{1,2}^{(1)}}. \tag{66}$$

In addition, the two constants E and F required in Eq. (65) are defined by a system of linear algebraic equations which we write as

$$\boldsymbol{N}\begin{bmatrix}E\\F\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1/\sigma_1\\1/\sigma_2\end{bmatrix}, \tag{67}$$

where the elements of $\boldsymbol{N}$ are given by

$$n_{1,1} = -\Phi_1 + \frac{5}{8}\frac{[\eta_{1,2}^{(2)}]^2}{\eta_{1,2}^{(1)}}, \tag{68a}$$

$$n_{1,2} = \eta_{1,2}^{(6)} - \frac{5}{8}r^3\frac{[\eta_{1,2}^{(2)}]^2}{\eta_{1,2}^{(1)}}, \tag{68b}$$

$$n_{2,1} = \eta_{2,1}^{(6)} - \frac{5}{8} s^3 \frac{[\eta_{2,1}^{(2)}]^2}{\eta_{2,1}^{(1)}} \tag{68c}$$

and

$$n_{2,2} = -\Phi_2 + \frac{5}{8} \frac{[\eta_{2,1}^{(2)}]^2}{\eta_{2,1}^{(1)}}, \tag{68d}$$

with

$$\Phi_1 = \eta_{1,1}^{(5)} + \eta_{1,2}^{(5)} - \eta_{1,1}^{(6)} \tag{69a}$$

and

$$\Phi_2 = \eta_{2,2}^{(5)} + \eta_{2,1}^{(5)} - \eta_{2,2}^{(6)}. \tag{69b}$$

At this point we can substitute Eq. (64) into a discrete-ordinates version of the boundary condition listed as Eq. (28) to define a system of linear algebraic equations. After solving the set of algebraic equations for the constants A and $\{A_j\}$, we can write our final results for the half-space thermal-creep problem as

$$u_1(\tau) = A - swE + \sum_{j=2}^{4N} A_j N_{u,1}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{70a}$$

$$u_2(\tau) = sA - rwF + \sum_{j=2}^{4N} A_j N_{u,2}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{70b}$$

$$p_\alpha(\tau) = \sum_{j=2}^{4N} A_j N_{p,\alpha}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{70c}$$

$$q_1(\tau) = \frac{5}{2} E + \sum_{j=2}^{4N} A_j N_{q,1}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j} \tag{70d}$$

and

$$q_2(\tau) = \frac{5}{2} F + \sum_{j=2}^{4N} A_j N_{q,2}(\nu_j)\, \mathrm{e}^{-\tau/\nu_j}, \tag{70e}$$

where we continue to use the definitions given by Eqs. (56). Considering that the thermal-slip coefficient for the mixture is given by

$$\zeta_T = \lim_{\tau\to\infty} u(\tau), \tag{71}$$

we can write

$$\zeta_T = (\varphi_{u,1} + s\varphi_{u,2})A - w(s\varphi_{u,1}E + r\varphi_{u,2}F). \tag{72}$$

In contrast to the viscous-slip problem, we see that here the slip coefficient depends on the factors $\varphi_{u,1}$ and $\varphi_{u,2}$, and so for this reason we intend to report

$$\zeta_1 = u_1(\infty) = A - swE \tag{73a}$$

and

$$\zeta_2 = u_2(\infty) = sA - rwF \tag{73b}$$

as well as species-specific profiles $u_\alpha(\tau)$ and $q_\alpha(\tau)$ for selected sets of data. It follows that once adaptation factors are specified, the thermal-slip coefficient for the mixture can be evaluated from

$$\zeta_T = \varphi_{u,1}\zeta_1 + \varphi_{u,2}\zeta_2. \tag{74}$$

As our solutions are complete, we continue with an implementation of the algorithms defined here to establish numerical results with what we consider to be a very good standard of accuracy.

5. Numerical results

The first thing to note in regard to our numerical work is the way we defined the quadrature scheme for the analytical discrete-ordinates method used in this work. To keep matters simple, we used the transformation

$$v(\xi) = \mathrm{e}^{-\xi} \tag{75}$$

to map $\xi \in [0, \infty)$ onto $v \in [0, 1]$, and we then used the Gauss–Legendre scheme mapped (linearly) onto the interval $[0, 1]$. In order to evaluate the merits of the solutions developed here for the half-space viscous-slip and thermal-creep problems, we have elected to use the three data cases defined by Sharipov and Kalempa [14]. These three data cases refer to a mixture of the species: (i) Ne–Ar, (ii) He–Ar and (iii) He–Xe. As we are reporting numerical work only for the case of rigid-sphere interactions, we can see that the McCormack model requires, for this case, only three ratios: the mass ratio (m_1/m_2), the diameter ratio (d_1/d_2) and the density ratio (n_1/n_2). In addition, by formulating the McCormack model in terms of a convenient mean-free path and by observing the ratios of parameters that result, we can see that the constant factor $(\pi k T_0/32)^{1/2}$ in Eq. (A.35) of Appendix A need not be specified.

