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The McCormack model for gas mixtures: The temperature-jump problem

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Abstract. An analytical version of the discrete-ordinates method (the ADO method) is used to establish a concise and particularly accurate solution to the temperature-jump problem for a binary gas mixture described by the McCormack kinetic model. The solution yields, in addition to the temperature-jump coefficient 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. Numerical results are reported for two binary mixtures (Ne-Ar and He-Xe) with various molar concentrations. 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.

Keywords. Rarefied gas dynamics, temperature jump coefficient, binary gas mixture, discrete ordinates.

1. Introduction

The classical temperature-jump problem as defined by Welander [1] for single-species gases has, over the years, been studied and solved in numerous ways and for various kinetic models, as well as for the linearized Boltzmann equation. We do not discuss here many important works on this subject, but we refer instead to the books of Cercignani [2, 3], Williams [4] and Ferziger and Kaper [5], as well as a review paper by Sharipov and Seleznev [6], for general background material. However, since this paper is another contribution to our study of the temperature-jump problem, we comment briefly on two of our preceding works [7–14] on this subject. The first definitive result for the temperature-jump coefficient for a single-species gas defined by the BGK model [15] was reported by Kriese, Chang and Siewert [7]. Considerably more recently, we reported [12, 13] a numerical implementation of a semi-analytical solution of this same temperature-jump problem, with Maxwell and with Cercignani-Lampis [16] boundary conditions, based on the linearized Boltzmann equation for rigid-sphere interactions. In this work, we consider the temperature-jump problem for the case of a binary-gas mixture. While in Ref. [14] we reported a concise and accurate solution of the temperature-jump problem for

gas mixtures, that work was based on the Hamel model [17], and so our work here with the McCormack kinetic model [18] is thought to yield physically more meaningful results.

2. 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 [18] published in 1973. While we use this model as defined in Ref. [18], we use 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 [19] in two recent works [20, 21] 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-parallel channels (Poiseuille flow, thermal-creep flow and flow driven by density gradients), and so some of our introductory material here is repeated from Refs. [20, 21]. We consider that the required functions $h_\alpha(x, \boldsymbol{v})$ for the two types of particles ($\alpha = 1$ and 2) denote perturbations from Maxwellian distributions for each species, i.e,

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

where

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

Here k is the Boltzmann constant, m_α and n_α are the mass and the equilibrium density of the 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 [18] 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 $\boldsymbol{c}$, 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

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

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 [18], we have introduced the dimensionless velocity $\boldsymbol{c}$ 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 $\boldsymbol{c} = \omega_2 \boldsymbol{v}$. 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 [22]. Here, following Ref. [22], we write

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

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 [22]

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

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 definitions given in Appendix A have been used,

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

and

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

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

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

In this work we consider the half-space temperature-jump problem, and so we seek solutions of Eqs. (18) that are valid for all $\tau > 0$, and we use Maxwell boundary conditions at the wall, viz.,

$$h_\alpha(0, c_x, c_y, c_z) = (1 - a_\alpha)h_\alpha(0, -c_x, c_y, c_z) + a_\alpha \mathcal{I}\{h_\alpha\}(0), \tag{19}$$

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

$$h_\alpha(\tau, \boldsymbol{c}) \Leftrightarrow h_\alpha(\tau, c_x, c_y, c_z) \tag{20}$$

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

$$\mathcal{I}\{h_\alpha\}(\tau) = \frac{2}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \mathrm{e}^{-c'^2} h_\alpha(\tau, -c'_x, c'_y, c'_z) c'_x \mathrm{d}c'_x \mathrm{d}c'_y \mathrm{d}c'_z \tag{21}$$

to denote the diffuse term in Eq. (19). In this formulation of the temperature-jump problem there is no driving term in Eq. (18), and so in addition to the boundary condition listed as Eq. (19), we will include in our statement of the problem a condition on $h_\alpha(\tau, \boldsymbol{c})$ as τ tends to infinity. This condition will be seen more clearly once we have expressed the density and temperature perturbations in terms of $h_\alpha(\tau, \boldsymbol{c})$.

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

$$N_\alpha(\tau) = \frac{1}{\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2} h_\alpha(\tau, \boldsymbol{c}) \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z \tag{22}$$

and

$$T_\alpha(\tau) = \frac{2}{3\pi^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2} h_\alpha(\tau, \boldsymbol{c})(c^2 - 3/2) \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z \tag{23}$$

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

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

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

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

Defining

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

and

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

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

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

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

$$\boldsymbol{\Sigma}=\mathrm{diag}\big\{\sigma_1,\sigma_1,\sigma_2,\sigma_2\big\} \tag{29}$$

and

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

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

$$\boldsymbol{G}(0,\xi)=\boldsymbol{S}\boldsymbol{G}(0,-\xi)+2\boldsymbol{D}\int_0^{\infty}\mathrm{e}^{-\xi'^2}\boldsymbol{G}(0,-\xi')\xi'\mathrm{d}\xi', \tag{31}$$

for $\xi>0$. Here

$$\boldsymbol{S}=\mathrm{diag}\{1-a_1,1-a_1,1-a_2,1-a_2\} \tag{32}$$

and

$$\boldsymbol{D}=\mathrm{diag}\{a_1,0,a_2,0\}. \tag{33}$$

So, if we can solve Eq. (28), subject to Eq. (31), we can compute the density and temperature perturbations we seek from

$$N_\alpha(\tau)=\int_{-\infty}^{\infty}\psi(\xi)g_{2\alpha-1}(\tau,\xi)\mathrm{d}\xi \tag{34}$$

and

$$T_\alpha(\tau)=\frac{2}{3}\int_{-\infty}^{\infty}\psi(\xi)[(\xi^2-1/2)g_{2\alpha-1}(\tau,\xi)+g_{2\alpha}(\tau,\xi)]\mathrm{d}\xi. \tag{35}$$

