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# A Discrete-Ordinates Solution for Heat Transfer in a Plane Channel

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A recently established version of the discrete-ordinates method is used to develop a solution to a class of problems in the theory of rarefied-gas dynamics where temperature and density effects are coupled. In particular, accurate solutions for the temperature perturbation, the density perturbation, and the heat flux are developed and evaluated for the flow, described by the Bhatnagar, Gross, and Krook model, of a rarefied gas between two parallel plates at which arbitrary and unequal accommodation is allowed. Numerical results are obtained for various choices of the accommodation coefficients and a wide range of the inverse Knudsen number. © 1999 Academic Press

## 1. INTRODUCTION

The method of discrete ordinates was introduced and used by Chandrasekhar [1] to solve well many basic problems in the area of radiative transfer. And while the method is somewhat less well developed and less often used in the general area of the kinetic theory of gases, we note that the early works of Wachman and Hamel [2], Huang and Giddens [3], and Bramlette and Huang [4] all illustrate that the discrete-ordinates method can be used to solve basic problems in this important branch of particle-transport theory. The idea of the discrete-ordinates method is very simple indeed: various integral terms in some form of the Boltzmann equation are replaced by numerical-quadrature approximations to those terms, and then a resulting set of ordinary differential equations is solved. However, there are many ways of introducing quadrature approximations and many ways of dealing with the resulting computational aspects of the relevant equations. In this work we define some elementary transformations that allow us to use a “half-range” quadrature scheme (considered superior to a “full-range” scheme) without having to do the careful numerical work required to define special purpose quadrature rules.

Needless to say, many numerical methods can yield meaningful results in low order. Our goal in this work has been somewhat different: we have defined and implemented our version of the discrete-ordinates method in such a way that very high quality results can be



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obtained in, say, intermediate order with a numerical method that is stable in high order. To illustrate the merits of our solution, which we hope will be used for even more challenging applications, we consider the quite difficult problem of the interaction of temperature and density effects in a plane channel. While the problem chosen to test our numerical work is not new, a uniqueness issue concerning the formulation of the problem is thought to be newly resolved here.

We consider a problem concerning heat transfer in a rarefied gas confined between two parallel plates, and since we are focusing our attention here on temperature and density effects as described by the linearized BGK equation [5], we can make use of the decomposition discussed by Cercignani [6] and thus base our work on the vector equation

$$\mu\frac{\partial}{\partial x}\mathbf{\Psi}(x,\mu)+\mathbf{\Psi}(x,\mu)=\pi^{-1/2}\mathbf{Q}(\mu)\int_{-\infty}^{\infty}\mathbf{Q}^{\mathrm{T}}(u)\mathbf{\Psi}(x,u)e^{-u^2}\,du, \tag{1}$$

for $x\in(-\delta/2,\delta/2)$ and $\mu\in(-\infty,\infty)$. Here we use the superscript T to denote the transpose operation, $x$ is the spatial distance (measured in dimensionless units) from the centerline between the two plates, $\mu$ is the non-dimensional $x$ component of the velocity, and

$$\mathbf{Q}(\mu)=\begin{bmatrix}\left(\frac{2}{3}\right)^{1/2}\left(\mu^2-\frac{1}{2}\right) & 1\\ \left(\frac{2}{3}\right)^{1/2} & 0\end{bmatrix}. \tag{2}$$

Following Ref. [7], we note that the components of

$$\mathbf{\Psi}(x,\mu)=\begin{bmatrix}\psi_1(x,\mu)\\ \psi_2(x,\mu)\end{bmatrix} \tag{3}$$

are related to the dimensionless perturbations in the number density and the temperature of the gas, *viz.*,

$$\Delta\rho(x)=\frac{1}{\pi}\int_{-\infty}^{\infty}\begin{bmatrix}1\\0\end{bmatrix}^{\mathrm{T}}\mathbf{\Psi}(x,\mu)e^{-\mu^2}\,d\mu \tag{4a}$$

and

$$\Delta T(x)=\frac{2}{3\pi}\int_{-\infty}^{\infty}\begin{bmatrix}\mu^2-\frac{1}{2}\\ 1\end{bmatrix}^{\mathrm{T}}\mathbf{\Psi}(x,\mu)e^{-\mu^2}\,d\mu. \tag{4b}$$