For the sake of our computations we consider that the data

$$m_2 = 39.948, \quad m_1 = 20.183, \quad \frac{d_2}{d_1} = 1.406 \quad \text{(Ne–Ar mixture)},$$

$$m_2 = 39.948, \quad m_1 = 4.0026, \quad \frac{d_2}{d_1} = 1.665 \quad \text{(He–Ar mixture)},$$

and

$$m_2 = 131.30, \quad m_1 = 4.0026, \quad \frac{d_2}{d_1} = 2.226 \quad \text{(He–Xe mixture)}$$

are exact. We follow Sharipov and Kalempa [14] and tabulate our results for these three cases in terms of the molar concentration defined (in terms of the first particle) as

$$C = \frac{n_1/n_2}{1 + n_1/n_2}. \tag{76}$$

In Tables 1–3 we list some typical results for the viscous-slip problem, and similar results for half-space thermal-creep problem are listed in Tables 4–7. Although we have computed all the basic quantities $u_\alpha(\tau)$, $q_\alpha(\tau)$ and $p_\alpha(\tau)$, we have (for economy of space) omitted $p_\alpha(\tau)$ from our tabulations, and we report results only for two choices of the accommodation coefficients.

While we have no definitive proof of the accuracy of our results, we believe the results listed in our tables are correct (within the context of the kinetic model used) to all digits given. To establish some confidence in our numerical results, we found stability in the results as we varied the only approximation parameter N from 20 to 100 and we obtained identical results from two independently implemented numerical codes: one based on MATLAB and the other on FORTRAN. In addition, we have also used the identity

$$\frac{n_1}{n} p_1'(\tau) + \frac{n_2}{n} p_2'(\tau) = 0, \tag{77}$$

Table 1
The viscous-slip coefficient

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
	$a_1 = 1.0$ $a_2 = 1.0$	$a_1 = 0.3$ $a_2 = 0.6$	$a_1 = 1.0$ $a_2 = 1.0$	$a_1 = 0.3$ $a_2 = 0.6$	$a_1 = 1.0$ $a_2 = 1.0$	$a_1 = 0.3$ $a_2 = 0.6$
C			ζ_P			
0.0	1.01837	2.26010	1.01837	2.26010	1.01837	2.26010
0.1	1.02446	2.40900	1.04375	2.37943	1.05671	2.38333
0.2	1.02980	2.57378	1.07010	2.51563	1.09891	2.52599
0.3	1.03424	2.75760	1.09715	2.67285	1.14546	2.69340
0.4	1.03759	2.96460	1.12434	2.85672	1.19678	2.89311
0.5	1.03963	3.20041	1.15059	3.07526	1.25300	3.13622
0.6	1.04008	3.47283	1.17386	3.34006	1.31339	3.43976
0.7	1.03862	3.79302	1.19002	3.66856	1.37452	3.83100
0.8	1.03486	4.17770	1.19034	4.08692	1.42417	4.35455
0.9	1.02831	4.65301	1.15387	4.62895	1.41346	5.06330
1.0	1.01837	5.26255	1.01837	5.26255	1.01837	5.26255

Table 2
The viscous-slip problem: velocity profiles for each species for the case $a_1 = 1.0$, $a_2 = 1.0$ and $C = 0.5$

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
τ	$u_1(\tau)$	$u_2(\tau)$	$u_1(\tau)$	$u_2(\tau)$	$u_1(\tau)$	$u_2(\tau)$
0.0	7.55303(−1)	9.64122(−1)	8.46368(−1)	2.46223	9.68271(−1)	4.83343
0.1	9.25139(−1)	1.22950	1.01778	3.05860	1.13443	5.92751
0.2	1.05946	1.43216	1.15358	3.51600	1.26763	6.76873
0.3	1.18367	1.61666	1.27907	3.93269	1.39123	7.53506
0.4	1.30233	1.79106	1.39884	4.32666	1.50949	8.25931
0.5	1.41738	1.95887	1.51487	4.70573	1.62428	8.95576
0.6	1.52989	2.12199	1.62824	5.07417	1.73660	9.63227
0.7	1.64049	2.28160	1.73962	5.43462	1.84708	1.02937(1)
0.8	1.74962	2.43848	1.84944	5.78883	1.95611	1.09433(1)
0.9	1.85756	2.59319	1.95802	6.13805	2.06400	1.15833(1)
1.0	1.96453	2.74612	2.06558	6.48319	2.17095	1.22156(1)
2.0	3.00483	4.22178	3.10979	9.80986	3.21183	1.82941(1)
5.0	6.03383	8.48848	6.14308	1.94062(1)	6.24416	3.57470(1)
9.0	1.00388(1)	1.41233(1)	1.01494(1)	3.20639(1)	1.02513(1)	5.87116(1)

