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The temperature-jump problem based on the linearized Boltzmann equation for a binary mixture of rigid spheres

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Abstract

An analytical version of the discrete-ordinates method (the ADO method) is used with recently reported analytical forms for the rigid-sphere scattering kernels to establish a concise and particularly accurate solution to the temperature-jump problem for a binary gas mixture described by the linearized Boltzmann equation. 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, the temperature and the heat-flow profiles for both types of particles. Numerical results are reported for two binary mixtures (Ne–Ar and He–Xe) with various molar concentrations.

Keywords: Rarefied gas dynamics; Binary mixtures; Rigid spheres; Temperature-jump coefficient

1. Introduction

While the classical temperature-jump problem in rarefied gas dynamics [1–3] has been extensively studied for the case of a single-species gas (see, for example, Refs. [4–11]), there are relatively few works [12–20] devoted to gas mixtures. Almost all of the works on gas mixtures are based on model equations [13,16–19], with the exception of a few that report variational estimates for the temperature-jump coefficient [12,14,15] but do not treat the density and temperature effects in detail and a work [20] that provides a full treatment of the collision term in the linearized Boltzmann equation (LBE) for a binary mixture of rigid-sphere gas particles. As the work in Ref. [20] is based on numerical procedures applied to a fully discretized form of the LBE and is devoted to the special case of complete accommodation for both species at the half-space boundary, we propose in this work a solution of the LBE that is based on recently derived explicit forms of the rigid-sphere collision kernels for binary gas mixtures [21] and the analytical discrete-ordinates (ADO) method [22], and allows a free choice of the accommodation coefficient for each species at the confining surface. Our approach relies on a continuous treatment of both the space and speed variables that has proved to be particularly efficient and accurate.

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2. Basic formulation

Before starting our work that is specific to the temperature-jump problem, we review here our analytical formulation of the linearized Boltzmann equation for a binary mixture of rigid spheres. This formulation was started in Ref. [21] and was further developed in Refs. [23] and [24]. Considering what has gone before this work, we write the coupled linearized Boltzmann equation (for variations only in the z direction) for the considered binary mixture of rigid spheres as

$$c\mu\frac{\partial}{\partial z}\boldsymbol{H}(z,\boldsymbol{c})+\varepsilon_0\boldsymbol{V}(c)\boldsymbol{H}(z,\boldsymbol{c})=\varepsilon_0\int \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}(\boldsymbol{c}':\boldsymbol{c})\boldsymbol{H}(z,\boldsymbol{c}')\,\mathrm{d}^3c', \tag{2.1}$$

where

$$\boldsymbol{H}(z,\boldsymbol{c})=\begin{bmatrix}h_1(z,\boldsymbol{c})\\ h_2(z,\boldsymbol{c})\end{bmatrix}. \tag{2.2}$$

At this point ε_0 is an arbitrary parameter that we (soon) will use to define a dimensionless spatial variable. Since Eq. (2.1) is written in terms of a dimensionless velocity variable $\boldsymbol{c}$, we note that the basic velocity distribution functions are available from

$$f_\alpha(z,\boldsymbol{v})=f_{\alpha,0}(v)\big[1+h_\alpha\big(z,\lambda_\alpha^{1/2}\boldsymbol{v}\big)\big],\quad \alpha=1,2, \tag{2.3}$$

where $\lambda_\alpha=m_\alpha/(2kT_0)$ and where

$$f_{\alpha,0}(v)=n_\alpha(\lambda_\alpha/\pi)^{3/2}\,\mathrm{e}^{-\lambda_\alpha v^2} \tag{2.4}$$

is the Maxwellian distribution for n_α particles of mass m_α in equilibrium at temperature T_0. Here, k is the Boltzmann constant. Continuing, we note that we use spherical coordinates $\{c,\theta,\phi\}$, with $\mu=\cos\theta$, to describe the dimensionless velocity vector, so that $\boldsymbol{H}(z,\boldsymbol{c})\Leftrightarrow\boldsymbol{H}(z,c,\mu,\phi)$. In addition,

$$\boldsymbol{V}(c)=(1/\varepsilon_0)\boldsymbol{\Sigma}(c) \tag{2.5}$$

and

$$\boldsymbol{\mathcal{K}}(\boldsymbol{c}':\boldsymbol{c})=(1/\varepsilon_0)\boldsymbol{K}(\boldsymbol{c}':\boldsymbol{c}), \tag{2.6}$$

where $\boldsymbol{\Sigma}(c)$ and $\boldsymbol{K}(\boldsymbol{c}':\boldsymbol{c})$ are as defined in Ref. [24]: first of all,

$$\boldsymbol{\Sigma}(c)=\begin{bmatrix}\varpi_1(c) & 0\\ 0 & \varpi_2(c)\end{bmatrix}, \tag{2.7}$$

with

$$\varpi_\alpha(c)=\varpi_\alpha^{(1)}(c)+\varpi_\alpha^{(2)}(c), \tag{2.8}$$

$$\varpi_\alpha^{(\beta)}(c)=4\pi^{1/2}n_\beta\sigma_{\alpha,\beta}a_{\beta,\alpha}\nu(a_{\alpha,\beta}c), \tag{2.9}$$

and

$$\nu(c)=\frac{2c^2+1}{c}\int_0^c \mathrm{e}^{-x^2}\,\mathrm{d}x+\mathrm{e}^{-c^2}. \tag{2.10}$$

Here

$$a_{\alpha,\beta}=(m_\beta/m_\alpha)^{1/2},\quad \alpha,\beta=1,2, \tag{2.11}$$

and to be clear, we note that we use $\sigma_{\alpha,\beta}$ to denote the differential-scattering cross section, which for the case of rigid-sphere scattering that is isotropic in the center-of-mass system, we write, after consultation with Chapman and Cowling [25], as

$$\sigma_{\alpha,\beta}=\frac{1}{4}\left(\frac{d_\alpha+d_\beta}{2}\right)^2, \tag{2.12}$$

where d_1 and d_2 are the atomic diameters of the two types of gas particles. Next, we again consult Ref. [24] and write

$$\boldsymbol{K}(\boldsymbol{c}' : \boldsymbol{c}) = \begin{bmatrix} K_{1,1}(\boldsymbol{c}' : \boldsymbol{c}) & K_{1,2}(\boldsymbol{c}' : \boldsymbol{c}) \\ K_{2,1}(\boldsymbol{c}' : \boldsymbol{c}) & K_{2,2}(\boldsymbol{c}' : \boldsymbol{c}) \end{bmatrix}, \tag{2.13}$$

where

$$K_{1,1}(\boldsymbol{c}' : \boldsymbol{c}) = 4n_1\sigma_{1,1}\pi^{1/2}\mathcal{P}(\boldsymbol{c}' : \boldsymbol{c}) + n_2\sigma_{1,2}\pi^{1/2}\mathcal{F}_{1,2}(\boldsymbol{c}' : \boldsymbol{c}), \tag{2.14}$$

$$K_{1,2}(\boldsymbol{c}' : \boldsymbol{c}) = 4n_2\sigma_{1,2}\pi^{1/2}\mathcal{G}_{1,2}(\boldsymbol{c}' : \boldsymbol{c}), \tag{2.15}$$

$$K_{2,1}(\boldsymbol{c}' : \boldsymbol{c}) = 4n_1\sigma_{2,1}\pi^{1/2}\mathcal{G}_{2,1}(\boldsymbol{c}' : \boldsymbol{c}), \tag{2.16}$$

and

$$K_{2,2}(\boldsymbol{c}' : \boldsymbol{c}) = 4n_2\sigma_{2,2}\pi^{1/2}\mathcal{P}(\boldsymbol{c}' : \boldsymbol{c}) + n_1\sigma_{2,1}\pi^{1/2}\mathcal{F}_{2,1}(\boldsymbol{c}' : \boldsymbol{c}). \tag{2.17}$$

Here

$$\mathcal{P}(\boldsymbol{c}' : \boldsymbol{c}) = \frac{1}{\pi}\left(\frac{2}{|\boldsymbol{c}' - \boldsymbol{c}|}\exp\left\{\frac{|\boldsymbol{c}' \times \boldsymbol{c}|^2}{|\boldsymbol{c}' - \boldsymbol{c}|^2}\right\} - |\boldsymbol{c}' - \boldsymbol{c}|\right) \tag{2.18}$$

is the basic kernel for a single-species gas used by Pekeris [26]. In addition,

$$\mathcal{F}_{\alpha,\beta}(\boldsymbol{c}' : \boldsymbol{c}) = \mathcal{F}(a_{\alpha,\beta}; \boldsymbol{c}' : \boldsymbol{c}) \tag{2.19}$$

and

$$\mathcal{G}_{\alpha,\beta}(\boldsymbol{c}' : \boldsymbol{c}) = \mathcal{G}(a_{\alpha,\beta}; \boldsymbol{c}' : \boldsymbol{c}), \tag{2.20}$$

where [23]

$$\mathcal{F}(a; \boldsymbol{c}' : \boldsymbol{c}) = \frac{(a^2+1)^2}{a^3\pi|\boldsymbol{c}' - \boldsymbol{c}|}\exp\left\{a^2\frac{|\boldsymbol{c}' \times \boldsymbol{c}|^2}{|\boldsymbol{c}' - \boldsymbol{c}|^2} - \frac{(1-a^2)^2(c'^2 + c^2)}{4a^2} - \frac{(a^4-1)\boldsymbol{c}' \cdot \boldsymbol{c}}{2a^2}\right\}, \tag{2.21}$$

and

$$\mathcal{G}(a; \boldsymbol{c}' : \boldsymbol{c}) = \frac{1}{a\pi}|\boldsymbol{c}' - a\boldsymbol{c}|\big[J(a; \boldsymbol{c}' : \boldsymbol{c}) - 1\big], \tag{2.22}$$

with

$$J(a; \boldsymbol{c}' : \boldsymbol{c}) = \frac{(a+1/a)^2}{2\Delta(a; \boldsymbol{c}' : \boldsymbol{c})}\exp\left\{\frac{-2C(a; \boldsymbol{c}' : \boldsymbol{c})}{(a-1/a)^2}\right\}\sinh\left\{\frac{2\Delta(a; \boldsymbol{c}' : \boldsymbol{c})}{(a-1/a)^2}\right\}, \quad a \neq 1, \tag{2.23a}$$

and

$$J(a; \boldsymbol{c}' : \boldsymbol{c}) = \frac{1}{|\boldsymbol{c}' - \boldsymbol{c}|^2}\exp\left\{\frac{|\boldsymbol{c}' \times \boldsymbol{c}|^2}{|\boldsymbol{c}' - \boldsymbol{c}|^2}\right\}, \quad a = 1. \tag{2.23b}$$

