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The temperature-jump problem for a mixture of two gases

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Abstract

An analytical variation of the discrete-ordinates method is used to establish a concise and accurate solution to the temperature-jump problem for a binary gas mixture. The analysis is based on Boltzmann equations of the BGK type subject to Maxwell's boundary conditions with arbitrary accommodation coefficients. The results include the complete temperature and density fields for specified mass, density and collision frequency ratios. The numerical results are of benchmark quality, and the required computational time is only a few seconds on a typical PC. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The problem of heat conduction in a slightly rarefied gas adjacent to a solid wall is a classical problem in kinetic theory. It is well known as the temperature-jump problem, and over the years a complete treatment [1–3] has been given for the case of a single-component gas. However, the corresponding problem for a multi-component gas mixture has received much less attention. This is mainly due to the fact that for mixtures a system of coupled kinetic equations must be solved, and so naturally the computational effort required is significantly increased. Most of the existing work in this direction is focused on the case of purely diffuse molecular reflection at the wall [4,5], or it is concerned only with the estimation of the macroscopic discontinuities at the surface of the wall [6,7].

Recently, a complete investigation of the temperature-jump problem for a two-component gas was reported by Onishi [8]. In that work [8] linearized versions of the Boltzmann equation of the

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BGK type [9], along with specular-diffuse boundary conditions, were transformed into a set of integral equations, and the unknown temperature and density fields were computed by the application of a refined moment method [4,10]. It is the purpose of the present work to solve Onishi's temperature-jump problem [8] for a binary gas mixture by following, however, a completely different mathematical procedure. A semi-analytical, numerical approach, based on an analytical version of the discrete-ordinates method [11–14] and some new computational ideas [15], complimented by aspects of the method of elementary solutions [16], are used for this work. While this present version of the discrete-ordinates method has been used recently to solve a collection [17–21] of classical problems for single-component gases, the method has been used for a binary mixture, so far, only for the Couette-flow problem [22]. The present work is the first implementation of the method for the coupled temperature–density problem relevant to two-component gas mixtures. Here, a system of four coupled kinetic equations (two for each gas) is solved. The focus of this work is on the formulation of a particularly elegant, concise and accurate solution that defines an algorithm that is especially easy to implement.

2. Kinetic equations and boundary conditions

To begin our analysis, we consider that our mixture of two species of gas particles can be modeled by a pair of coupled linearized Boltzmann–BGK equations which we write as

$$\left(c_x \frac{\partial}{\partial x} + 1\right) h_1(x, c_x, c_y, c_z) = N_1(x) + (c^2 - 3/2)[c_{11} T_1(x) + c_{12} T_2(x)] \tag{1a}$$

and

$$\left(c_x \frac{\partial}{\partial x} + \sigma\right) h_2(x, c_x, c_y, c_z) = \sigma N_2(x) + \sigma(c^2 - 3/2)[c_{21} T_1(x) + c_{22} T_2(x)] \tag{1b}$$

where for $i = 1$ and 2

$$N_i(x) = \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h_i(x, c_x, c_y, c_z) \mathrm{e}^{-c^2} \, \mathrm{d}c_x \, \mathrm{d}c_y \, \mathrm{d}c_z \tag{2a}$$

and

$$T_i(x) = \frac{2}{3} \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (c^2 - 3/2) h_i(x, c_x, c_y, c_z) \mathrm{e}^{-c^2} \, \mathrm{d}c_x \, \mathrm{d}c_y \, \mathrm{d}c_z. \tag{2b}$$

Here our basic unknowns $h_i(x, c_x, c_y, c_z)$, for $i = 1,2$, are perturbations from Maxwellian distributions for the two species of gas particles, x is the dimensionless spatial variable and the normalized particle velocity vector has components c_x, c_y, c_z and magnitude c. As we intend to compare our final results with those of Onishi [8], we chose to define the physical parameters relevant to this model in terms of those previously used, and so we write [8]

$$\sigma = \frac{a_{22} + a_{21}}{1 + a_{12}} M^{1/2}, \tag{3}$$

$c_{11} = 1 - c_{12}$ and $c_{22} = 1 - c_{21}$ where

$$c_{12} = \frac{2\mu_1\mu_2 a_{12}}{1 + a_{12}} \quad \text{and} \quad c_{21} = \frac{2\mu_1\mu_2 a_{21}}{a_{21} + a_{22}}. \tag{4a,b}$$

Here $M = m_2/m_1$ is the ratio of particle masses, $\mu_i = m_i/(m_1 + m_2)$, for $i = 1,2$, are the reduced masses,

$$a_{12} = \frac{n_2 k_{12}}{n_1 k_{11}}, \quad a_{21} = \frac{k_{12}}{k_{11}} \quad \text{and} \quad a_{22} = \frac{n_2 k_{22}}{n_1 k_{11}}, \tag{5a,b,c}$$

where n_2/n_1 is the ratio of particle densities and the various k_{ij} are collision-interaction parameters.