Table 3
The viscous-slip problem: heat-flow profiles for the case $a_1 = 1.0$, $a_2 = 1.0$ and $C = 0.5$

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
τ	$q_1(\tau)$	$q_2(\tau)$	$q_1(\tau)$	$q_2(\tau)$	$q_1(\tau)$	$q_2(\tau)$
0.0	1.89366(−1)	2.20338(−1)	2.01585(−1)	5.44563(−1)	2.29190(−1)	1.09101
0.1	1.54414(−1)	1.66050(−1)	1.62946(−1)	4.12577(−1)	1.88953(−1)	8.49530(−1)
0.2	1.35151(−1)	1.39133(−1)	1.42141(−1)	3.46192(−1)	1.66994(−1)	7.24066(−1)
0.3	1.20599(−1)	1.20029(−1)	1.26690(−1)	2.98938(−1)	1.50595(−1)	6.32992(−1)
0.4	1.08780(−1)	1.05257(−1)	1.14298(−1)	2.62360(−1)	1.37376(−1)	5.61368(−1)
0.5	9.88249(−2)	9.33169(−2)	1.03960(−1)	2.32786(−1)	1.26292(−1)	5.02669(−1)
0.6	9.02527(−2)	8.33959(−2)	9.51224(−2)	2.08213(−1)	1.16764(−1)	4.53306(−1)
0.7	8.27593(−2)	7.49926(−2)	8.74385(−2)	1.87401(−1)	1.08431(−1)	4.11047(−1)
0.8	7.61370(−2)	6.77728(−2)	8.06745(−2)	1.69523(−1)	1.01050(−1)	3.74389(−1)
0.9	7.02355(−2)	6.15014(−2)	7.46631(−2)	1.53996(−1)	9.44481(−2)	3.42263(−1)
1.0	6.49414(−2)	5.60054(−2)	6.92799(−2)	1.40391(−1)	8.84958(−2)	3.13877(−1)
2.0	3.21782(−2)	2.47749(−2)	3.58737(−2)	6.30190(−2)	5.02212(−2)	1.47335(−1)
5.0	5.77450(−3)	3.66393(−3)	7.48265(−3)	9.93901(−3)	1.32122(−2)	2.50836(−2)
9.0	8.46370(−4)	4.53106(−4)	1.32329(−3)	1.35016(−3)	3.00230(−3)	3.63951(−3)

Table 4
The thermal-slip coefficients for the case $a_1 = 1.0$ and $a_2 = 1.0$

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
C	ζ_1	ζ_2	ζ_1	ζ_2	ζ_1	ζ_2
0.0	6.04774(−1)	5.87362(−1)	4.70214(−1)	5.87362(−1)	4.42313(−1)	5.87362(−1)
0.1	6.00986(−1)	5.83201(−1)	4.73861(−1)	5.80695(−1)	4.54594(−1)	6.04903(−1)
0.2	5.97620(−1)	5.79717(−1)	4.78681(−1)	5.76174(−1)	4.68238(−1)	6.25615(−1)
0.3	5.94687(−1)	5.76933(−1)	4.85008(−1)	5.74625(−1)	4.83582(−1)	6.50701(−1)
0.4	5.92196(−1)	5.74871(−1)	4.93284(−1)	5.77203(−1)	5.01099(−1)	6.82026(−1)
0.5	5.90161(−1)	5.73553(−1)	5.04090(−1)	5.85548(−1)	5.21483(−1)	7.22615(−1)
0.6	5.88592(−1)	5.73006(−1)	5.18165(−1)	6.02021(−1)	5.45779(−1)	7.77615(−1)
0.7	5.87506(−1)	5.73255(−1)	5.36343(−1)	6.30009(−1)	5.75544(−1)	8.56322(−1)
0.8	5.86919(−1)	5.74333(−1)	5.59045(−1)	6.74031(−1)	6.12694(−1)	9.76405(−1)
0.9	5.86859(−1)	5.76278(−1)	5.83581(−1)	7.37580(−1)	6.54585(−1)	1.16839
1.0	5.87362(−1)	5.79143(−1)	5.87362(−1)	8.01401(−1)	5.87362(−1)	1.28637