To write Eq. (2.23a), we have used the definitions [23]

$$\Delta(a; \boldsymbol{c}' : \boldsymbol{c}) = \left\{C^2(a; \boldsymbol{c}' : \boldsymbol{c}) + (a-1/a)^2|\boldsymbol{c}' \times \boldsymbol{c}|^2\right\}^{1/2} \tag{2.24}$$

and

$$C(a; \boldsymbol{c}' : \boldsymbol{c}) = c'^2 + c^2 - (a+1/a)\boldsymbol{c}' \cdot \boldsymbol{c}. \tag{2.25}$$

We wish to make use of a dimensionless spatial variable that is based on the physical properties of both species of particles, and so we choose to follow Ref. [24] and let

$$\varepsilon_0 = (n_1+n_2)\pi^{1/2}\left(\frac{n_1d_1 + n_2d_2}{n_1+n_2}\right)^2 \tag{2.26}$$

and then

$$\tau = z\varepsilon_0. \tag{2.27}$$

Introducing the spatial variable τ and noting that the considered (temperature-jump) problem has azimuthal symmetry, we find it convenient to define our work in terms of

$$\boldsymbol{\Psi}(\tau, c, \mu) = \frac{1}{2\pi} \int_0^{2\pi} \boldsymbol{H}(\tau/\varepsilon_0, \boldsymbol{c})\, \mathrm{d}\phi \tag{2.28}$$

and deduce from Eq. (2.1) that

$$c\mu \frac{\partial}{\partial \tau} \boldsymbol{\Psi}(\tau, c, \mu) + \boldsymbol{V}(c)\boldsymbol{\Psi}(\tau, c, \mu) = \int_0^{\infty} \int_{-1}^{1} \mathrm{e}^{-c'^2} \boldsymbol{\mathcal{K}}(c', \mu' : c, \mu) \boldsymbol{\Psi}(\tau, c', \mu') c'^2 \, \mathrm{d}\mu' \, \mathrm{d}c'. \tag{2.29}$$

Here

$$\boldsymbol{\mathcal{K}}(c', \mu' : c, \mu) = \int_0^{2\pi} \boldsymbol{\mathcal{K}}(\boldsymbol{c}' : \boldsymbol{c})\, \mathrm{d}\phi. \tag{2.30}$$

We find from Ref. [24] that we can write

$$\boldsymbol{\mathcal{K}}(c', \mu' : c, \mu) = \frac{1}{2} \sum_{n=0}^{\infty} (2n+1) P_n(\mu') P_n(\mu) \boldsymbol{\mathcal{K}}_n(c', c), \tag{2.31}$$

where

$$\boldsymbol{\mathcal{K}}_n(c', c) = \begin{bmatrix} \mathcal{K}_n^{(1,1)}(c', c) & \mathcal{K}_n^{(1,2)}(c', c) \\ \mathcal{K}_n^{(2,1)}(c', c) & \mathcal{K}_n^{(2,2)}(c', c) \end{bmatrix}, \tag{2.32}$$

with

$$\mathcal{K}_n^{(1,1)}(c', c) = p_1 \mathcal{P}^{(n)}(c', c) + (g_2/4) \mathcal{F}^{(n)}(a_{1,2}; c', c), \tag{2.33a}$$

$$\mathcal{K}_n^{(1,2)}(c', c) = g_2 \mathcal{G}^{(n)}(a_{1,2}; c', c), \tag{2.33b}$$

$$\mathcal{K}_n^{(2,1)}(c', c) = g_1 \mathcal{G}^{(n)}(a_{2,1}; c', c), \tag{2.33c}$$

and

$$\mathcal{K}_n^{(2,2)}(c', c) = p_2 \mathcal{P}^{(n)}(c', c) + (g_1/4) \mathcal{F}^{(n)}(a_{2,1}; c', c). \tag{2.33d}$$

We also can write

$$\boldsymbol{V}(c) = \begin{bmatrix} v_1(c) & 0 \\ 0 & v_2(c) \end{bmatrix}, \tag{2.34}$$

where now

$$v_1(c) = p_1 \nu(c) + g_2 a_{2,1} \nu(a_{1,2} c) \tag{2.35a}$$

and

$$v_2(c) = p_2 \nu(c) + g_1 a_{1,2} \nu(a_{2,1} c). \tag{2.35b}$$

In writing Eqs. (2.33) and (2.35), we have used

$$p_\alpha = c_\alpha \left(\frac{n d_\alpha}{n_1 d_1 + n_2 d_2} \right)^2, \quad \alpha = 1, 2, \tag{2.36a}$$

and

$$g_\alpha = c_\alpha \left(\frac{n d_{\mathrm{avg}}}{n_1 d_1 + n_2 d_2} \right)^2, \quad \alpha = 1, 2, \tag{2.36b}$$

where

$$c_\alpha = n_\alpha/n, \quad n = n_1 + n_2, \quad \text{and} \quad d_{\text{avg}} = (d_1 + d_2)/2. \tag{2.37a–c}$$

In order to avoid too much repetition, we do not list here our expressions for the Legendre moments $\mathcal{P}^{(n)}(c', c)$, $\mathcal{F}^{(n)}(a; c', c)$, and $\mathcal{G}^{(n)}(a; c', c)$ since they are explicitly given in Ref. [24].

At the confining surface of the considered half-space, we use a combination of specular and diffuse reflection, and so, in regard to Eq. (2.1), we write the boundary condition as

$$\boldsymbol{H}(0, c, \mu, \phi) - (\boldsymbol{I} - \boldsymbol{\alpha})\boldsymbol{H}(0, c, -\mu, \phi) - \frac{2}{\pi}\boldsymbol{\alpha}\int_0^\infty\int_0^1\int_0^{2\pi} \mathrm{e}^{-c'^2}\boldsymbol{H}(0, c', -\mu', \phi')c'^3\mu'\,\mathrm{d}\phi'\,\mathrm{d}\mu'\,\mathrm{d}c' = \boldsymbol{0}, \tag{2.38}$$

for $\mu \in (0, 1]$ and all c and all ϕ. Here, $\boldsymbol{I}$ is the 2×2 identity matrix and

$$\boldsymbol{\alpha} = \text{diag}\{\alpha_1, \alpha_2\}, \tag{2.39}$$

where α_1 and α_2 are the accommodation coefficients to be used for the two species of gas particles. Taking note of Eq. (2.28), we find from Eq. (2.38) the boundary condition subject to which we must solve Eq. (2.29), viz.

$$\boldsymbol{\Psi}(0, c, \mu) - (\boldsymbol{I} - \boldsymbol{\alpha})\boldsymbol{\Psi}(0, c, -\mu) - 4\boldsymbol{\alpha}\int_0^\infty\int_0^1 \mathrm{e}^{-c'^2}\boldsymbol{\Psi}(0, c', -\mu')c'^3\mu'\,\mathrm{d}\mu'\,\mathrm{d}c' = \boldsymbol{0}, \tag{2.40}$$

for $\mu \in (0, 1]$ and all c.

In this work, we intend to compute the density, the temperature, and the heat-flow perturbations (see Appendix A for a discussion of these and other macroscopic quantities of interest), i.e.,

$$N_\alpha(z) = \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z, \boldsymbol{c})\,\mathrm{d}^3c, \tag{2.41a}$$

$$T_\alpha(z) = \frac{2}{3\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z, \boldsymbol{c})\big(c^2 - 3/2\big)\,\mathrm{d}^3c, \tag{2.41b}$$

and

$$Q_\alpha(z) = \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z, \boldsymbol{c})\big(c^2 - 5/2\big)c\mu\,\mathrm{d}^3c, \tag{2.41c}$$

for $\alpha = 1$ and 2. Thus, making use of the dimensionless spatial variable and matrix notation, we can express the desired perturbations as

$$\boldsymbol{N}(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} \mathrm{e}^{-c^2}\boldsymbol{H}(\tau/\varepsilon_0, \boldsymbol{c})c^2\,\mathrm{d}\phi\,\mathrm{d}\mu\,\mathrm{d}c, \tag{2.42a}$$

$$\boldsymbol{T}(\tau) = \frac{2}{3\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} \mathrm{e}^{-c^2}\boldsymbol{H}(\tau/\varepsilon_0, \boldsymbol{c})\big(c^2 - 3/2\big)c^2\,\mathrm{d}\phi\,\mathrm{d}\mu\,\mathrm{d}c, \tag{2.42b}$$

and

$$\boldsymbol{Q}(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty\int_{-1}^1\int_0^{2\pi} \mathrm{e}^{-c^2}\boldsymbol{H}(\tau/\varepsilon_0, \boldsymbol{c})\big(c^2 - 5/2\big)c^3\mu\,\mathrm{d}\phi\,\mathrm{d}\mu\,\mathrm{d}c \tag{2.42c}$$

or

$$\boldsymbol{N}(\tau) = \frac{2}{\pi^{1/2}}\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c^2}\boldsymbol{\Psi}(\tau, c, \mu)c^2\,\mathrm{d}\mu\,\mathrm{d}c, \tag{2.43a}$$

$$\boldsymbol{T}(\tau) = \frac{4}{3\pi^{1/2}} \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} \boldsymbol{\Psi}(\tau, c, \mu)\big(c^2 - 3/2\big)c^2 \,\mathrm{d}\mu \,\mathrm{d}c, \tag{2.43b}$$

and

$$\boldsymbol{Q}(\tau) = \frac{2}{\pi^{1/2}} \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} \boldsymbol{\Psi}(\tau, c, \mu)\big(c^2 - 5/2\big)c^3\mu \,\mathrm{d}\mu \,\mathrm{d}c. \tag{2.43c}$$

Now, since there is no driving term in Eq. (2.1) we require that the solutions $h_\alpha(z, \boldsymbol{c})$ diverge as z tends to infinity, but at the same time we impose a (generalized) Welander condition [1] on the temperature of the gas mixture, viz.

$$\lim_{\tau\to\infty} [c_1 \quad c_2] \frac{\mathrm{d}}{\mathrm{d}\tau} \boldsymbol{T}(\tau) = \mathcal{K}. \tag{2.44}$$

Here $\mathcal{K}$ is a normalizing constant which we henceforth set equal to unity. At this point we are ready to discuss the ADO method and to develop a (diverging as τ tends to infinity) solution of the problem defined by Eqs. (2.29), (2.40) and (2.44).