In regard to the boundary conditions, subject to which we must solve Eq. (1), we continue to follow Ref. [7] and write

$$\mathbf{\Psi}(-a,\mu)=(1-\alpha_1)\mathbf{\Psi}(-a,-\mu)+\alpha_1\pi^{1/2}\begin{bmatrix}\mu^2+b_1\\ 1\end{bmatrix} \tag{5a}$$

and

$$\mathbf{\Psi}(a,-\mu)=(1-\alpha_2)\mathbf{\Psi}(a,\mu)-\alpha_2\pi^{1/2}\begin{bmatrix}\mu^2+b_2\\ 1\end{bmatrix} \tag{5b}$$

for $\mu \in (0, \infty)$. Here we use $a = \delta/2$ for the channel half-width and $\alpha_1$ and $\alpha_2$ for the accommodation coefficients at the two walls that confine the gas. In addition the constants $b_1$ and $b_2$ used in Eqs. (5) are to be defined so that the condition of no net flow in the $x$ direction can be satisfied not only for $x \in (-a, a)$ but also at two boundaries $x = \pm a$. We express this condition of no net flow in the $x$ direction as it was done in Ref. [7], *viz.*,

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}^{\mathrm{T}} \int_{-\infty}^{\infty} \mathbf{\Psi}(x, \mu) e^{-\mu^2} \mu \, d\mu = 0 \tag{6}$$

for $x \in [-a, a]$. We can now substitute Eqs. (5) into Eq. (6) to find

$$b_1 = -1 + 2\pi^{-1/2} \int_0^{\infty} \psi_1(-a, -\mu) e^{-\mu^2} \mu \, d\mu \tag{7a}$$

and

$$b_2 = -1 - 2\pi^{-1/2} \int_0^{\infty} \psi_1(a, \mu) e^{-\mu^2} \mu \, d\mu, \tag{7b}$$

where $\psi_1(x, \mu)$ is the first component of $\mathbf{\Psi}(x, \mu)$. We can use Eqs. (7) to rewrite Eqs. (5) as

$$\mathbf{\Psi}(-a, \mu) = (1 - \alpha_1)\mathbf{\Psi}(-a, -\mu) + 2\alpha_1 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \int_0^{\infty} \mathbf{\Psi}(-a, -u) e^{-u^2} u \, du + \mathbf{K}_1(\mu) \tag{8a}$$

and

$$\mathbf{\Psi}(a, -\mu) = (1 - \alpha_2)\mathbf{\Psi}(a, \mu) + 2\alpha_2 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \int_0^{\infty} \mathbf{\Psi}(a, u) e^{-u^2} u \, du - \mathbf{K}_2(\mu) \tag{8b}$$

for $\mu \in (0, \infty)$. Here the known functions are

$$\mathbf{K}_1(\mu) = \alpha_1 \pi^{1/2} \begin{bmatrix} \mu^2 - 1 \\ 1 \end{bmatrix} \tag{9a}$$

and

$$\mathbf{K}_2(\mu) = \alpha_2 \pi^{1/2} \begin{bmatrix} \mu^2 - 1 \\ 1 \end{bmatrix}. \tag{9b}$$

In this work we intend to compute $\Delta\rho(x)$ and $\Delta T(x)$ as given by Eqs. (4) and the normalized heat flux $q$ defined as [8, 9]

$$q = -\left( \frac{\alpha_1 + \alpha_2 - \alpha_1\alpha_2}{\alpha_1\alpha_2} \right) \pi^{-1/2} \int_{-\infty}^{\infty} \begin{bmatrix} \mu^2 + 1 \\ 1 \end{bmatrix}^{\mathrm{T}} \mathbf{\Psi}(x, \mu) e^{-\mu^2} \mu \, d\mu. \tag{10}$$