We note that Eqs. (1) are valid for $x > 0$ and c_x, c_y, c_z all $\in(-\infty, \infty)$, and in addition to Eqs. (1), we consider boundary conditions (at the wall) written as

$$h_i(0, c_x, c_y, c_z) = (1 - \alpha_i)h_i(0, -c_x, c_y, c_z) + (\mathscr{I}h_i)(0) \tag{6}$$

for $c_x \in (0, \infty)$ and all c_y and c_z. Here

$$(\mathscr{I}h_i)(0) = \frac{2\alpha_i}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \mathrm{e}^{-c^2}h_i(0, -c_x, c_y, c_z)c_x\,\mathrm{d}c_x\,\mathrm{d}c_y\,\mathrm{d}c_z \tag{7}$$

and the α_i, $i = 1,2$, are accommodation coefficients. Having defined the basic starting equations for this work, we will consider that the six basic parameters

$$m_1/m_2, \quad n_1/n_2, \quad k_{12}/k_{11}, \quad k_{22}/k_{11}, \quad \alpha_1 \text{ and } \alpha_2$$

which characterize the gas mixture are prescribed, and subsequently we seek solutions for various moments of $h_i(x, c_x, c_y, c_z)$ for $i = 1$ and 2.

Of course, if we sought to compute the complete distribution functions $h_i(x, c_x, c_y, c_z)$ then we would have to work explicitly with Eqs. (1) and (2); however, here we seek only the temperature and density perturbations $T_i(x)$ and $N_i(x)$, for $i = 1,2$, which we can express in terms of moments (integrals) of $h_i(x, c_x, c_y, c_z)$. Defining the quantities

$$H_{1i}(x, c_x) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-(c_y^2 + c_z^2)}h_i(x, c_x, c_y, c_z)\,\mathrm{d}c_y\,\mathrm{d}c_z \tag{8a}$$

and

$$H_{2i}(x, c_x) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-(c_y^2 + c_z^2)}(c_y^2 + c_z^2 - 1)h_i(x, c_x, c_y, c_z)\,\mathrm{d}c_y\,\mathrm{d}c_z \tag{8b}$$

for $i = 1,2$, we find we can rewrite Eqs. (2) as

$$N_i(x) = \pi^{-1/2}\int_{-\infty}^{\infty} H_{1i}(x, c_x)\mathrm{e}^{-c_x^2}\,\mathrm{d}c_x \tag{9a}$$

and

$$T_i(x) = \frac{2}{3}\pi^{-1/2}\int_{-\infty}^{\infty} [(c_x^2 - 1/2)H_{1i}(x, c_x) + H_{2i}(x, c_x)]\mathrm{e}^{-c_x^2}\,\mathrm{d}c_x. \tag{9b}$$

Now to find defining equations for $H_{1i}(x, c_x)$ and $H_{2i}(x, c_x)$, we first multiply Eqs. (1) and (6) by

$$\phi_1(c_y, c_z) = \pi^{-1/2} e^{-(c_y^2 + c_z^2)} \tag{10a}$$

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

$$\phi_2(c_y, c_z) = \pi^{-1/2} e^{-(c_y^2 + c_z^2)}(c_y^2 + c_z^2 - 1) \tag{10b}$$

instead of $\phi_1(c_y, c_z)$. In this way we find, after changing c_x to ξ,

$$\xi \frac{\partial}{\partial x} \boldsymbol{Y}(x,\xi) + \boldsymbol{\Sigma Y}(x,\xi) = \pi^{-1/2} \boldsymbol{\Sigma A}(\xi) \int_{-\infty}^{\infty} \boldsymbol{B}(\xi') \boldsymbol{Y}(x,\xi') e^{-\xi'^2} \, d\xi', \tag{11}$$

for $x \in (0, \infty)$ and $\xi \in (-\infty, \infty)$, and

$$\boldsymbol{Y}(0,\xi) = \boldsymbol{\mathcal{A} Y}(0, -\xi) + 2\boldsymbol{\mathcal{B}} \int_0^{\infty} \xi' \boldsymbol{Y}(0, -\xi') e^{-\xi'^2} \, d\xi', \tag{12}$$

for $\xi \in (0, \infty)$. At this point the vector-valued function

$$\boldsymbol{Y}(x,\xi) = \begin{bmatrix} H_{11}(x,\xi) \\ H_{12}(x,\xi) \\ H_{21}(x,\xi) \\ H_{22}(x,\xi) \end{bmatrix} \tag{13}$$

is our basic unknown. In addition, the known quantities in Eqs. (11) and (12) are

$$\boldsymbol{A}(\xi) = \begin{bmatrix} (2/3)^{1/2}(\xi^2 - 1/2)\boldsymbol{C} & \boldsymbol{I} \\ (2/3)^{1/2}\boldsymbol{C} & \boldsymbol{0} \end{bmatrix}, \tag{14}$$