3. An expansion in the speed variable

In order to account for the c dependence of $\boldsymbol{\Psi}(\tau, c, \mu)$ we introduce the (approximate) representation

$$\boldsymbol{\Psi}(\tau, c, \mu) = \sum_{k=0}^{K} \Pi_k(c) \boldsymbol{G}_k(\tau, \mu), \tag{3.1}$$

where $\{\Pi_k(c)\}$ is a collection of basis functions to be specified. And so we substitute Eq. (3.1) into Eqs. (2.29) and (2.40), multiply the resulting equations by

$$c^2 \exp\big\{-c^2\big\}\Pi_l(c)$$

and integrate over all c to find

$$\mu \frac{\partial}{\partial\tau} \boldsymbol{A}\boldsymbol{G}(\tau, \mu) + \boldsymbol{S}\boldsymbol{G}(\tau, \mu) = \int_{-1}^1 \boldsymbol{C}(\mu' : \mu)\boldsymbol{G}(\tau, \mu') \,\mathrm{d}\mu' \tag{3.2}$$

and

$$\boldsymbol{F}\boldsymbol{G}(0, \mu) - \boldsymbol{H}\boldsymbol{G}(0, -\mu) - \boldsymbol{J} \int_0^1 \boldsymbol{G}(0, -\mu')\mu' \,\mathrm{d}\mu' = \boldsymbol{0}, \quad \mu \in (0, 1]. \tag{3.3}$$

Here

$$\boldsymbol{G}(\tau, \mu) = \big[\boldsymbol{G}_0(\tau, \mu), \boldsymbol{G}_1(\tau, \mu), \ldots, \boldsymbol{G}_K(\tau, \mu)\big]^{\mathrm{T}}, \tag{3.4}$$

where the superscript T denotes the transpose operation, and the $2(K + 1) \times 2(K + 1)$ matrices $\boldsymbol{A}$, $\boldsymbol{S}$ and $\boldsymbol{C}(\mu' : \mu)$ have 2×2 elements given by

$$\boldsymbol{A}_{l,k} = \boldsymbol{I} \int_0^\infty \mathrm{e}^{-c^2} c^3 \Pi_l(c)\Pi_k(c) \,\mathrm{d}c, \tag{3.5a}$$

$$\boldsymbol{S}_{l,k} = \int_0^\infty \mathrm{e}^{-c^2} c^2 \Pi_l(c)\boldsymbol{V}(c)\Pi_k(c) \,\mathrm{d}c, \tag{3.5b}$$

and

$$\boldsymbol{C}_{l,k}(\mu' : \mu) = \int_0^\infty \int_0^\infty \mathrm{e}^{-c^2}\, \mathrm{e}^{-c'^2} c^2 c'^2 \Pi_l(c) \mathcal{K}(c', \mu' : c, \mu) \Pi_k(c')\, \mathrm{d}c'\, \mathrm{d}c. \tag{3.5c}$$

In addition, we define the $2(K+1) \times 2(K+1)$ matrices

$$\boldsymbol{F} = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c) \boldsymbol{P}(c) c^2\, \mathrm{d}c, \tag{3.6a}$$

$$\boldsymbol{H} = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c) (\boldsymbol{I} - \boldsymbol{\alpha}) \boldsymbol{P}(c) c^2\, \mathrm{d}c, \tag{3.6b}$$

and

$$\boldsymbol{J} = 4 \boldsymbol{P}_0^{\mathrm{T}} \boldsymbol{\alpha} \boldsymbol{P}_1, \tag{3.6c}$$

where

$$\boldsymbol{P}_n = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}(c) c^{n+2}\, \mathrm{d}c, \tag{3.7}$$

with the $2 \times 2(K+1)$ matrix $\boldsymbol{P}(c)$ given by

$$\boldsymbol{P}(c) = \big[\Pi_0(c) \boldsymbol{I} \quad \Pi_1(c) \boldsymbol{I} \cdots \Pi_K(c) \boldsymbol{I} \big]. \tag{3.8}$$

And so we now proceed to develop our ADO (analytical discrete ordinates) solution of Eqs. (3.2) and (3.3) in order to compute the density, temperature, and heat-flow perturbations as defined by Eqs. (2.43).

4. Elementary (ADO) solutions

Seeking separable solutions of Eq. (3.2), we substitute

$$\boldsymbol{G}(\tau, \mu) = \boldsymbol{\Phi}(\nu, \mu)\, \mathrm{e}^{-\tau/\nu} \tag{4.1}$$

into that equation to find

$$\boldsymbol{S}\boldsymbol{U}(\nu, \mu) - \int_0^1 \boldsymbol{C}_+(\mu' : \mu) \boldsymbol{U}(\nu, \mu')\, \mathrm{d}\mu' = (\mu/\nu) \boldsymbol{A}\boldsymbol{V}(\nu, \mu) \tag{4.2a}$$

and

$$\boldsymbol{S}\boldsymbol{V}(\nu, \mu) - \int_0^1 \boldsymbol{C}_-(\mu' : \mu) \boldsymbol{V}(\nu, \mu')\, \mathrm{d}\mu' = (\mu/\nu) \boldsymbol{A}\boldsymbol{U}(\nu, \mu), \tag{4.2b}$$

where

$$\boldsymbol{C}_\pm(\mu' : \mu) = \boldsymbol{C}(\mu' : \mu) \pm \boldsymbol{C}(-\mu' : \mu). \tag{4.3}$$

Here

$$\boldsymbol{U}(\nu, \mu) = \boldsymbol{\Phi}(\nu, \mu) + \boldsymbol{\Phi}(\nu, -\mu) \tag{4.4a}$$

and

$$\boldsymbol{V}(\nu, \mu) = \boldsymbol{\Phi}(\nu, \mu) - \boldsymbol{\Phi}(\nu, -\mu). \tag{4.4b}$$

We can now substitute $\boldsymbol{U}(\nu,\mu)$ from Eq. (4.2b) into Eq. (4.2a) to find

$$\left(1/\mu^2\right)\left[\boldsymbol{\Sigma}^2\boldsymbol{V}(\nu,\mu)-\int_0^1 \boldsymbol{\mathcal{B}}(\mu':\mu)\boldsymbol{V}(\nu,\mu')\,\mathrm{d}\mu'\right]=\lambda\boldsymbol{V}(\nu,\mu), \tag{4.5}$$

where

$$\lambda=1/\nu^2, \tag{4.6}$$

$$\boldsymbol{\mathcal{B}}(\mu':\mu)=(\mu/\mu')\boldsymbol{B}_+(\mu':\mu)\boldsymbol{\Sigma}+\boldsymbol{\Sigma}\boldsymbol{B}_-(\mu':\mu)-\int_0^1(\mu/\mu'')\boldsymbol{B}_+(\mu'':\mu)\boldsymbol{B}_-(\mu':\mu'')\,\mathrm{d}\mu'', \tag{4.7}$$

$$\boldsymbol{\Sigma}=\boldsymbol{A}^{-1}\boldsymbol{S}, \tag{4.8}$$

and

$$\boldsymbol{B}_\pm(\mu':\mu)=\frac{1}{2}\sum_{n=0}^{\infty}(2n+1)\left[1\pm(-1)^n\right]P_n(\mu')P_n(\mu)\boldsymbol{B}_n, \tag{4.9}$$

where

$$\boldsymbol{B}_n=\boldsymbol{A}^{-1}\boldsymbol{C}_n \tag{4.10}$$

and where the $2(K+1)\times 2(K+1)$ matrices $\boldsymbol{C}_n$ have 2×2 elements given by

$$\boldsymbol{C}_{l,k}^{(n)}=\int_0^\infty\int_0^\infty \mathrm{e}^{-c^2}\,\mathrm{e}^{-c'^2}c^2c'^2\Pi_l(c)\boldsymbol{\mathcal{K}}_n(c',c)\Pi_k(c')\,\mathrm{d}c'\,\mathrm{d}c. \tag{4.11}$$

We rewrite Eq. (4.7) as

$$\boldsymbol{\mathcal{B}}(\mu':\mu)=(\mu/\mu')\boldsymbol{B}_+(\mu':\mu)\boldsymbol{\Sigma}+\boldsymbol{\Sigma}\boldsymbol{B}_-(\mu':\mu)-\mu\sum_{m=0}^{\infty}\sum_{m'=m}^{\infty}\Delta_{m,m'}P_{2m}(\mu)P_{2m'+1}(\mu')\boldsymbol{B}_{2m}\boldsymbol{B}_{2m'+1}, \tag{4.12}$$

where

$$\Delta_{m,m'}=(4m+1)(4m'+3)\int_0^1 P_{2m}(x)P_{2m'+1}(x)\frac{\mathrm{d}x}{x} \tag{4.13}$$

or

$$\Delta_{m,m'}=\left[(2m'+1)P_{2m'}(0)\right]^{-1}(4m+1)(4m'+3)P_{2m}(0),\quad m\leqslant m', \tag{4.14}$$

with

$$P_{\alpha+2}(0)=-\left(\frac{\alpha+1}{\alpha+2}\right)P_\alpha(0),\quad \alpha=0,2,\ldots,\quad \text{and}\quad P_0(0)=1. \tag{4.15a,b}$$

We now introduce a "half-range" quadrature scheme (with weights and nodes w_k and μ_k) and rewrite Eqs. (4.5) and (4.2b) evaluated at the quadrature points as

$$\left(1/\mu_i^2\right)\left[\boldsymbol{\Sigma}^2\boldsymbol{V}(\nu_j,\mu_i)-\sum_{k=1}^{N}w_k\boldsymbol{\mathcal{B}}(\mu_k:\mu_i)\boldsymbol{V}(\nu_j,\mu_k)\right]=\lambda_j\boldsymbol{V}(\nu_j,\mu_i) \tag{4.16a}$$

and

$$\boldsymbol{U}(\nu_j,\mu_i)=(\nu_j/\mu_i)\left[\boldsymbol{\Sigma}\boldsymbol{V}(\nu_j,\mu_i)-\sum_{k=1}^{N}w_k\boldsymbol{B}_-(\mu_k:\mu_i)\boldsymbol{V}(\nu_j,\mu_k)\right], \tag{4.16b}$$

for $i = 1, 2, \ldots, N$. Equation (4.16a) 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

$$\boldsymbol{\Phi}(\nu_j, \mu_i) = (1/2)\big[\boldsymbol{U}(\nu_j, \mu_i) + \boldsymbol{V}(\nu_j, \mu_i)\big] \tag{4.17a}$$

and

$$\boldsymbol{\Phi}(\nu_j, -\mu_i) = (1/2)\big[\boldsymbol{U}(\nu_j, \mu_i) - \boldsymbol{V}(\nu_j, \mu_i)\big]. \tag{4.17b}$$

Note that the separation constants defined by

$$\nu_j = \pm\lambda_j^{-1/2} \tag{4.18}$$

occur in $\pm$ pairs. From this point, we take ν_j to be the positive root listed in Eq. (4.18). Once we have solved the eigenvalue problem defined by Eq. (4.16a), we can write our general (discrete-ordinates) solution to Eq. (3.2) as

$$\boldsymbol{G}(\tau, \pm\mu_i) = \sum_{j=1}^{J} \big[A_j \boldsymbol{\Phi}(\nu_j, \pm\mu_i)\, \mathrm{e}^{-\tau/\nu_j} + B_j \boldsymbol{\Phi}(\nu_j, \mp\mu_i)\, \mathrm{e}^{\tau/\nu_j}\big], \tag{4.19}$$

for $i = 1, 2, \ldots, N$. Here $J = 2N(K+1)$, and the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the boundary conditions of a specific problem.