## 2. A QUESTION OF UNIQUENESS

We wish to point out that the heat-transfer problem defined by Eqs. (1), (8), and (9) does not have a unique solution. This observation is easily made once we see that if $\mathbf{\Psi}(x, \mu)$ is a solution of Eqs. (1), (8), and (9) then so is

$$\hat{\mathbf{\Psi}}(x, \mu) = \mathbf{\Psi}(x, \mu) + K \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{11}$$

for any value of $K$. In Ref. [7] Thomas *et al.* solved, for the case of $\alpha_1 = \alpha_2$, the coupled temperature–density problem we are considering here. In that work [7] the authors imposed the antisymmetry condition

$$\mathbf{\Psi}(-x, -\mu) = -\mathbf{\Psi}(x, \mu) \tag{12}$$

which, when utilized in Eqs. (7) and (11), shows that the Thomas *et al.* formulation of the $\alpha_1 = \alpha_2$ case has $K = 0$ and $b_1 = b_2$. Here, in order to define the constant $K$ we follow a suggestion offered by Chang [10] and impose the conservation condition

$$\int_{-a}^{a} \Delta\rho(x)\, dx = 0, \tag{13}$$

and so if we substitute Eq. (11) into Eq. (4a) and the resulting equation into Eq. (13) we find that

$$K = -\frac{\pi^{-1/2}}{2a} \int_{-a}^{a} \int_{-\infty}^{\infty} \psi_1(x, \mu) e^{-\mu^2}\, d\mu\, dx. \tag{14}$$

To see the effect of the constant $K$ on the quantities we intend to compute we substitute $\hat{\mathbf{\Psi}}(x, \mu)$ into Eqs. (4b) and (10) and note that the term added to $\mathbf{\Psi}(x, \mu)$ in Eq. (11) does not affect the temperature perturbation $\Delta T(x)$ or the heat flux $q$. However, substituting Eq. (11) into Eq. (4a), we find that

$$\Delta\rho(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \begin{bmatrix} 1 \\ 0 \end{bmatrix}^{\mathrm{T}} \mathbf{\Psi}(x, \mu) e^{-\mu^2}\, d\mu + K\pi^{-1/2} \tag{15}$$

does depend on the constant $K$. It is clear that by defining the constant $K$ as we have done in Eq. (14) we have removed the multiplicity of solutions as expressed by Eq. (11); on the other hand, we clearly have not proved that the problem, as we now have it defined, does in fact have a unique solution.

## 3. A DISCRETE-ORDINATES SOLUTION

In a recent paper [11] concerning a radiative-transfer problem for a model that included some polarization effects, a discrete-ordinates solution was developed that is very similar to what we require here to solve Eq. (1) subject to the boundary conditions given by Eqs. (8) and (9). In order to make use immediately of Ref. [11] we multiply Eq. (1) by $\mathbf{Q}^{-1}(\mu)$ and define

$$\mathbf{G}(x, \mu) = \mathbf{Q}^{-1}(\mu)\mathbf{\Psi}(x, \mu) \tag{16}$$

and

$$\boldsymbol{\Psi}(u) = \pi^{-1/2}\mathbf{Q}^{\mathrm{T}}(u)\mathbf{Q}(u)e^{-u^2} \tag{17}$$

so we can obtain

$$\mu\frac{\partial}{\partial x}\mathbf{G}(x,\mu) + \mathbf{G}(x,\mu) = \int_{-\infty}^{\infty}\boldsymbol{\Psi}(u)\mathbf{G}(x,u)\,du \tag{18}$$

for $x \in (-a, a)$ and $\mu \in (-\infty, \infty)$. As the basic elements of the discrete-ordinates solution we wish to develop have already been reported in Ref. [11], we now repeat (only briefly) a part of Ref. [11] we can use in this work, and then we will make some modifications to the solution that are specific to the heat-transfer problem considered here.

We note first of all that (what we call) the characteristic matrix $\boldsymbol{\Psi}(u)$ as defined by Eq. (17) is symmetric. Also $\boldsymbol{\Psi}(u) = \boldsymbol{\Psi}(-u)$, and so we write our discrete-ordinates equations as

$$\mu_i\frac{d}{dx}\mathbf{G}(x,\mu_i) + \mathbf{G}(x,\mu_i) = \sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\mu_k)[\mathbf{G}(x,\mu_k) + \mathbf{G}(x,-\mu_k)] \tag{19a}$$

and

$$-\mu_i\frac{d}{dx}\mathbf{G}(x,-\mu_i) + \mathbf{G}(x,-\mu_i) = \sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\mu_k)[\mathbf{G}(x,\mu_k) + \mathbf{G}(x,-\mu_k)] \tag{19b}$$

for $i = 1, 2, \ldots, N$. In writing Eqs. (19) as we have, we clearly are considering that the $N$ quadrature points $\{\mu_k\}$ 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 attribute the especially good accuracy we have obtained from the solution reported here.