Now, since there is no driving term in Eq. (28) we require that the solutions $h_\alpha(\tau,\boldsymbol{c})$ diverge as τ tends to infinity, but at the same time we impose the (generalized) Welander condition [1], viz.

$$\lim_{\tau\to\infty}\frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{T}(\tau)=\mathcal{K}\begin{bmatrix}1\\1\end{bmatrix}. \tag{36}$$

Here $\mathcal{K}$ is a normalizing constant, and the vector-valued function $\boldsymbol{T}(\tau)$ has the perturbed temperatures $T_\alpha(\tau)$ as components. At this point we are ready to discuss the ADO method and to develop our solution of the formulated problem.

3. The elementary solutions

As the temperature-jump problem has (in our formulation) no inhomogeneous diving term in the balance equation, we require only basic solutions of the homogeneous equation, and so here we establish (in terms of the ADO method) the elementary solutions of

$$\xi\frac{\partial}{\partial\tau}\boldsymbol{G}(\tau,\xi)+\boldsymbol{\Sigma}\boldsymbol{G}(\tau,\xi)=\boldsymbol{\Sigma}\int_{-\infty}^{\infty}\psi(\xi')\boldsymbol{K}(\xi',\xi)\boldsymbol{G}(\tau,\xi')\mathrm{d}\xi'. \tag{37}$$

We seek solutions of Eq. (37) of the form

$$\boldsymbol{G}(\tau,\xi)=\boldsymbol{\Phi}(\nu,\xi)\mathrm{e}^{-\tau/\nu} \tag{38}$$

where the separation constants ν and the elementary solutions $\boldsymbol{\Phi}(\nu,\xi)$ are to be determined. Substituting Eq. (38) into Eq. (37), we find

$$(\nu\boldsymbol{\Sigma}-\xi\boldsymbol{I})\boldsymbol{\Phi}(\nu,\xi)=\nu\boldsymbol{\Sigma}\int_{0}^{\infty}\psi(\xi')[\boldsymbol{K}(\xi',\xi)\boldsymbol{\Phi}(\nu,\xi')+\boldsymbol{K}(-\xi',\xi)\boldsymbol{\Phi}(\nu,-\xi')]\mathrm{d}\xi' \tag{39}$$

and

$$(\nu\boldsymbol{\Sigma}+\xi\boldsymbol{I})\boldsymbol{\Phi}(\nu,-\xi)=\nu\boldsymbol{\Sigma}\int_{0}^{\infty}\psi(\xi')[\boldsymbol{K}(\xi',-\xi)\boldsymbol{\Phi}(\nu,\xi')+\boldsymbol{K}(-\xi',-\xi)\boldsymbol{\Phi}(\nu,-\xi')]\mathrm{d}\xi' \tag{40}$$

from which we conclude, since

$$\boldsymbol{K}(\xi',-\xi)=\boldsymbol{K}(-\xi',\xi), \tag{41}$$

that

$$\boldsymbol{\Phi}(\nu,\xi)=\boldsymbol{\Phi}(-\nu,-\xi). \tag{42}$$

Now, adding and subtracting Eqs. (39) and (40), one from the other, we find that

$$(1/\xi^2)\big[\boldsymbol{\Sigma}^2\boldsymbol{V}(\nu,\xi)-\int_{0}^{\infty}\psi(\xi')\boldsymbol{\mathcal{K}}(\xi',\xi)\boldsymbol{V}(\nu,\xi')\mathrm{d}\xi'\big]=\lambda\boldsymbol{V}(\nu,\xi) \tag{43}$$

and

$$\boldsymbol{U}(\nu,\xi)=(\nu/\xi)\boldsymbol{\Sigma}\big[\boldsymbol{V}(\nu,\xi)-\int_{0}^{\infty}\psi(\xi')\boldsymbol{K}_{-}(\xi',\xi)\boldsymbol{V}(\nu,\xi')\mathrm{d}\xi'\big], \tag{44}$$

where

$$\boldsymbol{U}(\nu,\xi)=\boldsymbol{\Phi}(\nu,\xi)+\boldsymbol{\Phi}(\nu,-\xi) \tag{45}$$

and

$$\boldsymbol{V}(\nu,\xi)=\boldsymbol{\Phi}(\nu,\xi)-\boldsymbol{\Phi}(\nu,-\xi). \tag{46}$$

Here

$$\lambda=1/\nu^2, \tag{47}$$

$$\boldsymbol{K}_{+}(\xi',\xi)=\boldsymbol{K}(\xi',\xi)+\boldsymbol{K}(-\xi',\xi), \tag{48}$$

$$\boldsymbol{K}_{-}(\xi',\xi)=\boldsymbol{K}(\xi',\xi)-\boldsymbol{K}(-\xi',\xi) \tag{49}$$

and

$$\boldsymbol{\mathcal{K}}(\xi',\xi) = (\xi/\xi')\boldsymbol{\Sigma}\boldsymbol{K}_+(\xi',\xi)\boldsymbol{\Sigma} + \boldsymbol{\Sigma}^2\boldsymbol{K}_-(\xi',\xi) - \int_0^\infty \psi(\xi'')(\xi/\xi'')\boldsymbol{\Sigma}\boldsymbol{K}_+(\xi'',\xi)\boldsymbol{\Sigma}\boldsymbol{K}_-(\xi',\xi'')\mathrm{d}\xi''. \tag{50}$$