5. The complete speed-dependent ADO solution

If we combine Eqs. (3.1), (3.8) and (4.19) we can write our (approximate) solution as

$$\boldsymbol{\Psi}(\tau, c, \pm\mu_i) = \boldsymbol{P}(c) \sum_{j=1}^{J} \big[A_j \boldsymbol{\Phi}(\nu_j, \pm\mu_i)\, \mathrm{e}^{-\tau/\nu_j} + B_j \boldsymbol{\Phi}(\nu_j, \mp\mu_i)\, \mathrm{e}^{\tau/\nu_j}\big], \tag{5.1}$$

for $i = 1, 2, \ldots, N$. While Eq. (5.1) is our general (discrete-ordinates) solution, we can make some improvements in that result. We have found that the eigenvalue problem defined by Eq. (4.16a) yields three 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. (5.1) and rewrite that equation as

$$\boldsymbol{\Psi}(\tau, c, \pm\mu_i) = \boldsymbol{\Psi}_*(\tau, c, \pm\mu_i) + \boldsymbol{P}(c) \sum_{j=4}^{J} \big[A_j \boldsymbol{\Phi}(\nu_j, \pm\mu_i)\, \mathrm{e}^{-\tau/\nu_j} + B_j \boldsymbol{\Phi}(\nu_j, \mp\mu_i)\, \mathrm{e}^{\tau/\nu_j}\big], \tag{5.2}$$

for $i = 1, 2, \ldots, N$. We note that $\boldsymbol{\Psi}_*(\tau, c, \mu)$ is defined in terms of the elementary solutions we reported in a previous work [24], viz.

$$\begin{aligned}\boldsymbol{\Psi}_*(\tau, c, \mu) &= A_1 \boldsymbol{H}_1 + A_2 \boldsymbol{H}_2 + A_3 \boldsymbol{H}_3(c) + B_1 \boldsymbol{H}_4(c, \mu) + B_2\big[\tau \boldsymbol{\Phi}_1(c) - \mu \boldsymbol{A}^{(1)}(c)\big] + B_3\big[\tau \boldsymbol{\Phi}_2(c) - \mu \boldsymbol{A}^{(2)}(c)\big], \end{aligned} \tag{5.3}$$

where

$$\boldsymbol{H}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \boldsymbol{H}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \boldsymbol{H}_3(c) = c^2 \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \text{and} \quad \boldsymbol{H}_4(c, \mu) = c\mu \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix}. \tag{5.4a–d}$$

In addition, the $\boldsymbol{A}^{(\alpha)}(c)$ are [24] solutions of the two generalized Chapman–Enskog (vector-valued) integral equations

$$\boldsymbol{V}(c)\boldsymbol{A}^{(\alpha)}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{\mathcal{K}}_1(c', c) \boldsymbol{A}^{(\alpha)}(c') c'^2 \, \mathrm{d}c' = c \boldsymbol{\Phi}_\alpha(c), \quad \alpha = 1, 2, \tag{5.5}$$

for $c \in [0, \infty)$. Here

$$\boldsymbol{\Phi}_\alpha(c) = \boldsymbol{\Phi}_{\alpha,0} + \big(c^2 - 5/2\big)\boldsymbol{\Phi}_{\alpha,2}, \quad \alpha = 1, 2, \tag{5.6}$$

with

$$\boldsymbol{\Phi}_{1,0}=\begin{bmatrix} c_1-1 \\ c_1 \end{bmatrix}, \quad \boldsymbol{\Phi}_{1,2}=\begin{bmatrix} c_1 \\ c_1 \end{bmatrix}, \quad \boldsymbol{\Phi}_{2,0}=\begin{bmatrix} c_2 \\ c_2-1 \end{bmatrix}, \quad \text{and} \quad \boldsymbol{\Phi}_{2,2}=\begin{bmatrix} c_2 \\ c_2 \end{bmatrix}. \tag{5.7a–d}$$

Note that Eqs. (2.32) and (2.34) are required to complete the definition of Eq. (5.5). And finally, since Eq. (5.5) does not uniquely define $\boldsymbol{A}^{(\alpha)}(c)$, we have, as in our previous work [24], imposed the normalization conditions

$$[c_1 \quad c_2]\int_0^\infty \mathrm{e}^{-c^2}\boldsymbol{A}^{(\alpha)}(c)c^3\,\mathrm{d}c=0, \quad \alpha=1,2, \tag{5.8}$$

to determine λ_α after adding

$$\boldsymbol{A}_{h,\alpha}(c)=\lambda_\alpha c\begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix} \tag{5.9}$$

to any computed solution of Eq. (5.5).

6. The temperature-jump problem

Having completed our general development, we are ready to solve the temperature-jump problem for a binary mixture of rigid spheres. Noting Eqs. (2.43b) and (2.44), we conclude that we must delete the terms in Eq. (5.2) that diverge exponentially as τ tends to infinity. We thus now have

$$\boldsymbol{\Psi}(\tau,c,\pm\mu_i)=\boldsymbol{\Psi}_*(\tau,c,\pm\mu_i)+\boldsymbol{P}(c)\sum_{j=4}^{J}A_j\boldsymbol{\Phi}(\nu_j,\pm\mu_i)\,\mathrm{e}^{-\tau/\nu_j}. \tag{6.1}$$

We can use Eqs. (5.3) and (6.1) to find from Eqs. (2.43a) and (2.43b)

$$\boldsymbol{N}(\tau)=\boldsymbol{N}_*(\tau)+\sum_{j=4}^{J}A_j\boldsymbol{N}_j\,\mathrm{e}^{-\tau/\nu_j} \tag{6.2a}$$

and

$$\boldsymbol{T}(\tau)=\boldsymbol{T}_*(\tau)+\sum_{j=4}^{J}A_j\boldsymbol{T}_j\,\mathrm{e}^{-\tau/\nu_j}, \tag{6.2b}$$

where

$$\boldsymbol{N}_*(\tau)=\begin{bmatrix} A_1+(3/2)A_3-B_2\tau \\ A_2+(3/2)A_3-B_3\tau \end{bmatrix} \tag{6.3a}$$

and

$$\boldsymbol{T}_*(\tau)=\begin{bmatrix} A_3+(c_1B_2+c_2B_3)\tau \\ A_3+(c_1B_2+c_2B_3)\tau \end{bmatrix}. \tag{6.3b}$$

In addition,

$$\boldsymbol{N}_j=\frac{2}{\pi^{1/2}}\boldsymbol{P}_0\boldsymbol{X}_j \tag{6.4a}$$

and

$$\boldsymbol{T}_j=\frac{4}{3\pi^{1/2}}\big[\boldsymbol{P}_2-(3/2)\boldsymbol{P}_0\big]\boldsymbol{X}_j, \tag{6.4b}$$

where $\boldsymbol{P}_0$ and $\boldsymbol{P}_2$ are defined by Eq. (3.7), and where

$$\boldsymbol{X}_j=\sum_{k=1}^{N}w_k\big[\boldsymbol{\Phi}(\nu_j,\mu_k)+\boldsymbol{\Phi}(\nu_j,-\mu_k)\big]. \tag{6.5}$$

Using Eq. (2.44) and the fact that we have imposed the normalization $\mathcal{K} = 1$, we find

$$c_1 B_2 + c_2 B_3 = 1, \tag{6.6}$$

which allows us to rewrite Eq. (6.3b) as

$$\boldsymbol{T}_*(\tau) = (\zeta + \tau)\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \tag{6.7}$$

where

$$\zeta = A_3 \tag{6.8}$$

is the temperature-jump coefficient.

In order to determine the required constants in our solution, we start by rewriting the boundary condition listed as Eq. (2.40) in the discrete-ordinates form

$$\boldsymbol{\Psi}(0, c, \mu_i) - (\boldsymbol{I} - \boldsymbol{\alpha})\boldsymbol{\Psi}(0, c, -\mu_i) - 4\boldsymbol{\alpha}\int_0^\infty \mathrm{e}^{-c'^2} c'^3 \sum_{k=1}^{N} w_k \boldsymbol{\Psi}(0, c', -\mu_k)\mu_k \,\mathrm{d}c' = \boldsymbol{0}, \tag{6.9}$$

for $i = 1, 2, \ldots, N$. We next use Eqs. (5.3) and (6.1) in Eq. (6.9), multiply the resulting equation by

$$c^2 \exp\{-c^2\}\boldsymbol{P}^{\mathrm{T}}(c),$$

and integrate over all c to find

$$A_3\boldsymbol{M}_3 + B_1\boldsymbol{N}_{1,i} + B_2\boldsymbol{N}_{2,i} + B_3\boldsymbol{N}_{3,i} + \sum_{j=4}^{J} A_j \boldsymbol{M}_{j,i} = \boldsymbol{0}, \tag{6.10}$$

where

$$\boldsymbol{M}_3 = \left[\boldsymbol{P}_2^{\mathrm{T}} - 2\boldsymbol{P}_0^{\mathrm{T}}\right]\boldsymbol{\alpha}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \tag{6.11a}$$

$$\boldsymbol{N}_{1,i} = \left[\mu_i \boldsymbol{P}_1^{\mathrm{T}}(2\boldsymbol{I} - \boldsymbol{\alpha}) + \left(\pi^{1/2}/2\right)\boldsymbol{P}_0^{\mathrm{T}}\boldsymbol{\alpha}\right]\begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix}, \tag{6.11b}$$

$$\boldsymbol{N}_{\beta+1,i} = -\mu_i \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c)(2\boldsymbol{I} - \boldsymbol{\alpha})\boldsymbol{A}^{(\beta)}(c)c^2 \,\mathrm{d}c - (4/3)\boldsymbol{P}_0^{\mathrm{T}}\boldsymbol{\alpha}\int_0^\infty \mathrm{e}^{-c^2}\boldsymbol{A}^{(\beta)}(c)c^3 \,\mathrm{d}c, \quad \beta = 1, 2, \tag{6.11c}$$