Following Ref. [11], we substitute

$$\mathbf{G}(x, \pm\mu_i) = \boldsymbol{\Phi}(\nu, \pm\mu_i)e^{-x/\nu} \tag{20}$$

into Eqs. (19) to find

$$(\nu - \mu_i)\boldsymbol{\Phi}(\nu,\mu_i) = \nu\sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\mu_k)[\boldsymbol{\Phi}(\nu,\mu_k) + \boldsymbol{\Phi}(\nu,-\mu_k)] \tag{21a}$$

and

$$(\nu + \mu_i)\boldsymbol{\Phi}(\nu,-\mu_i) = \nu\sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\mu_k)[\boldsymbol{\Phi}(\nu,\mu_k) + \boldsymbol{\Phi}(\nu,-\mu_k)] \tag{21b}$$

for $i = 1, 2, \ldots, N$. If we now let $\Phi_1(\nu, \pm\mu_i)$ and $\Phi_2(\nu, \pm\mu_i)$ denote the two components of $\boldsymbol{\Phi}(\nu, \pm\mu_i)$ and if we use

$$\boldsymbol{\Phi}_{1\pm} = [\Phi_1(\nu,\pm\mu_1), \Phi_1(\nu,\pm\mu_2), \ldots, \Phi_1(\nu,\pm\mu_N)]^{\mathrm{T}} \tag{22a}$$

and

$$\boldsymbol{\Phi}_{2\pm} = [\Phi_2(\nu,\pm\mu_1), \Phi_2(\nu,\pm\mu_2), \ldots, \Phi_2(\nu,\pm\mu_N)]^{\mathrm{T}} \tag{22b}$$

then we can write rewrite Eqs. (21) as

$$\frac{1}{\nu}\mathbf{M}\mathbf{\Phi}_{+} = (\mathbf{I} - \mathbf{W})\mathbf{\Phi}_{+} - \mathbf{W}\mathbf{\Phi}_{-} \tag{23a}$$

and

$$-\frac{1}{\nu}\mathbf{M}\mathbf{\Phi}_{-} = (\mathbf{I} - \mathbf{W})\mathbf{\Phi}_{-} - \mathbf{W}\mathbf{\Phi}_{+}. \tag{23b}$$

Here $\mathbf{I}$ is the $2N \times 2N$ identity matrix, the two vector elements of $\mathbf{\Phi}_{\pm}$ are $\mathbf{\Phi}_{1\pm}$ and $\mathbf{\Phi}_{2\pm}$, the four $N \times N$ matrix elements of $\mathbf{W}$, *viz.*, $\mathbf{W}_{m,n}$, for $m, n = 1, 2,$ are given by

$$(\mathbf{W}_{m,n})_{i,j} = w_j \Psi_{m,n}(\mu_j), \tag{24}$$

where $\Psi_{m,n}(\mu)$, $m, n = 1, 2,$ are the elements of $\mathbf{\Psi}(\mu)$, and

$$\mathbf{M} = \text{diag}\{\mu_1, \mu_2, \ldots, \mu_N, \mu_1, \mu_2, \ldots, \mu_N\}. \tag{25}$$

Continuing to follow Ref. [11], we now let

$$\mathbf{U} = \mathbf{\Phi}_{+} + \mathbf{\Phi}_{-} \tag{26a}$$

and

$$\mathbf{V} = \mathbf{\Phi}_{+} - \mathbf{\Phi}_{-} \tag{26b}$$

so that we can eliminate between the sum and the difference of Eqs. (23) to find

$$(\mathbf{D} - 2\mathbf{M}^{-1}\mathbf{W}\mathbf{M}^{-1})\mathbf{M}\mathbf{U} = \lambda\mathbf{M}\mathbf{U}, \tag{27}$$

where $\lambda = 1/\nu^2$ and

$$\mathbf{D} = \text{diag}\left\{\mu_1^{-2}, \mu_2^{-2}, \ldots, \mu_N^{-2}, \mu_1^{-2}, \mu_2^{-2}, \ldots, \mu_N^{-2}\right\}. \tag{28}$$