We now introduce a "half-range" quadrature scheme (with weights and nodes, w_k and ξ_k) and rewrite Eqs. (43) and (44) evaluated at the quadrature points as

$$(1/\xi_i^2)\big[\boldsymbol{\Sigma}^2\boldsymbol{V}(\nu_j,\xi_i) - \sum_{k=1}^{N} w_k\psi(\xi_k)\boldsymbol{\mathcal{K}}(\xi_k,\xi_i)\boldsymbol{V}(\nu_j,\xi_k)\big] = \lambda_j\boldsymbol{V}(\nu_j,\xi_i) \tag{51}$$

and

$$\boldsymbol{U}(\nu_j,\xi_i) = (\nu_j/\xi_i)\boldsymbol{\Sigma}\big[\boldsymbol{V}(\nu_j,\xi_i) - \sum_{k=1}^{N} w_k\psi(\xi_k)\boldsymbol{K}_-(\xi_k,\xi_i)\boldsymbol{V}(\nu_j,\xi_k)\big], \tag{52}$$

for $i = 1,2,...,N$. Equation (51) 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

$$\boldsymbol{\Phi}(\nu_j,\xi_i) = (1/2)[\boldsymbol{U}(\nu_j,\xi_i) + \boldsymbol{V}(\nu_j,\xi_i)] \tag{53}$$

and

$$\boldsymbol{\Phi}(\nu_j,-\xi_i) = (1/2)[\boldsymbol{U}(\nu_j,\xi_i) - \boldsymbol{V}(\nu_j,\xi_i)]. \tag{54}$$

Note that the separation constants defined by

$$\nu_j = \pm\lambda_j^{-1/2} \tag{55}$$

occur in $\pm$ pairs. From this point, we take ν_j to be the positive root listed in Eq. (55). Once we have solved the eigenvalue problem defined by Eq. (51), we can write our general (discrete ordinates) solution to Eq. (37) as

$$\boldsymbol{G}(\tau,\pm\xi_i) = \sum_{j=1}^{4N}\big[A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\mathrm{e}^{-\tau/\nu_j} + B_j\boldsymbol{\Phi}(\nu_j,\mp\xi_i)\mathrm{e}^{\tau/\nu_j}\big], \tag{56}$$

for $i = 1,2,...,N$. Here the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the boundary conditions of a specific problem. While Eq. (56) is our general discrete-ordinates solution, we can make some improvements in that result. We have found that the eigenvalue problem yields 3 separation constants, say ν_1, ν_2 and ν_3, that approximate the three expected unbounded separation constants. And so we ignore ν_1, ν_2 and ν_3, in Eq. (56) and rewrite that equation as

$$\boldsymbol{G}(\tau,\pm\xi_i) = \boldsymbol{G}_*(\tau,\pm\xi_i) + \sum_{j=4}^{4N}\big[A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\mathrm{e}^{-\tau/\nu_j} + B_j\boldsymbol{\Phi}(\nu_j,\mp\xi_i)\mathrm{e}^{\tau/\nu_j}\big], \tag{57}$$

$$\boldsymbol{G}_*(\tau,\xi) = A_1\boldsymbol{G}_1 + A_2\boldsymbol{G}_2 + A_3\boldsymbol{G}_3 + B_1\boldsymbol{G}_4(\xi) + B_2[\tau\boldsymbol{H}_1(\xi) + \boldsymbol{F}_1(\xi)] + B_3[\tau\boldsymbol{H}_2(\xi) + \boldsymbol{F}_2(\xi)]. \tag{58}$$

Here

$$\boldsymbol{G}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{G}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \boldsymbol{G}_3(\xi) = \begin{bmatrix} \xi^2 - 1/2 \\ 1 \\ \xi^2 - 1/2 \\ 1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{G}_4(\xi) = \begin{bmatrix} r\xi \\ 0 \\ \xi \\ 0 \end{bmatrix} \tag{59a, b, c, d}$$

are exact (linearly independent) solutions of Eq. (37). Note that, in general, we use

$$r = (m_1/m_2)^{1/2}, \quad s = (m_2/m_1)^{1/2} \quad \text{and} \quad n = n_1 + n_2. \tag{60a, b, c}$$

We also find that if we write

$$\boldsymbol{H}_1(\xi) = \begin{bmatrix} -1 + c_1(\xi^2 - 1/2) \\ c_1 \\ c_1(\xi^2 - 1/2) \\ c_1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{H}_2(\xi) = \begin{bmatrix} c_2(\xi^2 - 1/2) \\ c_2 \\ -1 + c_2(\xi^2 - 1/2) \\ c_2 \end{bmatrix}, \tag{61a, b}$$

with $c_1 = n_1/n$ and $c_2 = n_2/n$, then there exist vector-valued functions $\boldsymbol{F}_1(\xi)$ and $\boldsymbol{F}_2(\xi)$ that render

$$\tau\boldsymbol{H}_1(\xi) + \boldsymbol{F}_1(\xi) \quad \text{and} \quad \tau\boldsymbol{H}_2(\xi) + \boldsymbol{F}_2(\xi) \tag{62a, b}$$

also solutions of Eq. (37). While we have not found explicit expressions for $\boldsymbol{F}_1(\xi)$ and $\boldsymbol{F}_2(\xi)$, we have used a software package to conclude that these two functions can be defined in terms of solutions to two systems of linear algebraic equations. If we substitute Eqs. (62) into Eq. (37) and use the fact that $\boldsymbol{H}_1(\xi)$ and $\boldsymbol{H}_2(\xi)$ are exact solutions of that equation, then we find the integral equations