Table 5
The thermal-slip coefficients for the case $a_1 = 0.3$ and $a_2 = 0.6$

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
C	ζ_1	ζ_2	ζ_1	ζ_2	ζ_1	ζ_2
0.0	5.49447(−1)	5.09525(−1)	4.45575(−1)	5.09525(−1)	4.28722(−1)	5.09525(−1)
0.1	5.39213(−1)	4.96294(−1)	4.46866(−1)	4.95415(−1)	4.38344(−1)	5.11831(−1)
0.2	5.28974(−1)	4.83141(−1)	4.48563(−1)	4.81026(−1)	4.48693(−1)	5.13670(−1)
0.3	5.18723(−1)	4.70062(−1)	4.50765(−1)	4.66445(−1)	4.59883(−1)	5.14969(−1)
0.4	5.08450(−1)	4.57050(−1)	4.53588(−1)	4.51795(−1)	4.72056(−1)	5.15685(−1)
0.5	4.98144(−1)	4.44097(−1)	4.57144(−1)	4.37239(−1)	4.85384(−1)	5.15856(−1)
0.6	4.87787(−1)	4.31186(−1)	4.61492(−1)	4.22980(−1)	5.00052(−1)	5.15720(−1)
0.7	4.77358(−1)	4.18292(−1)	4.66449(−1)	4.09198(−1)	5.16120(−1)	5.15977(−1)
0.8	4.66824(−1)	4.05375(−1)	4.70961(−1)	3.95757(−1)	5.32701(−1)	5.18251(−1)
0.9	4.56133(−1)	3.92363(−1)	4.70646(−1)	3.80798(−1)	5.42127(−1)	5.24294(−1)
1.0	4.45192(−1)	3.79127(−1)	4.45192(−1)	3.52257(−1)	4.45192(−1)	4.72090(−1)

Table 6
The thermal-creep problem: velocity profiles for each species for the case $a_1 = 1.0$, $a_2 = 1.0$ and $C = 0.5$

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
τ	$u_1(\tau)$	$u_2(\tau)$	$u_1(\tau)$	$u_2(\tau)$	$u_1(\tau)$	$u_2(\tau)$
0.0	1.61427(−1)	1.33496(−1)	1.57774(−1)	1.34776(−1)	1.72434(−1)	1.58232(−1)
0.1	2.34650(−1)	2.03781(−1)	2.22911(−1)	1.98945(−1)	2.36530(−1)	2.27514(−1)
0.2	2.78299(−1)	2.45648(−1)	2.60670(−1)	2.37882(−1)	2.73967(−1)	2.70694(−1)
0.3	3.11995(−1)	2.78192(−1)	2.89263(−1)	2.68519(−1)	3.02416(−1)	3.05217(−1)
0.4	3.39637(−1)	3.05111(−1)	3.12347(−1)	2.94144(−1)	3.25453(−1)	3.34477(−1)
0.5	3.63026(−1)	3.28090(−1)	3.31610(−1)	3.16251(−1)	3.44727(−1)	3.60018(−1)
0.6	3.83201(−1)	3.48090(−1)	3.48021(−1)	3.35689(−1)	3.61190(−1)	3.82719(−1)
0.7	4.00838(−1)	3.65731(−1)	3.62208(−1)	3.53005(−1)	3.75454(−1)	4.03148(−1)
0.8	4.16409(−1)	3.81444(−1)	3.74605(−1)	3.68577(−1)	3.87948(−1)	4.21698(−1)
0.9	4.30262(−1)	3.95544(−1)	3.85530(−1)	3.82684(−1)	3.98982(−1)	4.38659(−1)
1.0	4.42663(−1)	4.08274(−1)	3.95225(−1)	3.95538(−1)	4.08793(−1)	4.54252(−1)
2.0	5.18478(−1)	4.88964(−1)	4.52587(−1)	4.80487(−1)	4.67313(−1)	5.61595(−1)
5.0	5.77603(−1)	5.57537(−1)	4.94838(−1)	5.61770(−1)	5.11187(−1)	6.77819(−1)
9.0	5.88323(−1)	5.71122(−1)	5.02555(−1)	5.81196(−1)	5.19526(−1)	7.12253(−1)

Table 7
The thermal-creep problem: heat-flow profiles for the case $a_1 = 1.0$, $a_2 = 1.0$ and $C = 0.5$

	Ne–Ar mixture		He–Ar mixture		He–Xe mixture	
τ	$-q_1(\tau)$	$-q_2(\tau)$	$-q_1(\tau)$	$-q_2(\tau)$	$-q_1(\tau)$	$-q_2(\tau)$
0.0	8.95414(−1)	7.52679(−1)	8.62425(−1)	7.74480(−1)	9.94638(−1)	8.54990(−1)
0.1	1.12207	9.71566(−1)	1.06318	9.78587(−1)	1.19797	1.06944
0.2	1.25061	1.09138	1.17530	1.09088	1.31439	1.19009
0.3	1.34625	1.17882	1.25793	1.17298	1.40150	1.27952
0.4	1.42232	1.24731	1.32318	1.23737	1.47117	1.35047
0.5	1.48495	1.30299	1.37662	1.28977	1.52887	1.40879
0.6	1.53768	1.34932	1.42140	1.33344	1.57774	1.45784
0.7	1.58275	1.38853	1.45955	1.37044	1.61979	1.49974
0.8	1.62174	1.42212	1.49245	1.40217	1.65640	1.53597
0.9	1.65576	1.45118	1.52111	1.42966	1.68859	1.56759
1.0	1.68568	1.47652	1.54627	1.45366	1.71709	1.59539
2.0	1.85623	1.61626	1.68953	1.58686	1.88563	1.75403
5.0	1.96928	1.70100	1.78730	1.66945	2.01414	1.85916
9.0	1.98609	1.71179	1.80371	1.68046	2.04045	1.87413