Considering that we have found the required separation constants $\{\pm\nu_j\}$ from the eigenvalues defined by Eq. (27), we go back to Eqs. (21) to find $\mathbf{\Phi}(\nu_j, \pm\mu_i)$, and so we write our general solution to Eqs. (19) as

$$\mathbf{G}(\tau, \pm\mu_i) = \sum_{j=1}^{2N}\left[A_j \frac{\nu_j}{\nu_j \mp \mu_i} e^{-(a+x)/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \mu_i} e^{-(a-x)/\nu_j}\right]\mathbf{F}(\nu_j). \tag{29}$$

Here $\mathbf{F}(\nu_j)$ is a vector in the null space of

$$\mathbf{\Omega}(\nu_j) = \mathbf{I} - 2\nu_j^2 \sum_{\alpha=1}^{N} w_\alpha \mathbf{\Psi}(\mu_\alpha) \frac{1}{\nu_j^2 - \mu_\alpha^2}, \tag{30}$$

$\mathbf{I}$ is now the $2 \times 2$ identity matrix, and the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the boundary conditions. Of course, we cannot allow $\nu_j = \mu_i$ in Eq. (29).

Having used Ref. [11] to obtain Eq. (29), we go back and use Eq. (16) to write a first version of our discrete-ordinates solution for $\mathbf{\Psi}(x, \mu)$ as

$$\mathbf{\Psi}(x, \pm\mu_i) = \mathbf{Q}(\mu_i) \sum_{j=1}^{2N} \left[ A_j \frac{\nu_j}{\nu_j \mp \mu_i} e^{-(a+x)/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \mu_i} e^{-(a-x)/\nu_j} \right] \mathbf{F}(\nu_j). \quad (31)$$

At this point we wish to introduce two basic modifications to Eq. (31) that are important for the problem considered in this work. First of all, it was shown in Ref. [12] that $\det \mathbf{\Omega}(z)$, where

$$\mathbf{\Omega}(z) = \mathbf{I} - 2z^2 \int_0^\infty \mathbf{\Psi}(\mu) \frac{d\mu}{z^2 - \mu^2}, \quad (32)$$

has a fourth-order zero at infinity, and so we choose to ignore the contributions in Eq. (31) from the two largest separation constants, $\nu_N$ and $\nu_{N-1}$ and, instead, to include the exact "discrete" solutions

$$\mathbf{F}_1(x, \mu) = \mathbf{F}_1(\mu) = \left(\frac{2}{3}\right)^{1/2} \begin{bmatrix} \mu^2 - \frac{1}{2} \\ 1 \end{bmatrix}, \quad (33a)$$

$$\mathbf{F}_2(x, \mu) = \mathbf{F}_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad (33b)$$

$$\mathbf{F}_3(x, \mu) = (\mu - x)\mathbf{F}_1(\mu), \quad (33c)$$

and

$$\mathbf{F}_4(x, \mu) = (\mu - x)\mathbf{F}_2 \quad (33d)$$

that Kriese *et al*. [12] found as a result of the fourfold eigenvalue at infinity. So, as a first modification, we choose to rewrite Eq. (31) as

$$\mathbf{\Psi}(x, \pm\mu_i) = \mathbf{\Psi}_*(x, \pm\mu_i) + \mathbf{Q}(\mu_i) \sum_{j=1}^{J} \left[ A_j \frac{\nu_j}{\nu_j \mp \mu_i} e^{-(a+x)/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \mu_i} e^{-(a-x)/\nu_j} \right] \mathbf{F}(\nu_j), \quad (34)$$

where

$$\mathbf{\Psi}_*(x, \pm\mu_i) = [A_1^* + B_1^*(x \mp \mu_i)]\mathbf{F}_1(\mu_i) + [A_2^* + B_2^*(x \mp \mu_i)]\mathbf{F}_2 \quad (35)$$

and where $J = 2N - 2$. Note that we still have $4N$ arbitrary constants to determine from the boundary conditions of our problem. In regard to a second modification of Eq. (31), we note from Eq. (17) that there can be some, say $N_0$, quadrature points $\{\mu_\alpha\}$ where the product $w_\alpha \mathbf{\Psi}(\mu_\alpha)$ is, from a computational point of view, effectively zero, and when this happens the right-hand sides of Eqs. (21) can be effectively zero, and so we can find $\nu_\alpha = \mu_\alpha$. In order to account for these special separation constants we label our quadrature points such that