$$\boldsymbol{B}(\xi) = \begin{bmatrix} (2/3)^{1/2}(\xi^2 - 1/2)\boldsymbol{I} & (2/3)^{1/2}\boldsymbol{I} \\ \boldsymbol{I} & \boldsymbol{0} \end{bmatrix}, \tag{15}$$

$$\boldsymbol{C} = \begin{bmatrix} 1 - c_{12} & c_{12} \\ c_{21} & 1 - c_{21} \end{bmatrix}, \tag{16}$$

$$\boldsymbol{\Sigma} = \mathrm{diag}\{1, \sigma, 1, \sigma\}, \tag{17}$$

$$\boldsymbol{\mathcal{A}} = \mathrm{diag}\{1 - \alpha_1, 1 - \alpha_2, 1 - \alpha_1, 1 - \alpha_2\}, \tag{18}$$

$$\boldsymbol{\mathcal{B}} = \mathrm{diag}\{\alpha_1, \alpha_2, 0, 0\} \tag{19}$$

and $\boldsymbol{I}$ is the 2×2 identity matrix. While Eq. (12) is the considered boundary condition at the wall ($x = 0$), we clearly must place constraints on the desired solution as x tends to infinity. Here, we follow Ref. [8] and impose the conditions

$$\lim_{x \to \infty} \frac{d}{dx} \boldsymbol{T}(x) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{20}$$

and

$$\lim_{x\to\infty} [\boldsymbol{T}(x) + \boldsymbol{N}(x)] = \mathbf{0}, \tag{21}$$

where the vector-valued functions $\boldsymbol{T}(x)$ and $\boldsymbol{N}(x)$ have, respectively, the perturbed temperature and densities $T_1(x)$ and $T_2(x)$ and $N_1(x)$ and $N_2(x)$ as components.

And so to be clear, we note that now we seek a solution of Eq. (11) that satisfies Eq. (12) and also Eqs. (20) and (21), once

$$\boldsymbol{N}(x) = \pi^{-1/2}\begin{bmatrix}\boldsymbol{I}\\ \mathbf{0}\end{bmatrix}^{\mathrm{T}}\int_{-\infty}^{\infty}\boldsymbol{Y}(x,\xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi \tag{22}$$

and

$$\boldsymbol{T}(x) = \frac{2}{3}\pi^{-1/2}\int_{-\infty}^{\infty}\begin{bmatrix}(\xi^2-1/2)\boldsymbol{I}\\ \boldsymbol{I}\end{bmatrix}^{\mathrm{T}}\boldsymbol{Y}(x,\xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi \tag{23}$$

have been used. We wish ultimately to compute $\boldsymbol{N}(x)$ and $\boldsymbol{T}(x)$ for all $x \geq 0$.

3. The discrete-ordinates solution

As we have already used our version of the discrete-ordinates method [15] to solve a collection [17–22] of problems in the area of rarefied gas dynamics, our discussion of the method here will be brief. To establish our discrete-ordinates equations, we replace the integral term in Eq. (11) by a numerical quadrature representation and then evaluate the resulting equation at the nodes of the quadrature scheme to obtain

$$\pm\xi_i\frac{\mathrm{d}}{\mathrm{d}x}\boldsymbol{Y}(x,\pm\xi_i) + \boldsymbol{\Sigma}\boldsymbol{Y}(x,\pm\xi_i) = \boldsymbol{\Sigma}\boldsymbol{A}(\xi_i)\sum_{k=1}^{N}\hat{w}_k\boldsymbol{B}(\xi_k)[\boldsymbol{Y}(x,\xi_k) + \boldsymbol{Y}(x,-\xi_k)] \tag{24}$$

where

$$\hat{w}_k = \pi^{-1/2}w_k\mathrm{e}^{-\xi_k^2} \tag{25}$$

for $i = 1, 2, \ldots, N$. In writing Eq. (24) as we have, we are clearly considering that the N quadrature points $\{\xi_k\}$ and the N weights $\{w_k\}$ are defined for use on the integration interval $[0,\infty)$. We note that it is to this feature of using a "half-range" quadrature scheme that we partially attribute the especially good accuracy we have obtained from the solution reported here. Now seeking exponential solutions, we substitute

$$\boldsymbol{Y}(x,\pm\xi_i) = \boldsymbol{\Phi}(\nu,\pm\xi_i)\mathrm{e}^{-x/\nu} \tag{26}$$

into Eq. (24) to find

$$(\nu\boldsymbol{\Sigma} \mp \xi_i\boldsymbol{I})\boldsymbol{\Phi}(\nu,\pm\xi_i) = \nu\boldsymbol{\Sigma}\boldsymbol{A}(\xi_i)\boldsymbol{F}(\nu) \tag{27}$$

where

$$\boldsymbol{F}(v) = \sum_{k=1}^{N} \hat{w}_k \boldsymbol{B}(\xi_k)[\boldsymbol{\Phi}(v, \xi_k) + \boldsymbol{\Phi}(v, -\xi_k)]. \tag{28}$$