where

$$n = n_1 + n_2, \tag{78}$$

to see that our computations confirmed (to the same number of digits listed in our tables) that

$$\Pi(\tau) = \frac{n_1}{n} p_1(\tau) + \frac{n_2}{n} p_2(\tau) \tag{79}$$

is constant. We have also been able (after taking note of some differing definitions) to confirm, for the case of rigid-sphere interactions, the three–four digit numerical results for the viscous-slip problem and the half-space thermal-creep problem reported for the case of purely diffuse boundary conditions, i.e., $a_1 = 1$ and $a_2 = 1$, by Sharipov and Kalempa [14,15] for the three mixtures defined in that work. Finally we have seen that our computations yield known results available from the S-model calculations [26] when we allow our data to collapse to the single-species gas. We have obtained this reduction to a single gas in three ways: (i) $n_1 = 0$, for which the quantities with subscript 2 yield the single-gas results, (ii) $n_2 = 0$, for which the quantities with subscript 1 yield the single-gas results, and (iii) $m_1 = m_2$ and $d_1 = d_2$. That we obtain identical results from these three limiting cases can be attributed, we believe, to the good way the mean-free path l_0 used in this work is defined [14]. We find it especially interesting to see that the S model can be obtained from the McCormack model when the data for the gas mixture is reduced to that of a single species.

In regard to adaptation factors, we note that

$$\varphi_{u,\alpha} = \frac{n_\alpha m_\alpha}{n_1 m_1 + n_2 m_2} \left(\frac{m}{m_\alpha} \right)^{1/2}, \quad \alpha = 1, 2, \tag{80}$$

can be used with our solutions, in the manner of Eq. (48a), to obtain the bulk velocity of the mixture and the slip coefficients as they are defined by Sharipov and Kalempa [14,15]. On the other hand, Sharipov and Kalempa [13] and Naris, Valougeorgis, Sharipov and Kalempa [18] have used the adaptation factors

$$\varphi_{u,\alpha} = \frac{n_\alpha}{n_1 + n_2} \left(\frac{m}{m_\alpha} \right)^{1/2}, \quad \alpha = 1, 2, \tag{81}$$

to define the velocity profile for a binary mixture. Note that the mean molecular mass m is defined in Eq. (9).

6. A relationship between the two considered problems

In a recent work [31] Sharipov used physical arguments to provide, within the context of the S model for a single-species gas, a relationship between the heat flow from Kramers' problem and the thermal-slip coefficient. In a following work [32], Siewert used the defining equations relevant to the linearized Boltzmann equation (and some kinetic models) and a form of the boundary condition (that includes the Maxwell and Cercignani-Lampis boundary conditions as special cases) to find and evaluate an explicit relationship between the heat flow from Kramers' problem and the thermal-slip coefficient. These two results [31,32] define, for the case of a single-species gas, a relationship between the viscous-slip problem and the half-space thermal-creep problem that can be used, for example, to help evaluate numerical results obtained for the two problems. We have extended the mentioned results [31,32] to the currently considered case of a binary-gas mixture described by the McCormack model. Since our derivation follows very closely the one given in [32], we list here only the final result. If we add subscripts K for the viscous-slip problem and T for the half-space thermal-creep problem, we find we can write

$$\frac{n_1}{n} Q_{K,1} + \frac{r n_2}{n} Q_{K,2} = \beta - \left(\frac{n_1}{n\sigma_1} \zeta_{T,1} + \frac{n_2}{n\sigma_2} \zeta_{T,2} \right), \tag{82}$$

where

$$\beta = -\left(\frac{n_1}{n\sigma_1} E + \frac{n_2}{n\sigma_2} F \right). \tag{83}$$

Here, E and F are the constants defined by Eq. (67), the thermal-slip coefficients $\zeta_{T,\alpha}$ are as defined by Eqs. (73) and

$$Q_{K,\alpha} = \int_0^\infty q_{K,\alpha}(\tau)\, \mathrm{d}\tau, \tag{84}$$

where the heat flow profiles for Kramers' problem are defined by Eq. (20c). We have confirmed, to many significant figures, Eq. (82) as part of our testing of the solutions reported in this work.

7. Concluding remarks

To conclude this work, we note that we believe our solutions to the considered problems of viscous slip and thermal creep are especially concise and easy to use. We have included a general form of the Maxwell boundary condition in our formulation, and we have reported what we believe to be highly accurate results for some test cases. It should be noted that our complete, species-specific results listed, for the two considered problems, in Eqs. (52) and (70) are continuous in the τ variable and thus are valid for all $\tau \geqslant 0$.