$$w_\alpha \mathbf{\Psi}(\mu_\alpha) = \mathbf{0}, \qquad \alpha = \alpha_0, \alpha_0 + 1, \dots, N, \quad (36)$$

where $\alpha_0 = N - N_0 + 1$, and then we can express the eigenvectors $\mathbf{\Phi}(\mu_\alpha, \pm\mu_i)$ for these cases as

$$\mathbf{\Phi}^{(1)}(\mu_\alpha, \mu_i) = \delta_{i,\alpha} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{37a}$$

and

$$\mathbf{\Phi}^{(2)}(\mu_\alpha, \mu_i) = \delta_{i,\alpha} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{37b}$$

with

$$\mathbf{\Phi}^{(1)}(\mu_\alpha, -\mu_i) = \mathbf{0} \tag{37c}$$

and

$$\mathbf{\Phi}^{(2)}(\mu_\alpha, -\mu_i) = \mathbf{0}. \tag{37d}$$

Here $\delta_{i,j}$ is the Kronecker delta. Now if we label the $2N - 2$ separation constants $\{\nu_j\}$ such that the first

$$J_* = 2N - 2 - 2N_0$$

of them are not contained in the collection $\mu_i$, $i = 1, 2, \ldots, N$, then we can incorporate the consequences of Eq. (36) into our discrete-ordinates solution and write

$$\mathbf{\Psi}(x, \pm\mu_i) = \mathbf{\Psi}_*^*(x, \pm\mu_i) + \mathbf{Q}(\mu_i) \sum_{j=1}^{J_*} \left[ A_j \frac{\nu_j}{\nu_j \mp \mu_i} e^{-(a+x)/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \mu_i} e^{-(a-x)/\nu_j} \right] \mathbf{F}(\nu_j), \tag{38}$$

where

$$\mathbf{\Psi}_*^*(x, \pm\mu_i) = \mathbf{\Psi}_*(x, \pm\mu_i) + \mathbf{\Delta}(x, \pm\mu_i) \tag{39}$$

with

$$\mathbf{\Delta}(x, \mu_i) = \sum_{\alpha=\alpha_0}^{N} \left[ A_\alpha^{(1)} \mathbf{F}_1(\mu_\alpha) + A_\alpha^{(2)} \mathbf{F}_2 \right] \delta_{i,\alpha} e^{-(a+x)/\mu_\alpha} \tag{40a}$$

and

$$\mathbf{\Delta}(x, -\mu_i) = \sum_{\alpha=\alpha_0}^{N} \left[ B_\alpha^{(1)} \mathbf{F}_1(\mu_\alpha) + B_\alpha^{(2)} \mathbf{F}_2 \right] \delta_{i,\alpha} e^{-(a-x)/\mu_\alpha}. \tag{40b}$$

Note that we still have $4N$ arbitrary constants to be used to satisfy the (approximated) boundary conditions of our problem.

## 4. COMPUTATIONAL DETAILS AND NUMERICAL RESULTS

We proceed now to use the discrete-ordinates result given by Eq. (38) to solve the heat-transfer problem defined by Eqs. (1) and (8). Since the first thing we wish to do is to constrain the expression given by Eq. (38) to meet the condition, as given by Eq. (6), of no net flow in the $x$ direction, we comment on our $\mu$-variable integration techniques when integrals involving $\mathbf{\Psi}(x, \mu)$ are required. Noting that Eq. (38) contains the "exact terms" $\mathbf{F}_\alpha(x, \mu)$, $\alpha = 1, 2, 3$, and 4, and terms that come directly from our discrete-ordinates approach, we use two different ways of evaluating the mentioned $\mu$-variable integrations. When integrating the exact terms we use exact integration, but when evaluating integrals containing the discrete-ordinates terms, we use our general quadrature formula, *viz.*,

$$\int_{-\infty}^{\infty} f(\mu)\, d\mu = \sum_{k=1}^{N} w_k [f(\mu_k) + f(-\mu_k)]. \tag{41}$$