and

$$\boldsymbol{M}_{j,i} = \boldsymbol{F}\boldsymbol{\Phi}(\nu_j, \mu_i) - \boldsymbol{H}\boldsymbol{\Phi}(\nu_j, -\mu_i) - 4\boldsymbol{P}_0^{\mathrm{T}}\boldsymbol{\alpha}\boldsymbol{P}_1 \sum_{k=1}^{N} w_k \mu_k \boldsymbol{\Phi}(\nu_j, -\mu_k) \tag{6.11d}$$

are vectors of size $2(K + 1)$. Clearly, Eq. (6.10) for $i = 1, 2, \ldots, N$ used in conjunction with Eq. (6.6) constitutes a system of $J + 1$ linear algebraic equations we can solve to find the $J + 1$ constants B_1, B_2, B_3, and A_j, $j = 3, 4, \ldots, J$. However, there is a problem: it can be noted that each of the solutions $\boldsymbol{H}_1$ and $\boldsymbol{H}_2$ associated respectively with A_1 and A_2 in Eq. (5.3) satisfy the boundary condition listed as Eq. (2.40), and so neither A_1 nor A_2 can be determined from that condition or from Eq. (2.44). Considering that the pressure perturbation on the gas mixture should approach zero as $\tau \to \infty$, we introduce the additional constraint

$$\lim_{\tau\to\infty} [c_1 \quad c_2]\left[\boldsymbol{N}(\tau) + \boldsymbol{T}(\tau)\right] = 0, \tag{6.12}$$

which we can satisfy by requiring that

$$c_1 A_1 + c_2 A_2 = -(5/2)\zeta, \tag{6.13}$$

where, at this point, the temperature-jump coefficient ζ is considered known. It thus follows, even after the use of Eq. (6.12), that there is still one degree of freedom in our solution. If we multiply Eq. (6.2a) on the left by $[c_1 \quad c_2]$ and use Eqs. (6.3a), (6.6), and (6.13), we find

$$[c_1 \quad c_2]\boldsymbol{N}(\tau) = -(\zeta + \tau) + [c_1 \quad c_2]\sum_{j=4}^{J} A_j \boldsymbol{N}_j \, \mathrm{e}^{-\tau/\nu_j}. \tag{6.14}$$

We thus conclude that Eq. (6.12) allows us to determine $[c_1 \quad c_2]\boldsymbol{N}(\tau)$ uniquely but not the individual components of $\boldsymbol{N}(\tau)$. Therefore, to be able to report some numerical results for the components of $\boldsymbol{N}(\tau)$, we choose to use

$$A_1 = A_2 = -(5/2)\zeta \tag{6.15}$$

to satisfy Eq. (6.13). With this arbitrary normalization, we find

$$\boldsymbol{N}(\tau) = -\begin{bmatrix} \zeta + B_2\tau \\ \zeta + B_3\tau \end{bmatrix} + \sum_{j=4}^{J} A_j \boldsymbol{N}_j \, \mathrm{e}^{-\tau/\nu_j}. \tag{6.16}$$

While the temperature-jump coefficient and the density and temperature distributions can be considered the principal quantities of interest for the considered problem, we can also compute the heat-flow distribution defined in Eqs. (2.42c) and/or (2.43c). Making use of Eqs. (5.3) and (6.1), we find

$$\boldsymbol{Q}(\tau) = \boldsymbol{Q}_* + \sum_{j=4}^{J} A_j \boldsymbol{Q}_j \, \mathrm{e}^{-\tau/\nu_j}, \tag{6.17}$$

where

$$\boldsymbol{Q}_* = -\frac{4}{3\pi^{1/2}} \int_0^\infty \mathrm{e}^{-c^2} \big[B_2 \boldsymbol{A}^{(1)}(c) + B_3 \boldsymbol{A}^{(2)}(c)\big]\big(c^2 - 5/2\big)c^3 \, \mathrm{d}c. \tag{6.18}$$

In addition,

$$\boldsymbol{Q}_j = \frac{2}{\pi^{1/2}}\big[\boldsymbol{P}_3 - (5/2)\boldsymbol{P}_1\big]\boldsymbol{Y}_j, \tag{6.19}$$

with

$$\boldsymbol{Y}_j = \sum_{k=1}^{N} w_k \mu_k \big[\boldsymbol{\Phi}(\nu_j, \mu_k) - \boldsymbol{\Phi}(\nu_j, -\mu_k)\big]. \tag{6.20}$$

In Ref. [27] it was proved for the McCormack model that

$$Q_0 = [\,\phi_1 \quad \phi_2\,]\,\boldsymbol{Q}(\tau), \tag{6.21}$$

where

$$\phi_1 = \frac{c_1}{c_1 + a_{2,1}c_2} \quad \text{and} \quad \phi_2 = \frac{a_{2,1}c_2}{c_1 + a_{2,1}c_2}, \tag{6.22a,b}$$

is a constant. In Appendix B of this work we report our proof of the fact that Q_0 as defined by Eq. (6.21) is a constant also for the linearized Boltzmann equation for a mixture of rigid spheres.

Finally we can use Eq. (2.40) and the constant-flow condition reported in Ref. [23] to show that

$$\boldsymbol{U}(\tau) = \boldsymbol{0}, \tag{6.23}$$

where

$$\boldsymbol{U}(\tau) = \frac{1}{\pi^{3/2}} \int_0^\infty \int_{-1}^{1} \int_0^{2\pi} \mathrm{e}^{-c^2} \boldsymbol{H}(\tau/\varepsilon_0, \boldsymbol{c})\mu c^3 \, \mathrm{d}\phi \, \mathrm{d}\mu \, \mathrm{d}c \tag{6.24}$$

or

$$\boldsymbol{U}(\tau) = \frac{2}{\pi^{1/2}} \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} \boldsymbol{\Psi}(\tau, c, \mu) \mu c^3 \, \mathrm{d}\mu \, \mathrm{d}c. \tag{6.25}$$

Using Eqs. (5.3) and (6.1) on the right side of Eq. (6.25) and noting Eq. (6.23), we find

$$\frac{\pi^{1/2}}{4} B_1 \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix} - \frac{2}{3} \int_0^\infty \mathrm{e}^{-c^2} \big[B_2 \boldsymbol{A}^{(1)}(c) + B_3 \boldsymbol{A}^{(2)}(c) \big] c^3 \, \mathrm{d}c + \boldsymbol{P}_1 \sum_{j=4}^{J} A_j \boldsymbol{Y}_j \, \mathrm{e}^{-\tau/\nu_j} = \boldsymbol{0}, \tag{6.26}$$

for any $\tau \in [0, \infty)$. When $\tau \to \infty$ this condition simplifies to

$$\frac{\pi^{1/2}}{4} B_1 \begin{bmatrix} 1 \\ a_{1,2} \end{bmatrix} - \frac{2}{3} \int_0^\infty \mathrm{e}^{-c^2} \big[B_2 \boldsymbol{A}^{(1)}(c) + B_3 \boldsymbol{A}^{(2)}(c) \big] c^3 \, \mathrm{d}c = \boldsymbol{0}. \tag{6.27}$$

At this point, we can multiply Eq. (6.27) on the left by $[c_1 \quad c_2]$ and note Eq. (5.8) to conclude that

$$B_1 = 0, \tag{6.28}$$

and so Eq. (6.27) reduces to

$$\int_0^\infty \mathrm{e}^{-c^2} \big[B_2 \boldsymbol{A}^{(1)}(c) + B_3 \boldsymbol{A}^{(2)}(c) \big] c^3 \, \mathrm{d}c = \boldsymbol{0}. \tag{6.29}$$

It is now clear that we can determine B_2 and B_3 by solving a system of two linear algebraic equations that consists of Eq. (6.6) and either one of the components of Eq. (6.29). We find, for $\alpha = 1$ (and $c_2 \neq 0$) or $\alpha = 2$ (and $c_1 \neq 0$),

$$B_2 = \Gamma_\alpha^{-1} \, [\, \delta_{1,\alpha} \quad \delta_{2,\alpha} \,] \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{A}^{(2)}(c) c^3 \, \mathrm{d}c \tag{6.30a}$$

and

$$B_3 = -\Gamma_\alpha^{-1} \, [\, \delta_{1,\alpha} \quad \delta_{2,\alpha} \,] \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{A}^{(1)}(c) c^3 \, \mathrm{d}c, \tag{6.30b}$$

where

$$\Gamma_\alpha = [\, \delta_{1,\alpha} \quad \delta_{2,\alpha} \,] \int_0^\infty \mathrm{e}^{-c^2} \big[c_1 \boldsymbol{A}^{(2)}(c) - c_2 \boldsymbol{A}^{(1)}(c) \big] c^3 \, \mathrm{d}c \tag{6.31}$$

and $\delta_{1,\alpha}$ and $\delta_{2,\alpha}$ are Kronecker deltas. In spite of the fact that Eqs. (6.28) and (6.30) provide explicit results for B_1, B_2, and B_3, we prefer to find these constants numerically from the solution of the linear system that consists of Eq. (6.10) for $i = 1, 2, \ldots, N$ combined with Eq. (6.6). The reason for this choice is that, in doing so, we can work with a square system. Nevertheless, to be sure of the adequacy of our approach, we have verified that the results for B_1, B_2, and B_3 that are obtained via solution of the linear system match very well the values that are obtained from Eqs. (6.28) and (6.30).

In conclusion, to be very clear about the temperature-jump problem formulated and solved in this work, we note that: we constructed a solution of Eq. (2.1) that diverges linearly in the spatial variable and that satisfies Eqs. (2.40), (2.44) and (6.12). It can be observed that we found a one-parameter family of solutions that satisfy these conditions, and while, in our computations, we fixed the one arbitrary parameter by choosing $A_1 = A_2$ in Eq. (6.13), it can be seen that this normalization does not affect either the reported temperature-jump coefficient or the reported temperature and heat-flow profiles.