If we now let

$$\boldsymbol{\Phi}_{\pm}(v) = [\boldsymbol{\Phi}^{\mathrm{T}}(v, \pm\xi_1) \quad \boldsymbol{\Phi}^{\mathrm{T}}(v, \pm\xi_2) \quad \cdots \quad \boldsymbol{\Phi}^{\mathrm{T}}(v, \pm\xi_N)]^{\mathrm{T}} \tag{29}$$

then we can rewrite the two ($\pm$) versions of Eq. (27) as

$$\frac{1}{v}\boldsymbol{M}\boldsymbol{\Phi}_{+}(v) = \boldsymbol{S}(\boldsymbol{I} - \boldsymbol{T}\boldsymbol{W})\boldsymbol{\Phi}_{+}(v) - \boldsymbol{S}\boldsymbol{T}\boldsymbol{W}\boldsymbol{\Phi}_{-}(v) \tag{30a}$$

and

$$-\frac{1}{v}\boldsymbol{M}\boldsymbol{\Phi}_{-}(v) = \boldsymbol{S}(\boldsymbol{I} - \boldsymbol{T}\boldsymbol{W})\boldsymbol{\Phi}_{-}(v) - \boldsymbol{S}\boldsymbol{T}\boldsymbol{W}\boldsymbol{\Phi}_{+}(v). \tag{30b}$$

In writing Eqs. (30), we have introduced the $4N \times 4N$ block diagonal matrices

$$\boldsymbol{M} = \mathrm{diag}\{\xi_1 \boldsymbol{I}, \xi_2 \boldsymbol{I}, \ldots, \xi_N \boldsymbol{I}\}, \tag{31}$$

$$\boldsymbol{S} = \mathrm{diag}\{\boldsymbol{\Sigma}, \boldsymbol{\Sigma}, \ldots, \boldsymbol{\Sigma}\} \tag{32}$$

and

$$\boldsymbol{T} = \mathrm{diag}\{\boldsymbol{A}(\xi_1), \boldsymbol{A}(\xi_2), \ldots, \boldsymbol{A}(\xi_N)\}. \tag{33}$$

In addition the $4N \times 4N$ matrix $\boldsymbol{W}$ has N block rows each given by

$$\boldsymbol{R} = [\hat{w}_1 \boldsymbol{B}(\xi_1) \quad \hat{w}_2 \boldsymbol{B}(\xi_2) \quad \cdots \quad \hat{w}_N \boldsymbol{B}(\xi_N)]. \tag{34}$$

Continuing, we now let

$$\boldsymbol{U}(v) = \boldsymbol{\Phi}_{+}(v) + \boldsymbol{\Phi}_{-}(v) \tag{35a}$$

and

$$\boldsymbol{V}(v) = \boldsymbol{\Phi}_{+}(v) - \boldsymbol{\Phi}_{-}(v) \tag{35b}$$

so that, we can eliminate between the sum and the difference of Eqs. (30a) and (30b) to find

$$(\boldsymbol{D} - 2\boldsymbol{S}\boldsymbol{M}^{-1}\boldsymbol{S}\boldsymbol{T}\boldsymbol{W}\boldsymbol{M}^{-1})\boldsymbol{M}\boldsymbol{U}(v) = \lambda \boldsymbol{M}\boldsymbol{U}(v), \tag{36}$$

where

$$\boldsymbol{D} = \mathrm{diag}\{\xi_1^{-2}\boldsymbol{\Sigma}^2, \xi_2^{-2}\boldsymbol{\Sigma}^2, \ldots, \xi_N^{-2}\boldsymbol{\Sigma}^2\} \tag{37}$$

is $4N \times 4N$ block diagonal and $\lambda = 1/v^2$.

Considering that we have solved the eigenvalue problem defined by Eq. (36) to obtain the $4N$ eigenvalues λ_j, we now have the $4N$ (positive) separation constants $v_j = \lambda_j^{-1/2}$ available, and so we can deduce from Eqs. (27) and (28) that

$$(v_j \boldsymbol{\Sigma} \mp \xi_i \boldsymbol{I})\boldsymbol{\Phi}(v_j, \pm\xi_i) = v_j \boldsymbol{\Sigma} \boldsymbol{A}(\xi_i) \boldsymbol{F}(v_j) \tag{38}$$

and

$$\boldsymbol{\Phi}(\nu_j, \pm\xi_i) = \nu_j(\nu_j\boldsymbol{\Sigma} \mp \xi_i\boldsymbol{I})^{-1}\boldsymbol{\Sigma}\boldsymbol{A}(\xi_i)\boldsymbol{F}(\nu_j) \tag{39}$$

where

$$\boldsymbol{\Omega}(\nu_j)\boldsymbol{F}(\nu_j) = \mathbf{0} \tag{40}$$

with

$$\boldsymbol{\Omega}(\nu_j) = \boldsymbol{I} - 2\nu_j^2 \sum_{k=1}^{N} \hat{w}_k \boldsymbol{B}(\xi_k)\boldsymbol{D}(\nu_j, \xi_k)\boldsymbol{A}(\xi_k). \tag{41}$$