Now substituting Eq. (38) into Eq. (6) and integrating as just mentioned, we find

$$\left(\frac{2}{3}\right)^{1/2} B_1^* + B_2^* = 0, \tag{42}$$

and so we rewrite our solution as

$$\mathbf{\Psi}(x, \pm\mu_i) = \mathbf{\Psi}_*^*(x, \pm\mu_i) + \mathbf{Q}(\mu_i) \sum_{j=1}^{J_*} \left[ A_j \frac{\nu_j}{\nu_j \mp \mu_i} e^{-(a+x)/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \mu_i} e^{-(a-x)/\nu_j} \right] \mathbf{F}(\nu_j), \tag{43}$$

where $\mathbf{\Psi}_*^*(x, \pm\mu_i)$ is given by Eq. (39) and now

$$\mathbf{\Psi}_*(x, \pm\mu_i) = A_1^* \mathbf{F}_1(\mu_i) + B_1^*(x \mp \mu_i)\mathbf{G}(\mu_i) \tag{44}$$

with

$$\mathbf{G}(\mu) = \left(\frac{2}{3}\right)^{1/2} \begin{bmatrix} \mu^2 - \frac{3}{2} \\ 1 \end{bmatrix}. \tag{45}$$

We note that since $\mathbf{F}_2$ is a solution of Eq. (1) that also satisfies homogeneous versions of Eqs. (8) we have dropped that term from Eq. (38) when writing Eq. (43).

If we now substitute Eq. (43) into Eqs. (8) evaluated at the quadrature points $\mu_i$, then we obtain a system of $4N$ equations for the $4N - 2$ unknown constants appearing in Eq. (43). This system of linear equations is clearly overly determined, and so we use a projection technique to obtain a "square" system. Since each quadrature point $\mu_i$ generates two equations on each of the two boundaries $x = -a$ and $x = a$, we choose to add together the two equations generated at $x = -a$ by the quadrature point $\mu_{N-N_0}$ and to ignore the second of the two equations generated, still at $x = -a$, from that same quadrature point. We then carry out the same procedure at the boundary $x = a$, and in this way we obtain the $2N - 2$ equations we solve (with Gaussian elimination) to find the $2N - 2$ constants required to complete the solution given by Eq. (43).

Of course, our solution is not defined until we specify a quadrature scheme, and so here we follow what was done in a recent work concerning Poiseuille flow [13]. First of all we have used either the transformation

$$u(\mu) = \frac{1}{1+\mu} \tag{46a}$$

or the transformation

$$u(\mu) = e^{-\mu} \tag{46b}$$

to map the interval $[0, \infty)$ onto $[0, 1]$, and we then used a Gauss–Legendre scheme mapped onto the interval $[0, 1]$. Of course other quadrature schemes could be used. In fact we note that recent works by Garcia [14] and Gander and Karp [15] have reported special quadrature schemes for use in the general area of particle-transport theory. Such an approach clearly could be used here. In fact the choice of a quadrature scheme based on the integration interval $[0, \infty)$ with a weight function

$$W(\mu) = e^{-\mu^2}$$

seems a natural choice for this work [see Ref. 3]. However, we have found the use of a mapping defined by either of Eqs. (46) followed by the use of the Gauss–Legendre integration formulas to be so effective that we have not tried other integration techniques.

Having defined our quadrature scheme, we found the required separation constants $\{\nu_j\}$ by using the driver program RG from the EISPACK collection [16] to find the eigenvalues defined by Eq. (27), and so we consider our solution complete.

Assuming that we have solved our linear system to find all of the required constants, we now substitute Eq. (43) into Eqs. (4b), (10), and (15) to find expressions for the physical quantites that we wish to compute, *viz*.,

$$\Delta T(x) = \left(\frac{2}{3\pi}\right)^{1/2} \left\{ A_1^* + B_1^* x + \sum_{j=1}^{J_*} \left[ A_j e^{-(a+x)/\nu_j} + B_j e^{-(a-x)/\nu_j} \right] f_1(\nu_j) \right\}, \tag{47}$$

$$q = -\frac{5}{8}\left(\frac{2}{3}\right)^{1/2} \left(\frac{\alpha_1 + \alpha_2 - \alpha_1\alpha_2}{\alpha_1\alpha_2}\right) B_1^*, \tag{48}$$

and

$$\Delta\rho(x) = \pi^{-1/2} \left\{ -\left(\frac{2}{3}\right)^{1/2} B_1^* x + \sum_{j=1}^{J_*} \left[ A_j e^{-(a+x)/\nu_j} + B_j e^{-(a-x)/\nu_j} \right] f_2(\nu_j) + K \right\}, \tag{49}$$

where $f_1(\nu_j)$ and $f_2(\nu_j)$ are the two components of the vector $\mathbf{F}(\nu_j)$. To be complete, we use Eq. (43) in Eq. (14) to find

$$K = -\frac{1}{2a} \sum_{j=1}^{J_*} \nu_j \left(1 - e^{-2a/\nu_j}\right)(A_j + B_j) f_2(\nu_j). \tag{50}$$

In order to test the discrete-ordinates solution developed in this work, we have confirmed to all figures given all of the numerical results given, for the case of $\alpha_1 = \alpha_2$, in Ref. [7].