7. Numerical results

Before reporting our numerical results for some representative cases and comparisons with results available in the literature, we would like to summarize the numerical methods we have used in this work. First of all, we note that our computational implementation was based on a truncated version of the kernel defined by Eq. (2.31). To this end, we have stopped the summations in Eqs. (2.31) and (4.9) at $n = L$ and, for consistency, we have stopped the summations in Eq. (4.12) at $m = \lfloor (L-1)/2 \rfloor$ and $m' = \lfloor (L-1)/2 \rfloor$, where $\lfloor x \rfloor$ denotes the floor (or integer part) of x. The Legendre components $\mathcal{K}_n(c', c)$ that are required in Eq. (4.11) were computed with the algorithms discussed in Appendix A of Ref. [24], which were found to work well in this work for L as high as 50 when a 200-point Gauss–Legendre quadrature set was used to perform the numerical integrations. In addition, we note that all integrals over the c variable that are required in this work [the integrals in Eqs. (3.5a), (3.5b), (3.6a), (3.6b), (3.7), and (4.11)] were evaluated by using the transformation $u = \mathrm{e}^{-c}$ to map the integration interval $[0, \infty)$ to $[0, 1]$, and then applying a Gauss–Legendre quadrature scheme of order M (with M even) mapped linearly onto $[0, 1]$. In the case of the inner integral over c' in Eq. (4.11), we have, for better accuracy, split the integration interval into $[0, c]$ and $[c, \infty)$. These two subintervals were then mapped onto $[0, 1]$ and a Gauss–Legendre quadrature of order $M/2$ (mapped onto $[0, 1]$) was used to evaluate the c' integral over each of these subintervals. Since in addition to these approximations we use the approximate representation of order K given by Eq. (3.1) with the choice $\Pi_k(c) = P_k(2\,\mathrm{e}^{-c} - 1)$ introduced in Ref. [9], a half-range quadrature scheme of order N in Eqs. (4.16), and a Hermite cubic spline representation with a number K_s of spline functions [24] to compute (without postprocessing) the generalized Chapman–Enskog vector functions $\boldsymbol{A}^{(\alpha)}(c)$, $\alpha = 1, 2$, we can see that our solution depends on the set of five approximation parameters $\{L, M, K, N, K_s\}$. Incidentally, we note that the required integrals of $\boldsymbol{A}^{(\alpha)}(c)$ (see Eqs. (6.11c) and (6.18)) were performed in this work as in Ref. [24], by applying a low-order Gaussian quadrature (order four being our choice here) to evaluate the integrals over each of the subintervals defined by two consecutive knots.

In regard to linear algebra, we note that have used the sequence of EISPACK [28] routines BALANC, ELMHES, ELTRAN, HQR2, and BALBAK to solve the eigensystem defined by Eq. (4.16a) for $i = 1, 2, \ldots, N$ and subroutines DGECO and DGESL of the LINPACK package [29] to solve the linear system defined by Eq. (6.10) for $i = 1, 2, \ldots, N$ and Eq. (6.6). We also note that for some choices of the approximation parameters $\{L, M, K, N\}$ a few eigenvalues of Eq. (4.16a) have shown up in our calculations as complex conjugate pairs slightly off the real axis. This situation is resolved in our code without having to resort to programming in complex mode.

Our test problems are defined in terms of two gas mixtures: Ne–Ar and He–Xe. The basic data for the Ne–Ar mixture are given by

$$m_2 = 39.948, \quad m_1 = 20.183, \quad d_2/d_1 = 1.406$$

and for the He–Xe mixture by

$$m_2 = 131.30, \quad m_1 = 4.0026, \quad d_2/d_1 = 2.226.$$

We report in Table 1 results of our computations of the temperature-jump coefficient ζ for several choices of the molar concentrations (c_1 as given in the table and $c_2 = 1 - c_1$) of the Ne–Ar mixture and various combinations of the accommodation coefficients α_1 and α_2. In Table 2, we show similar results for the He–Xe mixture. The numerical results in Tables 1 and 2 are thought to be accurate to within ± 1 in the last figure. To obtain these results, the code was executed several times for each case, increasing the values of the approximation parameters $\{L, M, K, N, K_s\}$ in steps, until numerical convergence was observed. Specifically, we have used $25 \leqslant L \leqslant 50$, $100 \leqslant M \leqslant 400$, $20 \leqslant K \leqslant 40$, $20 \leqslant N \leqslant 30$, and $80 \leqslant K_s - 2 \leqslant 1280$ in our calculations. To provide some detailed results for the temperature, density, and heat-flow profiles, we report in Table 3 our converged results for the case of the He–Xe mixture with $c_1 = 0.3$, $\alpha_1 = 0.3$, and $\alpha_2 = 0.6$. Typically, a calculation performed with $L = 25$, $M = 100$, $K = 20$, $N = 20$, and $K_s = 82$ yields at least five figures of accuracy for all quantities, and uses less than a minute of CPU time on an AMD Athlon 64 3200+ machine running at 2 GHz.

Now, in order to compare our results with those based on the McCormack model and reported in Ref. [18], we must take note of the differing definitions of the mean-free path used in the two works: this work and Ref. [18]. Recalling that we use τ, as defined by Eq. (2.27), to denote the dimensionless spatial variable adopted in this work and using τ_M for that of Ref. [18], we find that the relationship between these two quantities,

$$\xi_M = \frac{\tau}{\tau_M}, \tag{7.1}$$

can be computed from

$$\xi_M = \frac{c_2[\Upsilon_1 + X^{(4)}_{2,1}] + c_1[\Upsilon_2 + X^{(4)}_{1,2}]}{\Upsilon_1\Upsilon_2 - X^{(4)}_{1,2}X^{(4)}_{2,1}}, \tag{7.2}$$

where

$$X^{(3)}_{\alpha,\beta} = \left(\frac{10}{3} + \frac{2m_\beta}{m_\alpha}\right) F_{\alpha,\beta}, \tag{7.3}$$

$$X^{(4)}_{\alpha,\beta} = \frac{4}{3} F_{\alpha,\beta}, \tag{7.4}$$

$$F_{\alpha,\beta} = \frac{2c_\beta m_\alpha}{5m_\beta}\left(\frac{m_\beta}{m_\alpha + m_\beta}\right)^{3/2}\left(\frac{c_1 m_1 + c_2 m_2}{m_\alpha}\right)^{1/2}\left(\frac{d_\alpha + d_\beta}{c_1 d_1 + c_2 d_2}\right)^2, \tag{7.5}$$

$$\Upsilon_1 = X^{(3)}_{1,1} + X^{(3)}_{1,2} - X^{(4)}_{1,1}, \tag{7.6}$$

and

$$\Upsilon_2 = X^{(3)}_{2,2} + X^{(3)}_{2,1} - X^{(4)}_{2,2}. \tag{7.7}$$

And so, to compare our results for the temperature-jump coefficient reported in Tables 1 and 2 with the equivalent results of Ref. [18], we find that we must divide our results by the ξ_M factor given by Eq. (7.2). Having done this conversion for all cases reported in Tables 1 and 2 of this work, we have found that the relative deviations of the results of the McCormack model with respect to our results reach a maximum value of $\sim 2.4\%$ for the test cases

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

c_1	$\alpha_1 = 0.1$ $\alpha_2 = 0.1$	$\alpha_1 = 0.1$ $\alpha_2 = 0.3$	$\alpha_1 = 0.3$ $\alpha_2 = 0.5$	$\alpha_1 = 0.1$ $\alpha_2 = 0.8$	$\alpha_1 = 0.8$ $\alpha_2 = 0.9$	$\alpha_1 = 1.0$ $\alpha_2 = 1.0$
0.0	1.45095(1)	4.44448	2.41164	1.24705	1.02676	8.48578(−1)
0.1	1.43466(1)	4.92061	2.57270	1.53745	1.04473	8.38662(−1)
0.2	1.42142(1)	5.45123	2.73796	1.87360	1.06237	8.30661(−1)
0.3	1.41122(1)	6.04846	2.90850	2.27184	1.07996	8.24525(−1)
0.4	1.40413(1)	6.72812	3.08575	2.75662	1.09785	8.20276(−1)
0.5	1.40035(1)	7.51123	3.27149	3.36616	1.11648	8.18017(−1)
0.6	1.40021(1)	8.42629	3.46808	4.16359	1.13640	8.17943(−1)
0.7	1.40425(1)	9.51278	3.67863	5.26092	1.15831	8.20369(−1)
0.8	1.41322(1)	1.08268(1)	3.90732	6.87700	1.18314	8.25769(−1)
0.9	1.42825(1)	1.24507(1)	4.15990	9.50286	1.21214	8.34833(−1)
1.0	1.45095(1)	1.45095(1)	4.44448	1.45095(1)	1.24705	8.48578(−1)

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

c_1	$\alpha_1 = 0.1$ $\alpha_2 = 0.1$	$\alpha_1 = 0.1$ $\alpha_2 = 0.3$	$\alpha_1 = 0.3$ $\alpha_2 = 0.5$	$\alpha_1 = 0.1$ $\alpha_2 = 0.8$	$\alpha_1 = 0.8$ $\alpha_2 = 0.9$	$\alpha_1 = 1.0$ $\alpha_2 = 1.0$
0.0	1.45095(1)	4.44448	2.41164	1.24705	1.02676	8.48578(−1)
0.1	1.37362(1)	6.12437	2.85924	2.62533	1.03464	7.89842(−1)
0.2	1.31606(1)	7.28482	3.08204	3.71452	1.02442	7.50181(−1)
0.3	1.26892(1)	8.13530	3.19932	4.65641	1.00832	7.19952(−1)
0.4	1.22982(1)	8.78985	3.26334	5.52402	9.91552(−1)	6.96240(−1)
0.5	1.19899(1)	9.32784	3.30402	6.37073	9.77609(−1)	6.78523(−1)
0.6	1.17858(1)	9.82007	3.34426	7.25166	9.70102(−1)	6.67780(−1)
0.7	1.17339(1)	1.03498(1)	3.40894	8.24404	9.74309(−1)	6.66783(−1)
0.8	1.19351(1)	1.10472(1)	3.53631	9.48537	9.99978(−1)	6.81705(−1)
0.9	1.26262(1)	1.21810(1)	3.80587	1.12796(1)	1.06916	7.27386(−1)
1.0	1.45095(1)	1.45095(1)	4.44448	1.45095(1)	1.24705	8.48578(−1)

studied in Table 1 and $\sim 9.2\%$ for those of Table 2. In Table 4, we display a comparison of our results for the profiles reported in Table 3, now measured in McCormack units, with the equivalent results of Ref. [18]. In this case, the relative deviations of the profiles computed with the McCormack model can be as high as $\sim 12.7\%$.

Finally, to be able to compare our results with the results reported in Ref. [20] for some test cases characterized by complete accommodation ($\alpha_1 = 1$ and $\alpha_2 = 1$) and gas particles with the same diameter ($d_1 = d_2$), we note that if we let τ_K denote the dimensionless spatial variable used in Ref. [20], then we find that

$$\xi_K = \frac{\tau}{\tau_K} \tag{7.8}$$

can be computed from

$$\xi_K = 2^{1/2}\left(\frac{c_1 d_1 + c_2 d_2}{2 d_1}\right)^2. \tag{7.9}$$

Thus, upon dividing our converged numerical results for the temperature-jump coefficient by the ξ_K factor, we found agreement (within ± 1 in the fifth figure) with the five-figure results reported in Table XI of Ref. [20].