$$\boldsymbol{F}_\beta(\xi) = -\xi\boldsymbol{\Sigma}^{-1}\boldsymbol{H}_\beta(\xi) + \int_{-\infty}^{\infty} \psi(\xi')\boldsymbol{K}(\xi', \xi)\boldsymbol{F}_\beta(\xi')\mathrm{d}\xi', \tag{63}$$

for $\beta = 1, 2$ and $\xi \in (-\infty, \infty)$. Since any linear combination of the solutions listed in Eqs. (59 is a solution of the homogeneous version of Eq. (63), the functions $\boldsymbol{F}_1(\xi)$ and $\boldsymbol{F}_2(\xi)$ clearly are not uniquely defined.

After noting the inhomogeneous term in Eq. (63) and the explicit form of the scattering kernel $\boldsymbol{K}(\xi', \xi)$, we conclude that the functions $\boldsymbol{F}_1(\xi)$ and $\boldsymbol{F}_2(\xi)$ can be expressed as

$$\boldsymbol{F}_\beta(\xi) = \sum_{\alpha=0}^{3} P_\alpha(\xi)\boldsymbol{F}_{\beta,\alpha} \tag{64}$$

where the vectors $\boldsymbol{F}_{\beta,\alpha}$ are constants and the orthogonal polynomials are given by

$$P_0(\xi) = 1, \quad P_1(\xi) = \xi, \quad P_2(\xi) = \xi^2 - 1/2 \quad \text{and} \quad P_3(\xi) = \xi(\xi^2 - 3/2). \tag{65a, b, c, d}$$

At this point we substitute Eq. (64) into Eq. (63), multiply the resulting equation by $\psi(\xi)P_k(\xi)$, for $k = 0, 1, 2, 3$, and integrate over all ξ to find a system of 16 linear-algebraic equations (with rank 12) that can be solved to find the components of

the vectors $\boldsymbol{F}_{\beta,\alpha}$ required in Eq. (64). Of course, since the system is rank deficient, solutions exist only for certain inhomogeneous terms. It is for this reason that the vector-valued functions $\boldsymbol{H}_1(\xi)$ and $\boldsymbol{H}_2(\xi)$ in Eqs. (62) are as defined in Eqs. (61). In regard to Eq. (64) we can be more explicit. We have used the MAPLE 9 software package to conclude that we can write

$$\boldsymbol{F}_\beta(\xi) = \boldsymbol{U}_\beta P_1(\xi) + \boldsymbol{V}_\beta P_3(\xi) \tag{66}$$

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

$$(\boldsymbol{I} - \boldsymbol{\mathcal{A}})\boldsymbol{U}_1 - \boldsymbol{\mathcal{C}}\boldsymbol{V}_1 = \left[\begin{array}{cccc} c_2/\sigma_1 & -c_1/\sigma_1 & -c_1/\sigma_2 & -c_1/\sigma_2 \end{array}\right]^T, \tag{67}$$

$$(\boldsymbol{I} - \boldsymbol{\mathcal{D}})\boldsymbol{V}_1 - \boldsymbol{\mathcal{B}}\boldsymbol{U}_1 = \left[\begin{array}{cccc} -c_1/\sigma_1 & 0 & -c_1/\sigma_2 & 0 \end{array}\right]^T \tag{68}$$

and

$$\left[\begin{array}{cccc} 0 & 0 & 1 & 0 \end{array}\right]\boldsymbol{U}_1 = 0, \tag{69}$$

for $\beta = 1$, and by

$$(\boldsymbol{I} - \boldsymbol{\mathcal{A}})\boldsymbol{U}_2 - \boldsymbol{\mathcal{C}}\boldsymbol{V}_2 = \left[\begin{array}{cccc} -c_2/\sigma_1 & -c_2/\sigma_1 & c_1/\sigma_2 & -c_2/\sigma_2 \end{array}\right]^T, \tag{70}$$

$$(\boldsymbol{I} - \boldsymbol{\mathcal{D}})\boldsymbol{V}_2 - \boldsymbol{\mathcal{B}}\boldsymbol{U}_2 = \left[\begin{array}{cccc} -c_2/\sigma_1 & 0 & -c_2/\sigma_2 & 0 \end{array}\right]^T \tag{71}$$

and

$$\left[\begin{array}{cccc} 0 & 0 & 1 & 0 \end{array}\right]\boldsymbol{U}_2 = 0, \tag{72}$$

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

$$\boldsymbol{\mathcal{A}} = 2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}(\xi',\xi)P_1(\xi')P_1(\xi)\mathrm{d}\xi'\mathrm{d}\xi, \tag{73}$$

$$\boldsymbol{\mathcal{B}} = (4/3)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}(\xi',\xi)P_1(\xi')P_3(\xi)\mathrm{d}\xi'\mathrm{d}\xi, \tag{74}$$

$$\boldsymbol{\mathcal{C}} = 2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}(\xi',\xi)P_3(\xi')P_1(\xi)\mathrm{d}\xi'\mathrm{d}\xi \tag{75}$$

and

$$\boldsymbol{\mathcal{D}} = (4/3)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}(\xi',\xi)P_3(\xi')P_3(\xi)\mathrm{d}\xi'\mathrm{d}\xi \tag{76}$$

are listed explicitly in Appendix C. We note that Eqs. (69) and (72) have been made a part of the (9×8) linear systems to be sure that the systems have unique solutions.