Here

$$\boldsymbol{D}(\nu_j, \xi_k) = \mathrm{diag}\left\{\frac{1}{\nu_j^2 - \xi_k^2}, \frac{\sigma^2}{\sigma^2\nu_j^2 - \xi_k^2}, \frac{1}{\nu_j^2 - \xi_k^2}, \frac{\sigma^2}{\sigma^2\nu_j^2 - \xi_k^2}\right\}. \tag{42}$$

Now, assuming that we have used numerical linear-algebra techniques to find the separation constants ν_j and the vectors $\boldsymbol{F}(\nu_j)$, we write a first version of the solution to our discrete-ordinates equations as

$$\boldsymbol{Y}(x, \pm\xi_i) = \sum_{j=1}^{4N} [A_j\boldsymbol{\Phi}(\nu_j, \pm\xi_i)\mathrm{e}^{-x/\nu_j} + B_j\boldsymbol{\Phi}(\nu_j, \mp\xi_i)\mathrm{e}^{x/\nu_j}] \tag{43}$$

where the constants $\{A_j\}$ and $\{B_j\}$ are, at this point, arbitrary. Of course, we cannot allow $\nu_j = \xi_i$ or $\sigma\nu_j = \xi_i$ in Eq. (43).

At this point, we wish to introduce a modification to Eq. (43) that is important for the problem considered in this work. We have found that $\det\boldsymbol{\Omega}(\xi)$, where

$$\boldsymbol{\Omega}(\xi) = \boldsymbol{I} - 2\pi^{-1/2}\xi^2 \int_0^\infty \boldsymbol{B}(\xi')\boldsymbol{D}(\xi, \xi')\boldsymbol{A}(\xi')\mathrm{e}^{-\xi'^2}\,\mathrm{d}\xi', \tag{44}$$

has a sixth-order zero at infinity, and so we choose to ignore the contributions in Eq. (43) from the three largest eigenvalues, say ν_1, ν_2 and ν_3, and (instead) to include the exact solutions

$$\boldsymbol{Y}_1(\xi) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{Y}_2(\xi) = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{Y}_3(\xi) = (2/3)^{1/2} \begin{bmatrix} \xi^2 - 1/2 \\ \xi^2 - 1/2 \\ 1 \\ 1 \end{bmatrix}, \tag{45a,b,c}$$

$$\boldsymbol{Y}_4(x, \xi) = (\xi\boldsymbol{\Sigma}^{-1} - x\boldsymbol{I})\boldsymbol{Y}_1(\xi), \tag{46}$$

$$\boldsymbol{Y}_5(x, \xi) = (\xi\boldsymbol{\Sigma}^{-1} - x\boldsymbol{I})\boldsymbol{Y}_2(\xi) \tag{47}$$

and

$$\boldsymbol{Y}_6(x, \xi) = (\xi\boldsymbol{\Sigma}^{-1} - x\boldsymbol{I})\boldsymbol{Y}_3(\xi). \tag{48}$$

And so we now rewrite Eq. (43) as

$$\boldsymbol{Y}(x, \pm \xi_i) = \boldsymbol{Y}_*(x, \pm \xi_i) + \sum_{j=4}^{4N} [A_j \boldsymbol{\Phi}(\nu_j, \pm \xi_i)\mathrm{e}^{-x/\nu_j} + B_j \boldsymbol{\Phi}(\nu_j, \mp \xi_i)\mathrm{e}^{x/\nu_j}] \tag{49}$$

where in general

$$\boldsymbol{Y}_*(x, \xi) = \sum_{j=1}^{3} [A_j + B_j(\xi \boldsymbol{\Sigma}^{-1} - x\boldsymbol{I})]\boldsymbol{Y}_j(\xi). \tag{50}$$

To conclude this section, we note that the solution of our discrete-ordinates equations, as given by Eqs. (49) and (50), contains $8N$ arbitrary constants $\{A_j\}$ and $\{B_j\}$ that we must determine, from the boundary condition at the wall and the imposed conditions as x tends to infinity, so as to define the solution we seek.