Table 3
Temperature, density, and heat-flow profiles for the He–Xe mixture with $c_1 = 0.3, \alpha_1 = 0.3, \alpha_2 = 0.6$: $\zeta = 2.96255$, $B_2 = 0.560696$, $B_3 = 1.18827$, $Q_0 = -0.746239$

τ	$-N_1(\tau)$	$-N_2(\tau)$	$T_1(\tau)$	$T_2(\tau)$	$-Q_1(\tau)$	$-Q_2(\tau)$
0.0	2.95231	2.04655	2.94012	1.88234	6.22796(−1)	1.04925
0.1	3.04632	2.39513	3.10870	2.27584	6.34439(−1)	1.02067
0.2	3.11360	2.60941	3.22981	2.49972	6.44351(−1)	9.96335(−1)
0.3	3.17459	2.79601	3.33949	2.68578	6.53153(−1)	9.74729(−1)
0.4	3.23260	2.96842	3.44367	2.85213	6.61086(−1)	9.55259(−1)
0.5	3.28898	3.13181	3.54478	3.00597	6.68293(−1)	9.37568(−1)
0.6	3.34439	3.28881	3.64404	3.15106	6.74876(−1)	9.21409(−1)
0.7	3.39922	3.44095	3.74215	3.28962	6.80912(−1)	9.06594(−1)
0.8	3.45368	3.58924	3.83954	3.42311	6.86461(−1)	8.92972(−1)
0.9	3.50794	3.73436	3.93649	3.55253	6.91574(−1)	8.80422(−1)
1.0	3.56208	3.87684	4.03319	3.67861	6.96293(−1)	8.68837(−1)
2.0	4.10520	5.21248	5.00184	4.83443	7.28051(−1)	7.90884(−1)
5.0	5.76870	8.88917	7.96756	7.94773	7.54513(−1)	7.25930(−1)
9.0	8.00897	1.36561(1)	1.19628(1)	1.19617(1)	7.57911(−1)	7.17588(−1)

Table 4
Basic results in McCormack units ($\tau \Rightarrow \tau_M$) for the He–Xe mixture with $c_1 = 0.3, \alpha_1 = 0.3$, and $\alpha_2 = 0.6$: $\zeta_{LBE} = 7.93116$ and $\zeta_{McC} = 7.34595$

τ	McCormack model [18]				Linearized Boltzmann equation			
	$-N_1(\tau)$	$-N_2(\tau)$	$T_1(\tau)$	$T_2(\tau)$	$-N_1(\tau)$	$-N_2(\tau)$	$T_1(\tau)$	$T_2(\tau)$
0.0	6.90689	5.03578	6.87509	4.69618	7.90375	5.47892	7.87114	5.03929
0.1	7.11313	5.45593	7.13187	5.14852	8.02052	5.95423	8.07981	5.58783
0.2	7.24491	5.73415	7.30983	5.44479	8.10444	6.24325	8.23067	5.90954
0.3	7.35582	5.97246	7.46464	5.69461	8.17869	6.48793	8.36431	6.17397
0.4	7.45531	6.18862	7.60648	5.91793	8.24758	6.70918	8.48834	6.40730
0.5	7.54742	6.39019	7.73978	6.12346	8.31300	6.91541	8.60609	6.62033
0.6	7.63433	6.58123	7.86699	6.31596	8.37598	7.11099	8.71941	6.81880
0.7	7.71738	6.76423	7.98960	6.49842	8.43716	7.29853	8.82944	7.00617
0.8	7.79744	6.94085	8.10863	6.67283	8.49696	7.47973	8.93694	7.18473
0.9	7.87513	7.11223	8.22478	6.84061	8.55569	7.65576	9.04246	7.35612
1.0	7.95090	7.27924	8.33859	7.00283	8.61357	7.82748	9.14638	7.52150
2.0	8.65150	8.80252	9.40554	8.43799	9.16891	9.39991	1.01412(1)	8.97649
5.0	1.05938(1)	1.27604(1)	1.24056(1)	1.19876(1)	1.07967(1)	1.34985(1)	1.30457(1)	1.25521(1)
9.0	1.31507(1)	1.76004(1)	1.63721(1)	1.62245(1)	1.30000(1)	1.84994(1)	1.69732(1)	1.68042(1)

8. Concluding remarks

We have reported in this work what we believe to be a concise and accurate solution for the temperature-jump problem, as described by the (vector) linearized Boltzmann equation for a binary mixture of rigid spheres.

In addition to the comparisons with numerical results of other works for binary mixtures that are reported in Section 7, we have also performed a comparison with the single-gas results of Ref. [9], using three different ways of achieving the single-gas limit in our formulation: (i) $c_1 = 0$, (ii) $c_2 = 0$, and (iii) $m_1 = m_2$ and $d_1 = d_2$. We note that to convert our results to the same spatial units used in Ref. [9] we made use of the factor

$$\xi_S = 0.679630049\ldots,$$

which is the ratio between our dimensionless spatial variable, as defined by Eq. (2.27), and that of Ref. [9]. Doing this, we found agreement (within ± 1 in the fifth figure) with the five-figure results for the temperature-jump coefficient and the density and temperature profiles that are tabulated in Ref. [9].

Finally, it is important to note that in contrast to other works [9,10,30–32], where problems formulated in terms of the single-gas LBE were well solved with a truncation of the scattering kernel at $L = 8$, we have found that more terms (at least $L = 35$ for the more demanding cases based on the He–Xe mixture) had to be used to obtain the six-figure results reported in this work.

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Appendix A. Macroscopic quantities for mixtures

While the material reported in this appendix is well established and thus can be found in many sources, e.g., Refs. [2,3,33–35], there are some variations in the way different authors define the macroscopic quantities used in this work. And so, in order to be clear and explicit about the quantities we report here, we include in this appendix a brief discussion of our way of defining the relevant macroscopic quantities for each species and for a binary mixture.

A.1. Single-species quantities

For problems formulated in terms of one spatial variable z, the number density $n_\alpha(z)$, the average velocity in the z direction $u_\alpha(z)$, the temperature $t_\alpha(z)$, and the heat flux (also called heat flow) in the z direction $q_\alpha(z)$ for a species (with particle mass m_α and equilibrium number density n_α) are defined by

$$n_\alpha(z) = \int f_{\alpha,0}(v)\big[1 + h_\alpha\big(z, \lambda_\alpha^{1/2}\boldsymbol{v}\big)\big]\,\mathrm{d}^3 v, \tag{A.1a}$$

$$n_\alpha(z)u_\alpha(z) = \int f_{\alpha,0}(v)\big[1 + h_\alpha\big(z, \lambda_\alpha^{1/2}\boldsymbol{v}\big)\big]v_z\,\mathrm{d}^3 v, \tag{A.1b}$$

$$(3/2)kn_\alpha(z)t_\alpha(z) = \int f_{\alpha,0}(v)\big[1 + h_\alpha\big(z, \lambda_\alpha^{1/2}\boldsymbol{v}\big)\big](m_\alpha/2)\big[\boldsymbol{v} - u_\alpha(z)\boldsymbol{e}_z\big]^2\,\mathrm{d}^3 v, \tag{A.1c}$$

and

$$q_\alpha(z) = \int f_{\alpha,0}(v)\big[1 + h_\alpha\big(z, \lambda_\alpha^{1/2}\boldsymbol{v}\big)\big](m_\alpha/2)\big[\boldsymbol{v} - u_\alpha(z)\boldsymbol{e}_z\big]^2\big[v_z - u_\alpha(z)\big]\,\mathrm{d}^3 v, \tag{A.1d}$$

where the $\boldsymbol{e}_z$ that appears in Eqs. (A.1c) and (A.1d) is a unit vector in the positive z direction. While the above definitions apply to a given species in a mixture, these definitions remain valid for a single-species gas.

Using Eq. (2.4) and the change of variables $\boldsymbol{c} = \lambda_\alpha^{1/2}\boldsymbol{v}$, we find we can write Eqs. (A.1a)–(A.1c) as

$$n_\alpha(z) = \frac{n_\alpha}{\pi^{3/2}} \int \mathrm{e}^{-c^2}\big[1 + h_\alpha(z, \boldsymbol{c})\big]\,\mathrm{d}^3 c, \tag{A.2a}$$

$$u_\alpha(z) = v_{\alpha,0}\frac{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})]c\mu\,\mathrm{d}^3c}{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})]\,\mathrm{d}^3c}, \tag{A.2b}$$

where $v_{\alpha,0} = (2kT_0/m_\alpha)^{1/2}$, and

$$(3/2)kt_\alpha(z) = \frac{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})][kT_0c^2 - (2kT_0m_\alpha)^{1/2}c\mu u_\alpha(z) + (m_\alpha/2)u_\alpha^2(z)]\,\mathrm{d}^3c}{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})]\,\mathrm{d}^3c}. \tag{A.2c}$$

We can evaluate one of the terms in Eq. (A.2a) to find

$$n_\alpha(z) = n_\alpha\left[1 + \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\,\mathrm{d}^3c\right]. \tag{A.3}$$

Next, we use the approximation (correct to order h)

$$\frac{1}{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})]\,\mathrm{d}^3c} \approx \frac{1}{\int \mathrm{e}^{-c^2}\,\mathrm{d}^3c}\left[1 - \frac{\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\,\mathrm{d}^3c}{\int \mathrm{e}^{-c^2}\,\mathrm{d}^3c}\right] \tag{A.4}$$

in Eq. (A.2b) and neglect the resulting term of order h^2 to find the result (correct to order h)

$$u_\alpha(z) = v_{\alpha,0}\left(\frac{1}{\pi^{3/2}}\right)\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})c\mu\,\mathrm{d}^3c. \tag{A.5}$$

Turning our attention to the temperature, we can use Eq. (A.2b) to rewrite Eq. (A.2c) as

$$(3/2)kt_\alpha(z) = kT_0\frac{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})]c^2\,\mathrm{d}^3c}{\int \mathrm{e}^{-c^2}[1+h_\alpha(z,\boldsymbol{c})]\,\mathrm{d}^3c} - (m_\alpha/2)u_\alpha^2(z). \tag{A.6}$$

Since $u_\alpha^2(z)$ is of order h^2, we can neglect the last term on the right side of Eq. (A.6), use the approximation expressed by Eq. (A.4), and evaluate some integrals to find the result (correct to order h)

$$t_\alpha(z) = T_0\left[1 + \frac{2}{3\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\big(c^2 - 3/2\big)\,\mathrm{d}^3c\right]. \tag{A.7}$$

In regard to the heat flux, we first neglect terms of order h^2 or higher in Eq. (A.1d) to find that this equation yields, to order h,

$$q_\alpha(z) = \int f_{\alpha,0}(v)\big[1 + h_\alpha\big(z,\lambda_\alpha^{1/2}\boldsymbol{v}\big)\big](m_\alpha/2)v^2v_z\,\mathrm{d}^3v - u_\alpha(z)\int f_{\alpha,0}(v)(m_\alpha/2)\big(v^2 + 2v_z^2\big)\,\mathrm{d}^3v. \tag{A.8}$$

Using the change of variables $\boldsymbol{c} = \lambda_\alpha^{1/2}\boldsymbol{v}$ and evaluating some integrals, we find that Eq. (A.8) reduces to

$$q_\alpha(z) = p_{\alpha,0}v_{\alpha,0}\left(\frac{1}{\pi^{3/2}}\right)\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\big(c^2 - 5/2\big)c\mu\,\mathrm{d}^3c, \tag{A.9}$$

where $p_{\alpha,0} = n_\alpha kT_0$ is the equilibrium partial pressure of the αth component of a mixture.