As our elementary solutions are established, we are ready to use them to solve the considered temperature-jump problem.

4. The solution of the temperature-jump problem

Since the solution we seek is not allowed to diverge exponentially as τ tends to infinity, it follows from Eq. (57) that we must, in that equation, take $B_j = 0$, for $j = 4, 5, ..., 4N$. And so we now have

$$\boldsymbol{G}(\tau, \pm\xi_i) = \boldsymbol{G}_*(\tau, \pm\xi_i) + \sum_{j=4}^{4N} A_j \boldsymbol{\Phi}(\nu_j, \pm\xi_i) \mathrm{e}^{-\tau/\nu_j} \tag{77}$$

for $i = 1, 2, ..., N$. Considering that the solution to our "$\boldsymbol{G}$ problem" is given by Eq. (77), we can now use that result to compute the density and temperature profiles [defined initially in Eqs. (22) and (23)] from Eqs. (34) and (35). In regard to the asymptotic part of the density and temperature profiles, we let $N^*_\alpha(\tau)$ and $T^*_\alpha(\tau)$ denote the perturbations obtained from Eqs. (34) and (35) when the exponential terms in Eq. (77) are ignored. In this way, we find, after carrying out all required integrals analytically, that we can write

$$N^*_1(\tau) = A_1 - B_2\tau, \tag{78}$$

$$N^*_2(\tau) = A_2 - B_3\tau, \tag{79}$$

$$T^*_1(\tau) = A_3 + (c_1 B_2 + c_2 B_3)\tau \tag{80}$$

and

$$T^*_2(\tau) = A_3 + (c_1 B_2 + c_2 B_3)\tau. \tag{81}$$

We note that $\boldsymbol{G}_1$ and $\boldsymbol{G}_2$, as defined in Eqs. (59a,b), satisfy the boundary condition listed as Eq. (31) and so the constants A_1 and A_2 can not be determined from that condition. We see therefore that our solution will satisfy the boundary condition given as Eq. (19) and the (generalized) Welander condition written as Eq. (36), for any value of A_1 and A_2. It can be seen from Eqs. (78) and (79) that this arbitrariness illustrates simply that the density perturbations are not uniquely defined for this problem here. We choose to "normalize" our solution by taking $A_1 = -A_3$ and $A_2 = -A_3$, and so we now have

$$\boldsymbol{G}(\tau, \pm\xi_i) = \boldsymbol{G}_*(\tau, \pm\xi_i) + \sum_{j=4}^{4N} A_j \boldsymbol{\Phi}(\nu_j, \pm\xi_i) \mathrm{e}^{-\tau/\nu_j}, \tag{82}$$

where

$$\boldsymbol{G}_*(\tau, \xi) = A_3 \boldsymbol{R}(\xi) + B_1 \boldsymbol{G}_4(\xi) + B_2[\tau \boldsymbol{H}_1(\xi) + \boldsymbol{F}_1(\xi)] + B_3[\tau \boldsymbol{H}_2(\xi) + \boldsymbol{F}_2(\xi)] \tag{83}$$

and

$$\boldsymbol{R}(\xi) = \begin{bmatrix} \xi^2 - 3/2 \\ 1 \\ \xi^2 - 3/2 \\ 1 \end{bmatrix}. \tag{84}$$

The solution given by Eqs. (82–84) contains $4N + 1$ arbitrary constants, and so when that solution is used in a discrete-ordinates version of Eq. (31), viz.,

$$\boldsymbol{G}(0,\xi_i) = \boldsymbol{S}\boldsymbol{G}(0,-\xi_i) + 2\pi^{1/2}\boldsymbol{D}\sum_{k=1}^{N} w_k\xi_k\psi(\xi_k)\boldsymbol{G}(0,-\xi_k), \tag{85}$$

for $i = 1, 2..., N$, we obtain a system of $4N$ linear algebraic equations for the $4N+1$ unknowns; however, there is the normalization condition listed as Eq. (36). And so we add to our system the normalization condition

$$c_1B_2 + c_2B_3 = 1, \tag{86}$$

where (without loss of generality) we have taken $\mathcal{K} = 1$. Once we solve the defined system of linear algebraic equations, our solution is established. We therefore can write

$$\boldsymbol{N}(\tau) = -\begin{bmatrix} A_3 + B_2\tau \\ A_3 + B_3\tau \end{bmatrix} + \sum_{j=4}^{4N} A_j\boldsymbol{X}(\nu_j)\mathrm{e}^{-\tau/\nu_j} \tag{87}$$

and

$$\boldsymbol{T}(\tau) = (A_3 + \tau)\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{2}{3}\sum_{j=4}^{4N} A_j\boldsymbol{Y}(\nu_j)\mathrm{e}^{-\tau/\nu_j}. \tag{88}$$

Here

$$\boldsymbol{X}(\nu_j) = \sum_{k=1}^{N} w_k\psi(\xi_k)\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}\left[\boldsymbol{\Phi}(\nu_j,\xi_k) + \boldsymbol{\Phi}(\nu_j,-\xi_k)\right] \tag{89}$$

and

$$\boldsymbol{Y}(\nu_j) = \sum_{k=1}^{N} w_k\psi(\xi_k)\begin{bmatrix} \xi_k^2 - 1/2 & 1 & 0 & 0 \\ 0 & 0 & \xi_k^2 - 1/2 & 1 \end{bmatrix}\left[\boldsymbol{\Phi}(\nu_j,\xi_k) + \boldsymbol{\Phi}(\nu_j,-\xi_k)\right]. \tag{90}$$

To conclude this section, we note that the temperature-jump coefficient (for each species) is defined as

$$T_\alpha^*(0) = \zeta_\alpha\frac{\mathrm{d}}{\mathrm{d}\tau}T_\alpha^*(\tau)\Big|_{\tau=0}. \tag{91}$$

However, it is clear from Eq. (88) that the temperature-jump coefficient is, in fact, the same for both species. And so

$$\zeta = A_3 \tag{92}$$

is our result for the desired temperature-jump coefficient.