4. Computational details and numerical results

Having developed the basic elements of our discrete-ordinates solution, we now are ready to solve the problem of interest here, and so, restating from Section 2, we seek an unbounded (as x tends to infinity) solution of

$$\xi \frac{\partial}{\partial x}\boldsymbol{Y}(x, \xi) + \boldsymbol{\Sigma}\boldsymbol{Y}(x, \xi) = \pi^{-1/2}\boldsymbol{\Sigma}\boldsymbol{A}(\xi)\int_{-\infty}^{\infty} \boldsymbol{B}(\xi')\boldsymbol{Y}(x, \xi')\mathrm{e}^{-\xi'^2}\,\mathrm{d}\xi', \tag{51}$$

for $x \in (0, \infty)$ and $\xi \in (-\infty, \infty)$, that satisfies

$$\boldsymbol{Y}(0, \xi) = \boldsymbol{A}\boldsymbol{Y}(0, -\xi) + 2\boldsymbol{B}\int_0^{\infty} \xi' \boldsymbol{Y}(0, -\xi')\mathrm{e}^{-\xi'^2}\,\mathrm{d}\xi', \tag{52}$$

for $\xi \in (0, \infty)$. In addition, the desired solution must satisfy the conditions

$$\lim_{x\to\infty} \frac{\mathrm{d}}{\mathrm{d}x}\frac{2}{3}\pi^{-1/2}\int_{-\infty}^{\infty} \begin{bmatrix} (\xi^2 - 1/2)\boldsymbol{I} \\ \boldsymbol{I} \end{bmatrix}^{\mathrm{T}} \boldsymbol{Y}(x, \xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{53}$$

and

$$\lim_{x\to\infty} \int_{-\infty}^{\infty} \begin{bmatrix} (\xi^2 + 1)\boldsymbol{I} \\ \boldsymbol{I} \end{bmatrix}^{\mathrm{T}} \boldsymbol{Y}(x, \xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi = \boldsymbol{0} \tag{54}$$

that can be deduced from Eqs. (20) to (23). And so looking back to Eqs. (49) and (50), we see that Eq. (53) requires us to take $B_j = 0$, $j = 4, 5, \ldots, 4N$. Now substituting Eq. (50) into Eqs. (53) and (54), we conclude that these conditions can be satisfied if we (introduce A) and take

$$B_1 = 1, \quad B_2 = 1 \quad \text{and} \quad B_3 = -(3/2)^{-1/2} \tag{55a,b,c}$$

and

$$A_1 = -A, \quad A_2 = -A \quad \text{and} \quad A_3 = (3/2)^{-1/2}A. \tag{56a,b,c}$$

Making use of Eqs. (55) and (56), we express the desired solution as

$$\boldsymbol{Y}(x, \pm \xi_i) = (x\boldsymbol{I} \mp \xi_i \boldsymbol{\Sigma}^{-1})\boldsymbol{R}(\xi_i) + A\boldsymbol{R}(\xi_i) + \sum_{j=4}^{4N} A_j \boldsymbol{\Phi}(\nu_j, \pm \xi_i)\mathrm{e}^{-x/\nu_j} \tag{57}$$

where in general

$$\boldsymbol{R}(\xi) = \begin{bmatrix} \xi^2 - 3/2 \\ \xi^2 - 3/2 \\ 1 \\ 1 \end{bmatrix}. \tag{58}$$

We note that there are still $4N - 2$ unknown constants in the solution given by Eq. (57), and so we intend to determine these constants from the boundary condition at the wall. To pursue this, we write a discrete-ordinates version of Eq. (52) as

$$\boldsymbol{Y}(0, \xi_i) = \boldsymbol{A}\boldsymbol{Y}(0, -\xi_i) + 2\boldsymbol{B}\int_0^\infty \xi \boldsymbol{Y}(0, -\xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi \tag{59a}$$

or

$$\boldsymbol{Y}(0, \xi_i) = \boldsymbol{A}\boldsymbol{Y}(0, -\xi_i) + 2\pi^{1/2}\boldsymbol{B}\sum_{k=1}^{N} \hat{w}_k \xi_k \boldsymbol{Y}(0, -\xi_k) \tag{59b}$$

for $i = 1, 2, \dots, N$. We have written both of Eqs. (59) in order to emphasize a particular feature of the solution given by Eq. (57). We think of Eq. (57) as being comprised of two components, one having to do with the vector $\boldsymbol{R}(\xi)$ that is defined for all ξ and the remaining part that is defined only at $\{\pm \xi_i\}$. And so when we wish to evaluate integrals involving Eq. (57), we integrate the terms related to $\boldsymbol{R}(\xi)$ exactly (if we can) and we use our quadrature scheme to integrate the other component.

The collection of equations defined by either of Eqs. (59) consists of $4N$ linear equations for the $4N - 2$ unknowns A and A_j, for $j = 4, 5, \dots, 4N$, and so the linear system is clearly overly determined. While we could follow what was done in Ref. [18] and use a projection technique to obtain a "square" system, we intend to follow Ref. [21] and to solve the overly determined system in a "least-squares" sense. And so, we consider our solution complete. Of course, having defined the vector-valued function $\boldsymbol{Y}(x, \xi)$, we can find the temperature perturbations from Eq. (23) and the density perturbations from Eq. (22). We express these results as

$$\boldsymbol{T}(x) = (A + x)\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \left(\frac{2}{3}\right)^{1/2} \sum_{j=4}^{4N} A_j \begin{bmatrix} f_1(\nu_j) \\ f_2(\nu_j) \end{bmatrix} \mathrm{e}^{-x/\nu_j} \tag{60}$$

and

$$\boldsymbol{N}(x) = -(A + x)\begin{bmatrix} 1 \\ 1 \end{bmatrix} + \sum_{j=4}^{4N} A_j \begin{bmatrix} f_3(\nu_j) \\ f_4(\nu_j) \end{bmatrix} \mathrm{e}^{-x/\nu_j} \tag{61}$$

where $f_k(v_j)$ is the kth component of $\boldsymbol{F}(v_j)$. Finally

$$\zeta = A \tag{62}$$

is the so-called temperature-jump coefficient.