In this work we have considered only the case of rigid-sphere interactions, but as pointed out by Sharipov and Kalempa [14] the solutions can be used for other scattering laws such the one defined by the Lennard-Jones potential simply by using, instead of Eqs. (A.34) and (A.35), appropriate definitions of the omega integrals [1,2]. In addition, it is clear that we now have essentially all we need to solve well the classical flow problems (Poiseuille, thermal creep and Couette) in a plane channel for a binary gas mixture that can be described by the McCormack model. In developing our solutions here for the McCormack model, we have noted one aspect of the computation that made this work especially interesting when compared to our previous work [28,29] for mixtures described by the Hamel model. This aspect of the solution can be seen in Eq. (39) where there appears an integral term that we have not seen in any of our previous work with the ADO method. While this integral term has required some attention, the ensuing additional work is considered modest when we take into account the merits of the McCormack model. We also see that the way in which Eqs. (35) and (39) were formulated can be utilized for other problems in rarefied gas dynamics.

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 solves both problems for all quantities of interest with 5 or 6 figures of accuracy in less than 0.1 seconds on a 1.2 GHz mobile Pentium III machine – which confirms, we believe, the merit of this work.

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Appendix A. Basic elements of the defining equations

Here we list some basics 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

$$K_{\beta,\alpha}(\boldsymbol{c}',\boldsymbol{c}) = K^{(1)}_{\beta,\alpha}(\boldsymbol{c}',\boldsymbol{c}) + K^{(2)}_{\beta,\alpha}(\boldsymbol{c}',\boldsymbol{c}) + K^{(3)}_{\beta,\alpha}(\boldsymbol{c}',\boldsymbol{c}) + K^{(4)}_{\beta,\alpha}(\boldsymbol{c}',\boldsymbol{c}), \quad \alpha,\beta = 1,2, \tag{A.1}$$

where

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

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

$$K^{(3)}_{1,1}(\boldsymbol{c}',\boldsymbol{c}) = 2\varpi_1[(\boldsymbol{c}'\cdot\boldsymbol{c})^2 - (1/3)c'^2c^2], \tag{A.4}$$

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

$$K^{(1)}_{2,1}(\boldsymbol{c}',\boldsymbol{c}) = r\{2\eta^{(1)}_{1,2} + \eta^{(2)}_{1,2}[r^2(c'^2 - 5/2) + c^2 - 5/2]\}\boldsymbol{c}'\cdot\boldsymbol{c}, \tag{A.6}$$

$$K^{(2)}_{2,1}(\boldsymbol{c}',\boldsymbol{c}) = (4/3)r^*\eta^{(1)}_{1,2}(c'^2 - 3/2)(c^2 - 3/2), \tag{A.7}$$

$$K^{(3)}_{2,1}(\boldsymbol{c}',\boldsymbol{c}) = 2\eta^{(4)}_{1,2}[(\boldsymbol{c}'\cdot\boldsymbol{c})^2 - (1/3)c'^2c^2], \tag{A.8}$$

$$K^{(4)}_{2,1}(\boldsymbol{c}',\boldsymbol{c}) = (4/5)\eta^{(6)}_{1,2}(c'^2 - 5/2)(c^2 - 5/2)\boldsymbol{c}'\cdot\boldsymbol{c}, \tag{A.9}$$

$$K^{(1)}_{2,2}(\boldsymbol{c}',\boldsymbol{c}) = 1 + \{2[1-\eta^{(1)}_{2,1}] - \eta^{(2)}_{2,1}(c'^2 - 5/2)\}\boldsymbol{c}'\cdot\boldsymbol{c}, \tag{A.10}$$

$$K^{(2)}_{2,2}(\boldsymbol{c}',\boldsymbol{c}) = (2/3)[1-2s^*\eta^{(1)}_{2,1}](c'^2 - 3/2)(c^2 - 3/2), \tag{A.11}$$

$$K^{(3)}_{2,2}(\boldsymbol{c}',\boldsymbol{c}) = 2\varpi_2[(\boldsymbol{c}'\cdot\boldsymbol{c})^2 - (1/3)c'^2c^2], \tag{A.12}$$

$$K_{2,2}^{(4)}(\boldsymbol{c}',\boldsymbol{c}) = \left[(4/5)\beta_2\left(c'^2 - 5/2\right) - \eta_{2,1}^{(2)}\right]\left(c^2 - 5/2\right)\boldsymbol{c}'\cdot\boldsymbol{c}, \tag{A.13}$$