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

$$v(\xi) = \mathrm{e}^{-\xi} \tag{93}$$

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, we have elected to use two data cases defined by Sharipov and Kalempa [22]. These data cases refer to a mixture of the species: (i) Ne-Ar and (ii) 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 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

$$m_2 = 39.948 \quad m_1 = 20.183 \quad d_2/d_1 = 1.406 \quad \text{(Ne-Ar mixture)}$$

and

$$m_2 = 131.30 \quad m_1 = 4.0026 \quad d_2/d_1 = 2.226 \quad \text{(He-Xe mixture)}$$

are exact. We tabulate our results for these two cases in terms of the molar concentration defined (in terms of the first particle) as

$$C = \frac{n_1/n_2}{1 + n_1/n_2}. \tag{94}$$

In addition to computing the temperature-jump coefficient, we have computed both the density and temperature distributions, as given by Eqs. (87) and (88), for various combinations of the accommodation coefficients a_1 and a_2. And so, first of all, we list in Tables 1 and 2 our results for the temperature-jump coefficient as a function of the number mix of the two species of particles for several typical values of the accommodation coefficients a_1 and a_2. And then, to demonstrate the totality of our solution we report in Table 3 our complete results (including the constants B_2 and B_3) for a typical (non-special) case.

We have no definitive proof of the accuracy of our results, but we believe the results listed in Tables 1 – 3 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. Additional confidence in this work (analytical and numerical) has been achieved through the supporting work of Garcia [23], Knackfuss and Barichello [24] and Thomas [25]. In fact, Garcia [23] has confirmed all of the analytical derivations and all of the numerical results that are reported in this work.

In the process of testing our solutions, we looked at the special case of a single-species gas. This reduction to a single gas was achieved in three ways: (i) $n_1 = 0$,

Table 1. The temperature-jump coefficient ζ for the Ne-Ar mixture

C	$a_1 = 0.1$ $a_2 = 0.1$	$a_1 = 0.1$ $a_2 = 0.3$	$a_1 = 0.3$ $a_2 = 0.5$	$a_1 = 0.1$ $a_2 = 0.8$	$a_1 = 0.8$ $a_2 = 0.9$	$a_1 = 1.0$ $a_2 = 1.0$
0.0	3.217519(1)	9.945770	5.443688	2.849612	2.355397	1.954073
0.1	3.204931(1)	1.108708(1)	5.846473	3.541425	2.414712	1.947628
0.2	3.196034(1)	1.235509(1)	6.258400	4.343080	2.471826	1.943362
0.3	3.190331(1)	1.377357(1)	6.679777	5.290552	2.526664	1.940884
0.4	3.187412(1)	1.537269(1)	7.110970	6.437165	2.579178	1.939863
0.5	3.186951(1)	1.719128(1)	7.552432	7.865494	2.629358	1.940024
0.6	3.188708(1)	1.928033(1)	8.004756	9.710594	2.677239	1.941156
0.7	3.192549(1)	2.170812(1)	8.468756	1.220952(1)	2.722925	1.943118
0.8	3.198470(1)	2.456833(1)	8.945601	1.581984(1)	2.766615	1.945858
0.9	3.206648(1)	2.799312(1)	9.437041	2.155319(1)	2.808654	1.949434
1.0	3.217519(1)	3.217519(1)	9.945770	3.217519(1)	2.849612	1.954073

Table 2. The temperature-jump coefficient ζ for the He-Xe mixture

C	$a_1 = 0.1$ $a_2 = 0.1$	$a_1 = 0.1$ $a_2 = 0.3$	$a_1 = 0.3$ $a_2 = 0.5$	$a_1 = 0.1$ $a_2 = 0.8$	$a_1 = 0.8$ $a_2 = 0.9$	$a_1 = 1.0$ $a_2 = 1.0$
0.0	3.217519(1)	9.945770	5.443688	2.849612	2.355397	1.954073
0.1	3.096147(1)	1.372577(1)	6.493532	5.808954	2.431914	1.883572
0.2	3.080385(1)	1.695103(1)	7.280924	8.562522	2.515514	1.872570
0.3	3.115779(1)	1.988923(1)	7.950479	1.132311(1)	2.607910	1.892737
0.4	3.184507(1)	2.269384(1)	8.570618	1.422486(1)	2.711077	1.933886
0.5	3.280467(1)	2.547350(1)	9.181867	1.738174(1)	2.827455	1.992269
0.6	3.402541(1)	2.831853(1)	9.813221	2.091217(1)	2.959979	2.067018
0.7	3.551431(1)	3.130593(1)	1.048636(1)	2.494813(1)	3.111346	2.158302
0.8	3.722795(1)	3.444906(1)	1.120061(1)	2.959654(1)	3.278705	2.263097
0.9	3.861956(1)	3.725510(1)	1.179573(1)	3.451536(1)	3.413730	2.347510
1.0	3.217519(1)	3.217519(1)	9.945770	3.217519(1)	2.849612	1.954073

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 obtained 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 [22]. As we noted [20, 21] for flow problems based on the McCormack

Table 3. Temperature and density profiles for the He-Xe mixture with $C = 0.3$, $a_1 = 0.3$, $a_2 = 0.6$: $\zeta = 7.345950$, $B_2 = 0.6434143$, $B_3 = 1.152822$.