The macroscopic quantities for a single species can be written in a more compact form by defining the perturbations

$$N_\alpha(z) = \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\,\mathrm{d}^3c, \tag{A.10a}$$

$$U_\alpha(z) = \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})c\mu\,\mathrm{d}^3c, \tag{A.10b}$$

$$T_\alpha(z) = \frac{2}{3\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\big(c^2 - 3/2\big)\,\mathrm{d}^3c, \tag{A.10c}$$

and

$$Q_\alpha(z) = \frac{1}{\pi^{3/2}}\int \mathrm{e}^{-c^2}h_\alpha(z,\boldsymbol{c})\big(c^2 - 5/2\big)c\mu\,\mathrm{d}^3c. \tag{A.10d}$$

With these definitions, we can write the number density of the αth species as

$$n_\alpha(z) = n_\alpha\big[1 + N_\alpha(z)\big], \tag{A.11a}$$

the average velocity as

$$u_\alpha(z) = v_{\alpha,0} U_\alpha(z), \tag{A.11b}$$

the temperature as

$$t_\alpha(z) = T_0\big[1 + T_\alpha(z)\big], \tag{A.11c}$$

and the heat flux as

$$q_\alpha(z) = p_{\alpha,0} v_{\alpha,0} Q_\alpha(z). \tag{A.11d}$$

A.2. Mixture quantities

For the considered case of a binary gas mixture, the macroscopic quantities are defined in terms of the quantities for species 1 and 2 following the prescriptions of Ferziger and Kaper [33]. The number density of the mixture $n(z)$ is defined by

$$n(z) = n_1(z) + n_2(z), \tag{A.12a}$$

the mass density (or simply the density) of the mixture $\rho(z)$ by

$$\rho(z) = m_1 n_1(z) + m_2 n_2(z), \tag{A.12b}$$

the average velocity of the mixture $u(z)$ by

$$n(z)u(z) = n_1(z)u_1(z) + n_2(z)u_2(z), \tag{A.12c}$$

the bulk or hydrodynamic velocity $\hat{u}(z)$ by

$$\rho(z)\hat{u}(z) = m_1 n_1(z)u_1(z) + m_2 n_2(z)u_2(z), \tag{A.12d}$$

the temperature of the mixture $t(z)$ by

$$(3/2)n(z)kt(z) = (3/2)k\big[n_1(z)t_1(z) + n_2(z)t_2(z)\big], \tag{A.12e}$$

and the heat flux for the mixture $q(z)$ by

$$q(z) = q_1(z) + q_2(z). \tag{A.12f}$$

While Eqs. (A.12a), (A.12b), and (A.12f) are straightforward to use, Eqs. (A.12c)–(A.12e) can be simplified, by linearization, to yield expressions that are correct to order h. In this way, we find

$$u(z) = c_1 u_1(z) + c_2 u_2(z), \tag{A.13a}$$

where $c_\alpha = n_\alpha/n$ with $n = n_1 + n_2$,

$$\hat{u}(z) = \frac{1}{m}\big[c_1 m_1 u_1(z) + c_2 m_2 u_2(z)\big], \tag{A.13b}$$

where $m = c_1 m_1 + c_2 m_2$, and

$$t(z) = c_1 t_1(z) + c_2 t_2(z). \tag{A.13c}$$

Finally, we note that the macroscopic quantities for a binary mixture can be written in terms of the single-species perturbations, equilibrium quantities, and basic parameters as

$$n(z) = n + n_1 N_1(z) + n_2 N_2(z), \tag{A.14a}$$

$$\rho(z) = nm + n_1 m_1 N_1(z) + n_2 m_2 N_2(z), \tag{A.14b}$$

$$u(z) = v_0\big[c_1 (m/m_1)^{1/2} U_1(z) + c_2 (m/m_2)^{1/2} U_2(z)\big], \tag{A.14c}$$

$$\hat{u}(z) = v_0\big[c_1(m_1/m)^{1/2}U_1(z) + c_2(m_2/m)^{1/2}U_2(z)\big], \tag{A.14d}$$

$$t(z) = T_0\big[1 + c_1T_1(z) + c_2T_2(z)\big], \tag{A.14e}$$

and

$$q(z) = p_0v_0\big[c_1(m/m_1)^{1/2}Q_1(z) + c_2(m/m_2)^{1/2}Q_2(z)\big], \tag{A.14f}$$

where $v_0 = (2kT_0/m)^{1/2}$ and $p_0 = nkT_0$.

Appendix B. A condition on the heat flux for the mixture

We report in this appendix our proof that the quantity Q_0, as defined by Eq. (6.21), is a constant. We begin by multiplying Eq. (2.29) by

$$c^2\big(c^2 - 5/2\big)\exp\big\{-c^2\big\}$$

and integrating the resulting equation over all c and all μ to find

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{Q}(\tau) = \frac{2}{\pi^{1/2}}\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c^2}\left\{-c^2\boldsymbol{V}(c) + \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_0(c,c')c'^4\,\mathrm{d}c'\right\}\boldsymbol{\Psi}(\tau,c,\mu)c^2\,\mathrm{d}\mu\,\mathrm{d}c, \tag{B.1}$$

where, to simplify the right-hand side, we have used the identities expressed by Eqs. (29a) and (29b) of Ref. [24] multiplied by $1/\varepsilon_0$, i.e.

$$\left\{\boldsymbol{V}(c) - \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_0(c',c)c'^2\,\mathrm{d}c'\right\}\begin{bmatrix}1\\0\end{bmatrix} = \boldsymbol{0} \tag{B.2a}$$

and

$$\left\{\boldsymbol{V}(c) - \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_0(c',c)c'^2\,\mathrm{d}c'\right\}\begin{bmatrix}0\\1\end{bmatrix} = \boldsymbol{0}. \tag{B.2b}$$

Noting that

$$\boldsymbol{I} = \left(\frac{1}{c_1c_2}\right)\boldsymbol{S}\boldsymbol{R}, \tag{B.3}$$

where

$$\boldsymbol{S} = \begin{bmatrix}c_2 & 0\\ 0 & c_1a_{1,2}\end{bmatrix} \quad\text{and}\quad \boldsymbol{R} = \begin{bmatrix}c_1 & 0\\ 0 & c_2a_{2,1}\end{bmatrix}, \tag{B.4a,b}$$

and using the relation

$$\boldsymbol{\mathcal{K}}_0(c,c')\boldsymbol{S} = \boldsymbol{S}\boldsymbol{\mathcal{K}}_0^{\mathrm{T}}(c',c), \tag{B.5}$$

which follows from Eq. (37) of Ref. [24], we can rewrite Eq. (B.1) as

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{Q}(\tau) = \frac{2}{\pi^{1/2}}\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c^2}\left\{-c^2\boldsymbol{V}(c) + \left(\frac{1}{c_1c_2}\right)\int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{S}\boldsymbol{\mathcal{K}}_0^{\mathrm{T}}(c',c)\boldsymbol{R}c'^4\,\mathrm{d}c'\right\}\boldsymbol{\Psi}(\tau,c,\mu)c^2\,\mathrm{d}\mu\,\mathrm{d}c. \tag{B.6}$$

Next, we transpose Eq. (B.6), use again Eq. (B.3) with the $\boldsymbol{V}(c)$ term and multiply the resulting equation by $\boldsymbol{R}$ on the right to find

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\boldsymbol{Q}^{\mathrm{T}}(\tau)\boldsymbol{R} = \frac{2}{\pi^{1/2}}\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c^2}\boldsymbol{\Psi}^{\mathrm{T}}(\tau,c,\mu)\boldsymbol{R}\left\{-c^2\boldsymbol{V}(c) + \int_0^\infty \mathrm{e}^{-c'^2}\boldsymbol{\mathcal{K}}_0(c',c)c'^4\,\mathrm{d}c'\right\}c^2\,\mathrm{d}\mu\,\mathrm{d}c. \tag{B.7}$$

Finally, multiplying this equation on the right by $[1 \quad 1]^{\mathrm{T}}$ and using Eq. (29c) of Ref. [24] multiplied by $1/\varepsilon_0$, i.e.

$$\left\{ c^2 \boldsymbol{V}(c) - \int_0^\infty \mathrm{e}^{-c'^2} \boldsymbol{\mathcal{K}}_0(c', c) c'^4 \, \mathrm{d}c' \right\} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \mathbf{0}, \tag{B.8}$$

we find

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \big[Q_1(\tau) \quad Q_2(\tau) \big] \begin{bmatrix} c_1 \\ c_2 a_{2,1} \end{bmatrix} = 0, \tag{B.9}$$

from which Eq. (6.21) follows.

To close this appendix, we note that the quantity Q_0 is related to the heat flux for the mixture $q(z)$, as defined in Eq. (A.14f), by

$$q(z) = \gamma p_0 v_0 Q_0, \tag{B.10}$$

where

$$\gamma = c_1 (m/m_1)^{1/2} + c_2 (m/m_2)^{1/2}. \tag{B.11}$$

We thus conclude, after letting $\tau \to \infty$ in Eqs. (6.17) and (6.21), using Eq. (6.29) in Eq. (6.18), and noting Eqs. (6.30), that the heat flux

$$q(z) = -\frac{4}{3\pi^{1/2}} \gamma p_0 v_0 \, [\, \phi_1 \quad \phi_2 \,] \int_0^\infty \mathrm{e}^{-c^2} \big[B_2 \boldsymbol{A}^{(1)}(c) + B_3 \boldsymbol{A}^{(2)}(c) \big] c^5 \, \mathrm{d}c \tag{B.12}$$

not only is a constant but also does not depend on the accommodation coefficients α_1 and α_2 used to define the boundary condition for the problem in Eq. (2.38).

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