Having formulated our results, we are ready to discuss a few of the computational details concerning the numerical implementation of the solution. As much of this discussion follows directly from Refs. [15,17], we can be brief. To start, we note that our solution is not defined until we specify a quadrature scheme, and so, first of all, we have used either the transformation

$$u(\xi) = \frac{1}{1+\xi} \tag{63a}$$

or the transformation

$$u(\xi) = \mathrm{e}^{-\xi} \tag{63b}$$

to map the interval $\xi \in [0, \infty)$ onto $u \in [0,1]$, and we then used a Gauss–Legendre scheme mapped onto the interval [0,1]. Of course other quadrature schemes could be used, but the scheme mentioned has worked so well for us that we have not investigated other choices. In regard to the choice of quadrature points, we consider it important to note, because of the way our basic eigenvalue problem is formulated, that we must exclude zero from the set of quadrature points. Of course to exclude zero from the quadrature set is not considered a serious restriction since typical Gauss quadrature schemes do not include the end-points of the integration interval. Having defined our quadrature scheme, we found the required separation constants $\{v_j\}$ by using the driver program RG from the EISPACK collection [23] to find the eigenvalues defined by Eq. (36). We then used the subroutine DGECO from the LINPACK package [24] to compute the required null vectors $\boldsymbol{F}(v_j)$ as defined by Eq. (40), and so, after using the subroutines DQRCO and DQRSL, also from the LINPACK package [24], to solve in a least-squares sense the linear system derived from Eqs. (59) to find the constants A, A_j, for $j = 4, 5, \dots, 4N$, we consider our solution complete.

Finally, but importantly, we wish to take into account the fact that the right-hand side of Eq. (38) can perhaps, for some values of v_j and ξ_i, be zero from a computational point-of-view. Of course, in this event some of the constants from the collection $\{\sigma v_j, v_j\}$ will be equal to some of the nodes from the collection $\{\xi_k\}$, and this is clearly not allowed (without qualification) in Eq. (39). We have found that as long as we seek qualities, such as the temperature and density perturbations, that are defined in terms of integrals (that are evaluated by our defined quadrature scheme) of the basic

Table 1
The temperature-jump coefficient for $m_1/m_2 = 0.5$ with $k_{12}/k_{11} = 1$ and $k_{22}/k_{11} = 1$

α_1	α_2	$n_1/n_2 = 9$	$n_1/n_2 = 4$	$n_1/n_2 = 1$	$n_1/n_2 = \frac{1}{4}$	$n_1/n_2 = \frac{1}{9}$
1.0	1.0	1.280169	1.255537	1.165513	1.039218	9.846511 (−1)
1.0	0.8	1.304651	1.306836	1.315429	1.329035	1.335453
0.8	1.0	1.829406	1.755089	1.502462	1.186776	1.061017
0.8	0.8	1.865788	1.828863	1.695355	1.511631	1.433446
0.5	0.5	3.560517	3.486483	3.223743	2.874439	2.729898

Table 2
The temperature-jump coefficient for $m_1/m_2 = 2$ with $k_{12}/k_{11} = 1$ and $k_{22}/k_{11} = 1$

α_1	α_2	$n_1/n_2 = 9$	$n_1/n_2 = 4$	$n_1/n_2 = 1$	$n_1/n_2 = \frac{1}{4}$	$n_1/n_2 = \frac{1}{9}$
1.0	1.0	1.392507	1.469677	1.648284	1.775597	1.810432
1.0	0.8	1.500504	1.678355	2.124802	2.482070	2.587171
0.8	1.0	1.888616	1.879540	1.860298	1.848145	1.845055
0.8	0.8	2.027199	2.137769	2.397594	2.586403	2.638622
0.5	0.5	3.860659	4.065070	4.559061	4.930632	5.035332

Table 3
The temperature and density perturbations for the case $m_1/m_2 = 1/5.0415$ with $\alpha_1 = 0.5$, $\alpha_2 = 0.5$, $k_{12}/k_{11} = 1.339$ and $k_{22}/k_{11} = 0.642$