τ	$-N_1(\tau)$	$-N_2(\tau)$	$T_1(\tau)$	$T_2(\tau)$
0.0	6.90689	5.03578	6.87509	4.69618
0.1	7.11313	5.45593	7.13187	5.14852
0.2	7.24491	5.73415	7.30983	5.44479
0.3	7.35582	5.97246	7.46464	5.69461
0.4	7.45531	6.18862	7.60648	5.91793
0.5	7.54742	6.39019	7.73978	6.12346
0.6	7.63433	6.58123	7.86699	6.31596
0.7	7.71738	6.76423	7.98960	6.49842
0.8	7.79744	6.94085	8.10863	6.67283
0.9	7.87513	7.11223	8.22478	6.84061
1.0	7.95090	7.27924	8.33859	7.00283
2.0	8.65150	8.80252	9.40554	8.43799
5.0	1.05938(1)	1.27604(1)	1.24056(1)	1.19876(1)
9.0	1.31507(1)	1.76004(1)	1.63721(1)	1.62245(1)

model, we found again that the McCormack model reduces to the S model [6] when the data for the gas mixture is reduced to that of a single species.

While investigating the special case of a single-species gas we found that our results for the S model were not, as suggested by the form of the balance equation used by Sharipov [26], identical to those predicted by the BGK model. We have concluded that, while the S-model results (when expressed in terms of a mean-free path based on thermal conductivity) for the temperature-jump coefficient and the density and temperature perturbations at the wall where identical to known BGK results (see Ref. [9], for example), there is a (very slight) difference in the results from the BGK and the S kinetic models for the density and temperature perturbations within the gas. The observation that the S model and the BGK model yield different temperature and density distributions within the gas has been confirmed by the very recent work of Knackfuss and Barichello [24].

6. Concluding remarks

To conclude this work, we note that we believe our solution to the considered temperature-jump problem is 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 the temperature-jump

coefficient and the temperature and density profiles for some test cases. It should be noted that our complete, species-specific results for the density and temperature 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 as pointed out by Sharipov and Kalempa [22] the solutions can be used for other scattering laws, such the one defined by the Lennard-Jones potential, simply by using appropriate definitions of the omega integrals [5, 27] mentioned in Appendix A.

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 5 or 6 figures of accuracy.

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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

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

where

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

and

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

Here we used

$$r = (m_1/m_2)^{1/2} \quad \text{and} \quad s = (m_2/m_1)^{1/2}, \tag{A.18}$$

along with

$$r^* = r^2/(1 + r^2) \quad \text{and} \quad s^* = s^2/(1 + s^2). \tag{A.19}$$

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 [18], we write

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

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

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

$$\nu^{(4)}_{\alpha,\beta} = \frac{16}{5}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^2 \frac{m_\alpha}{m_\beta} n_\beta \Big(\frac{10}{3}\Omega^{11}_{\alpha,\beta} - \Omega^{22}_{\alpha,\beta}\Big), \tag{A.28}$$

$$\nu^{(5)}_{\alpha,\beta} = \frac{64}{15}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^3 \frac{m_\alpha}{m_\beta} n_\beta \Gamma^{(5)}_{\alpha,\beta} \tag{A.29}$$

and

$$\nu^{(6)}_{\alpha,\beta} = \frac{64}{15}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^3 \Big(\frac{m_\alpha}{m_\beta}\Big)^{3/2} n_\beta \Gamma^{(6)}_{\alpha,\beta}, \tag{A.30}$$

with

$$\Gamma^{(5)}_{\alpha,\beta} = \Omega^{22}_{\alpha,\beta} + \Big(\frac{15m_\alpha}{4m_\beta} + \frac{25m_\beta}{8m_\alpha}\Big)\Omega^{11}_{\alpha,\beta} - \Big(\frac{m_\beta}{2m_\alpha}\Big)\Big(5\Omega^{12}_{\alpha,\beta} - \Omega^{13}_{\alpha,\beta}\Big) \tag{A.31}$$

and, after a correction by Sharipov and Kalempa [22],

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

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 [5,27] which for the case of rigid-sphere interactions take the simple forms

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

with

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

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 components of the kernel $\boldsymbol{K}(\xi',\xi)$ required in Eq. (28) as follows:

$$k_{1,1}(\xi',\xi) = 1 + f_{1,1}(\xi',\xi)\xi'\xi + (2/3)[1 - 2r^*\eta^{(1)}_{1,2} + 2\varpi_1](\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B.1}$$