$$K_{1,2}^{(1)}(\boldsymbol{c}',\boldsymbol{c}) = s\left\{2\eta_{2,1}^{(1)} + \eta_{2,1}^{(2)}\left[s^2\left(c'^2 - 5/2\right) + c^2 - 5/2\right]\right\}\boldsymbol{c}'\cdot\boldsymbol{c}, \tag{A.14}$$

$$K_{1,2}^{(2)}(\boldsymbol{c}',\boldsymbol{c}) = (4/3)s^*\eta_{2,1}^{(1)}\left(c'^2 - 3/2\right)\left(c^2 - 3/2\right), \tag{A.15}$$

$$K_{1,2}^{(3)}(\boldsymbol{c}',\boldsymbol{c}) = 2\eta_{2,1}^{(4)}\left[(\boldsymbol{c}'\cdot\boldsymbol{c})^2 - (1/3)c'^2c^2\right] \tag{A.16}$$

and

$$K_{1,2}^{(4)}(\boldsymbol{c}',\boldsymbol{c}) = (4/5)\eta_{2,1}^{(6)}\left(c'^2 - 5/2\right)\left(c^2 - 5/2\right)\boldsymbol{c}'\cdot\boldsymbol{c}. \tag{A.17}$$

Here

$$r^* = r^2/\left(1 + r^2\right) \tag{A.18}$$

and

$$s^* = s^2/\left(1 + s^2\right). \tag{A.19}$$

In addition,

$$\varpi_1 = 1 + \eta_{1,1}^{(4)} - \eta_{1,1}^{(3)} - \eta_{1,2}^{(3)}, \tag{A.20}$$

$$\varpi_2 = 1 + \eta_{2,2}^{(4)} - \eta_{2,2}^{(3)} - \eta_{2,1}^{(3)}, \tag{A.21}$$

$$\beta_1 = 1 + \eta_{1,1}^{(6)} - \eta_{1,1}^{(5)} - \eta_{1,2}^{(5)} \tag{A.22}$$

and

$$\beta_2 = 1 + \eta_{2,2}^{(6)} - \eta_{2,2}^{(5)} - \eta_{2,1}^{(5)}, \tag{A.23}$$

where

$$\eta_{i,j}^{(k)} = \nu_{i,j}^{(k)}/\gamma_i. \tag{A.24}$$

Following McCormack [23], we write

$$\nu_{\alpha,\beta}^{(1)} = \frac{16}{3}\frac{m_{\alpha,\beta}}{m_\alpha}n_\beta\Omega_{\alpha\beta}^{11}, \tag{A.25}$$

$$\nu_{\alpha,\beta}^{(2)} = \frac{64}{15}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^2 n_\beta\left(\Omega_{\alpha\beta}^{12} - \frac{5}{2}\Omega_{\alpha\beta}^{11}\right), \tag{A.26}$$

$$\nu_{\alpha,\beta}^{(3)} = \frac{16}{5}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^2\frac{m_\alpha}{m_\beta}n_\beta\left(\frac{10}{3}\Omega_{\alpha\beta}^{11} + \frac{m_\beta}{m_\alpha}\Omega_{\alpha\beta}^{22}\right), \tag{A.27}$$

$$\nu_{\alpha,\beta}^{(4)} = \frac{16}{5}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^2\frac{m_\alpha}{m_\beta}n_\beta\left(\frac{10}{3}\Omega_{\alpha\beta}^{11} - \Omega_{\alpha\beta}^{22}\right), \tag{A.28}$$

$$\nu_{\alpha,\beta}^{(5)} = \frac{64}{15}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^3\frac{m_\alpha}{m_\beta}n_\beta\Gamma_{\alpha,\beta}^{(5)} \tag{A.29}$$

and

$$\nu_{\alpha,\beta}^{(6)} = \frac{64}{15}\left(\frac{m_{\alpha,\beta}}{m_\alpha}\right)^3\left(\frac{m_\alpha}{m_\beta}\right)^{3/2}n_\beta\Gamma_{\alpha,\beta}^{(6)}, \tag{A.30}$$

with

$$\Gamma_{\alpha,\beta}^{(5)} = \Omega_{\alpha\beta}^{22} + \left(\frac{15m_\alpha}{4m_\beta} + \frac{25m_\beta}{8m_\alpha}\right)\Omega_{\alpha\beta}^{11} - \left(\frac{m_\beta}{2m_\alpha}\right)\left(5\Omega_{\alpha\beta}^{12} - \Omega_{\alpha\beta}^{13}\right) \tag{A.31}$$

and, after a correction by Sharipov and Kalempa [14],

$$\Gamma_{\alpha,\beta}^{(6)} = -\Omega_{\alpha\beta}^{22} + \frac{55}{8}\Omega_{\alpha\beta}^{11} - \frac{5}{2}\Omega_{\alpha\beta}^{12} + \frac{1}{2}\Omega_{\alpha\beta}^{13}. \tag{A.32}$$