	$n_1/n_2 = 4$				$n_1/n_2 = \frac{1}{4}$			
x	$T_1(x)$	$T_2(x)$	$N_1(x)$	$N_2(x)$	$T_1(x)$	$T_2(x)$	$N_1(x)$	$N_2(x)$
0.0	2.79361	2.19366	− 2.95620	− 2.25879	2.56297	2.30764	− 2.72310	− 2.42364
0.1	3.04683	2.58867	− 3.18860	− 2.61688	2.79451	2.57526	− 2.93617	− 2.66804
0.2	3.22320	2.83683	− 3.34970	− 2.84750	2.95650	2.75702	− 3.08447	− 2.83460
0.3	3.37782	3.04426	− 3.49185	− 3.04442	3.09910	2.91506	− 3.21581	− 2.98107
0.4	3.52044	3.22885	− 3.62391	− 3.22241	3.23115	3.06011	− 3.33827	− 3.11688
0.5	3.65521	3.39827	− 3.74955	− 3.38764	3.35642	3.19673	− 3.45520	− 3.24593
0.6	3.78440	3.55667	− 3.87074	− 3.54343	3.47695	3.32737	− 3.56836	− 3.37024
0.7	3.90937	3.70664	− 3.98865	− 3.69187	3.59397	3.45352	− 3.67881	− 3.49105
0.8	4.03106	3.84995	− 4.10403	− 3.83437	3.70830	3.57618	− 3.78724	− 3.60914
0.9	4.15011	3.98782	− 4.21741	− 3.97196	3.82052	3.69603	− 3.89412	− 3.72506
1.0	4.26698	4.12120	− 4.32919	− 4.10542	3.93102	3.81359	− 3.99977	− 3.83922
2.0	5.36790	5.31322	− 5.39826	− 5.30366	4.98636	4.91802	− 5.02351	− 4.92586
3.0	6.41246	6.38961	− 6.42851	− 6.38492	6.00539	5.96399	− 6.02692	− 5.96633
4.0	7.43529	7.42499	− 7.44420	− 7.42273	7.01328	6.98767	− 7.02624	− 6.98817
5.0	8.44791	8.44295	− 8.45303	− 8.44183	8.01693	8.00085	− 8.02493	− 8.00076
6.0	9.45521	9.45269	− 9.45824	− 9.45212	9.01875	9.00855	− 9.02378	− 9.00831
7.0	10.4596	10.4582	− 10.4614	− 10.4579	10.0197	10.0132	− 10.0229	− 10.0130
8.0	11.4623	11.4615	− 11.4634	− 11.4613	11.0203	11.0161	− 11.0223	− 11.0159
9.0	12.4640	12.4635	− 12.4647	− 12.4634	12.0206	12.0179	− 12.0219	− 12.0177
10.0	13.4650	13.4648	− 13.4655	− 13.4647	13.0208	13.0190	− 13.0217	− 13.0189
20.0	23.4671	23.4670	− 23.4671	− 23.4670	23.0212	23.0212	− 23.0212	− 23.0212

discrete-ordinates solution, then we can simply omit, from some aspects our calculation, all N_0 offending quadrature points and all $4N_0$ offending separation constants. While this procedure can, we believe, be justified in terms of the numerics of the problem, a more elegant (and perhaps more complicated) procedure, as was reported in Ref. [18], could have been used here.

To complete this work, we use the accompanying tables to list our results, which we believe to be correct to all digits given, for the temperature-jump coefficient ζ and the temperature and density perturbations, $\boldsymbol{T}(x)$ and $\boldsymbol{N}(x)$ (Tables 1–3). Of course, we have no proof of the accuracy of our results, but we have done various things to establish the confidence we have. First of all, we have increased the value of N used in our computations until we found stability in the final results, and we have also used both nonlinear maps given by Eqs. (63) to obtain the same results as given in our tables. In regard to published results, we have found only Onishi's work [8], and so we have confirmed, except for two cases, all five of the significant figures for the temperature-jump coefficient reported by Onishi. Although Onishi [8] did not report his results for the temperature and density perturbations in tabular form (and so a definitive comparison with those results cannot be made), we have confirmed the qualitative form of Onishi's results (given in a graphical format). We have also obtained our final results from two independently developed FORTRAN and MATLAB implementations of our solution, and so we believe we can justify the confidence we have in our reported numerical results.

We note that we have typically used $N = 50$ to generate the results listed in our tables and that our FORTRAN implementation (no special effort was made to make the code especially efficient) of our discrete-ordinates solution (with $N = 50$) runs in less than a 3 s on a 400 MHz Pentium-based notebook PC. Finally, to have some idea about N_0, the number of quadrature points not included in some parts of our calculation, we note that using $\varepsilon = 10^{-14}$ to decide if an eigenvalue and a quadrature point were the same "computationally", we found $N_0 = 2$ when $N = 50$ and the map defined by Eq. (63b) were used.

5. Concluding remarks

The classical half-space temperature-jump problem has been solved for the case of a binary gas mixture. The solution is based on a concise analytical version of the discrete-ordinates method which has been implemented to yield numerical results of high accuracy for the temperature-jump coefficient and temperature and density fields. We believe the ease of use and particularly the accurate results obtained justify our confidence that the method can also be used to solve a much larger class of problems in the general area of rarefied-gas dynamics.

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