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

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

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

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

$$k_{2,2}(\xi',\xi) = (2/3)[1 - 2r^*\eta^{(1)}_{1,2}] + (1/3)\varpi_1 + (4/5)\beta_1\xi'\xi, \tag{B.6}$$

$$k_{2,3}(\xi',\xi) = [r\eta_{1,2}^{(2)}+(4/5)\eta_{1,2}^{(6)}(\xi'^2-3/2)]\xi'\xi+(2/3)[2r^*\eta_{1,2}^{(1)}-\eta_{1,2}^{(4)}](\xi'^2-1/2), \quad \text{(B.7)}$$

$$k_{2,4}(\xi',\xi) = (4/5)\eta_{1,2}^{(6)}\xi'\xi + (1/3)[4r^*\eta_{1,2}^{(1)} + \eta_{1,2}^{(4)}], \quad \text{(B.8)}$$

$$k_{3,1}(\xi',\xi) = f_{3,1}(\xi',\xi)\xi'\xi + (4/3)[s^*\eta_{2,1}^{(1)} + \eta_{2,1}^{(4)}](\xi'^2 - 1/2)(\xi^2 - 1/2), \quad \text{(B.9)}$$

$$k_{3,2}(\xi',\xi) = [s^3\eta_{2,1}^{(2)}+(4/5)\eta_{2,1}^{(6)}(\xi^2-3/2)]\xi'\xi+(2/3)[2s^*\eta_{2,1}^{(1)}-\eta_{2,1}^{(4)}](\xi^2-1/2), \quad \text{(B.10)}$$

$$k_{3,3}(\xi',\xi) = 1+f_{3,3}(\xi',\xi)\xi'\xi+(2/3)[1-2s^*\eta_{2,1}^{(1)}+2\varpi_2](\xi'^2-1/2)(\xi^2-1/2), \quad \text{(B.11)}$$

$$k_{3,4}(\xi',\xi) = [(4/5)\beta_2(\xi^2-3/2)-\eta_{2,1}^{(2)}]\xi'\xi+(2/3)[1-2s^*\eta_{2,1}^{(1)}-\varpi_2](\xi^2-1/2), \quad \text{(B.12)}$$

$$k_{4,1}(\xi',\xi) = [s\eta_{2,1}^{(2)}+(4/5)\eta_{2,1}^{(6)}(\xi'^2-3/2)]\xi'\xi+(2/3)[2s^*\eta_{2,1}^{(1)}-\eta_{2,1}^{(4)}](\xi'^2-1/2), \quad \text{(B.13)}$$

$$k_{4,2}(\xi',\xi) = (4/5)\eta_{2,1}^{(6)}\xi'\xi + (1/3)[4s^*\eta_{2,1}^{(1)} + \eta_{2,1}^{(4)}], \quad \text{(B.14)}$$

$$k_{4,3}(\xi',\xi) = [(4/5)\beta_2(\xi'^2-3/2)-\eta_{2,1}^{(2)}]\xi'\xi+(2/3)[1-2s^*\eta_{2,1}^{(1)}-\varpi_2](\xi'^2-1/2) \quad \text{(B.15)}$$

and

$$k_{4,4}(\xi',\xi) = (2/3)[1 - 2s^*\eta_{2,1}^{(1)}] + (1/3)\varpi_2 + (4/5)\beta_2\xi'\xi. \quad \text{(B.16)}$$

Here we have used

$$f_{1,1}(\xi',\xi) = 2[1 - \eta_{1,2}^{(1)}] - \eta_{1,2}^{(2)}(\xi'^2 + \xi^2 - 3) + (4/5)\beta_1(\xi'^2 - 3/2)(\xi^2 - 3/2), \quad \text{(B.17)}$$

$$f_{1,3}(\xi',\xi) = 2r\eta_{1,2}^{(1)} + r\eta_{1,2}^{(2)}[r^2(\xi'^2 - 3/2) + \xi^2 - 3/2] + (4/5)\eta_{1,2}^{(6)}(\xi'^2 - 3/2)(\xi^2 - 3/2), \quad \text{(B.18)}$$

$$f_{3,1}(\xi',\xi) = 2s\eta_{2,1}^{(1)} + s\eta_{2,1}^{(2)}[s^2(\xi'^2 - 3/2) + \xi^2 - 3/2] + (4/5)\eta_{2,1}^{(6)}(\xi'^2 - 3/2)(\xi^2 - 3/2) \quad \text{(B.19)}$$

and

$$f_{3,3}(\xi',\xi) = 2[1 - \eta_{2,1}^{(1)}] - \eta_{2,1}^{(2)}(\xi'^2 + \xi^2 - 3) + (4/5)\beta_2(\xi'^2 - 3/2)(\xi^2 - 3/2). \quad \text{(B.20)}$$

7. Appendix C: Basic elements for defining a linear system

We list here our results for the matrices $\boldsymbol{\mathcal{A}}$, $\boldsymbol{\mathcal{B}}$, $\boldsymbol{\mathcal{C}}$ and $\boldsymbol{\mathcal{D}}$ required to define Eqs. (67), (68), (70) and (71).

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} 1-\eta_{1,2}^{(1)} & -(1/2)\eta_{1,2}^{(2)} & r\eta_{1,2}^{(1)} & (r^3/2)\eta_{1,2}^{(2)} \\ -(1/2)\eta_{1,2}^{(2)} & (2/5)\beta_1 & (r/2)\eta_{1,2}^{(2)} & (2/5)\eta_{1,2}^{(6)} \\ s\eta_{2,1}^{(1)} & (s^3/2)\eta_{2,1}^{(2)} & 1-\eta_{2,1}^{(1)} & -(1/2)\eta_{2,1}^{(2)} \\ (s/2)\eta_{2,1}^{(2)} & (2/5)\eta_{2,1}^{(6)} & -(1/2)\eta_{2,1}^{(2)} & (2/5)\beta_2 \end{bmatrix}, \quad \text{(C.1)}$$

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

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

and

$$\boldsymbol{\mathcal{D}} = \begin{bmatrix} (3/5)\beta_1 & 0 & (3/5)\eta_{1,2}^{(6)} & 0 \\ 0 & 0 & 0 & 0 \\ (3/5)\eta_{2,1}^{(6)} & 0 & (3/5)\beta_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{C.4}$$

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