In addition,

$$m_{\alpha,\beta} = m_\alpha m_\beta/(m_\alpha + m_\beta) \tag{A.33}$$

and the Ω functions are the Chapman–Cowling integrals [1,2] which for the case of rigid-sphere interactions take the simple forms

$$\Omega^{12}_{\alpha,\beta} = 3\Omega^{11}_{\alpha,\beta}, \quad \Omega^{13}_{\alpha,\beta} = 12\Omega^{11}_{\alpha,\beta} \quad \text{and} \quad \Omega^{22}_{\alpha,\beta} = 2\Omega^{11}_{\alpha,\beta} \tag{A.34a–c}$$

with

$$\Omega^{11}_{\alpha\beta} = \frac{1}{4}\left(\frac{\pi k T_0}{2m_{\alpha,\beta}}\right)^{1/2}(d_\alpha + d_\beta)^2. \tag{A.35}$$

Appendix B. The basic kernels for flow problems

The components of the kernel $\boldsymbol{K}(\xi', \xi)$ required in Eq. (24) are as follows:

$$k_{1,1}(\xi', \xi) = 2\varpi_1\xi'\xi + 1 - \eta^{(1)}_{1,2} - \eta^{(2)}_{1,2}\big(\xi'^2 + \xi^2 - 1\big)/2 + 2\beta_1\big(\xi'^2 - 1/2\big)\big(\xi^2 - 1/2\big)/5, \tag{B.1}$$

$$k_{1,2}(\xi', \xi) = -(1/2)\eta^{(2)}_{1,2} + 2\beta_1\big(\xi^2 - 1/2\big)/5, \tag{B.2}$$

$$k_{1,3}(\xi', \xi) = 2\eta^{(4)}_{1,2}\xi'\xi + r\big\{\eta^{(1)}_{1,2} + \eta^{(2)}_{1,2}\big[r^2\big(\xi'^2 - 1/2\big) + \xi^2 - 1/2\big]/2\big\} + 2\eta^{(6)}_{1,2}\big(\xi'^2 - 1/2\big)\big(\xi^2 - 1/2\big)/5, \tag{B.3}$$

$$k_{1,4}(\xi', \xi) = (1/2)r^3\eta^{(2)}_{1,2} + 2\eta^{(6)}_{1,2}\big(\xi^2 - 1/2\big)/5, \tag{B.4}$$

$$k_{2,1}(\xi', \xi) = -\eta^{(2)}_{1,2} + 4\beta_1\big(\xi'^2 - 1/2\big)/5, \tag{B.5}$$

$$k_{2,2}(\xi', \xi) = (4/5)\beta_1, \tag{B.6}$$

$$k_{2,3}(\xi', \xi) = r\eta^{(2)}_{1,2} + 4\eta^{(6)}_{1,2}\big(\xi'^2 - 1/2\big)/5, \tag{B.7}$$

$$k_{2,4}(\xi', \xi) = (4/5)\eta^{(6)}_{1,2}, \tag{B.8}$$

$$k_{3,1}(\xi', \xi) = 2\eta^{(4)}_{2,1}\xi'\xi + s\big\{\eta^{(1)}_{2,1} + \eta^{(2)}_{2,1}\big[s^2\big(\xi'^2 - 1/2\big) + \xi^2 - 1/2\big]/2\big\} + 2\eta^{(6)}_{2,1}\big(\xi'^2 - 1/2\big)\big(\xi^2 - 1/2\big)/5, \tag{B.9}$$

$$k_{3,2}(\xi', \xi) = (1/2)s^3\eta^{(2)}_{2,1} + 2\eta^{(6)}_{2,1}\big(\xi^2 - 1/2\big)/5, \tag{B.10}$$

$$k_{3,3}(\xi', \xi) = 2\varpi_2\xi'\xi + 1 - \eta^{(1)}_{2,1} - \eta^{(2)}_{2,1}\big(\xi'^2 + \xi^2 - 1\big)/2 + 2\beta_2\big(\xi'^2 - 1/2\big)\big(\xi^2 - 1/2\big)/5, \tag{B.11}$$

$$k_{3,4}(\xi', \xi) = -(1/2)\eta^{(2)}_{2,1} + 2\beta_2\big(\xi^2 - 1/2\big)/5, \tag{B.12}$$

$$k_{4,1}(\xi', \xi) = s\eta^{(2)}_{2,1} + 4\eta^{(6)}_{2,1}\big(\xi'^2 - 1/2\big)/5, \tag{B.13}$$

$$k_{4,2}(\xi', \xi) = (4/5)\eta^{(6)}_{2,1}, \tag{B.14}$$

$$k_{4,3}(\xi', \xi) = -\eta^{(2)}_{2,1} + 4\beta_2\big(\xi'^2 - 1/2\big)/5 \tag{B.15}$$

and

$$k_{4,4}(\xi', \xi) = (4/5)\beta_2. \tag{B.16}$$

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