In that work [7], Thomas *et al*. computed and reported the heat flux $q$ with six figures of accuracy and the temperature and density perturbations with five figures of accuracy for various values of the accommodation coefficient and a wide range, our $a \in [0.0005, 5]$, of the inverse Knudsen number. Considering now that $\alpha_1 \neq \alpha_2$, we note that Thomas [8] has reported results of a calculation that was based on exact analysis and that Valougeorgis and Thomas [9] used the $F_N$ method [17] to solve the same class of problems. While the formulation of the basic problem introduced and used in Refs. [8, 9] is different from what we have here, we find that the results can be easily related. If we let $q^\dagger$, $\Delta T^\dagger(x)$, and $\Delta\rho^\dagger(x)$ denote the heat flux, the temperature perturbation, and the density perturbation defined and calculated by Thomas [8] and by Valougeorgis and Thomas [9], then we find that the following relations relate the quantities from Refs. [8, 9] to what we have here,

$$q^\dagger = q, \tag{51a}$$

$$\Delta T^\dagger(x) = \tfrac{1}{2}[1 - \Delta T(x)] \tag{51b}$$

and

$$\Delta\rho^\dagger(x) = \tfrac{1}{2}\left[K\pi^{-1/2} + b_1 + \tfrac{1}{2} - \Delta\rho(x)\right], \tag{51c}$$

where $K$ is given by Eq. (50) and $b_1$ is given by Eq. (7a) or, after we use Eq. (43) in Eq. (7a),

$$b_1 = -1 + 2\pi^{-1/2}\left[\frac{6^{1/2}}{12}(A_1^* + aB_1^*) + S\right], \tag{52}$$

where

$$S = \sum_{k=1}^{N}\sum_{j=1}^{J_*} w_k\mu_k e^{-\mu_k^2}\left[\frac{A_j\nu_j}{\nu_j + \mu_k} + \frac{B_j\nu_j}{\nu_j - \mu_k}e^{-2a/\nu_j}\right]\left[\left(\frac{2}{3}\right)^{1/2}\left(\mu_k^2 - \frac{1}{2}\right) f_1(\nu_j) + f_2(\nu_j)\right]. \tag{53}$$

As a first test of our solution for a case of two different accommodation coefficients we have used our solution (with $N = 60$) to confirm to six significant figures all of the

**TABLE I**
**The Temperature and Density Profiles for $a = 1.0$, $\alpha_1 = 0.7$, and $\alpha_2 = 0.3$**

| $\eta$ | $\Delta T(-a + 2\eta a)$ | $\Delta\rho(-a + 2\eta a)$ |
|---|---|---|
| 0.0 | 6.74584(−1) | −2.64589(−1) |
| 0.1 | 5.96370(−1) | −1.93097(−1) |
| 0.2 | 5.39984(−1) | −1.41190(−1) |
| 0.3 | 4.88604(−1) | −9.34717(−2) |
| 0.4 | 4.39293(−1) | −4.74422(−2) |
| 0.5 | 3.90627(−1) | −1.94045(−3) |
| 0.6 | 3.41552(−1) | 4.38749(−2) |
| 0.7 | 2.90927(−1) | 9.09189(−2) |
| 0.8 | 2.36995(−1) | 1.40637(−1) |
| 0.9 | 1.75849(−1) | 1.96382(−1) |
| 1.0 | 8.40673(−2) | 2.79763(−1) |

**TABLE II**
**The Temperature and Density Profiles for**
**$a = 2.5$, $\alpha_1 = 1.0$, and $\alpha_2 = 0.5$**

| $\eta$ | $\Delta T(-a + 2\eta a)$ | $\Delta\rho(-a + 2\eta a)$ |
|---|---|---|
| 0.0 | 8.26728(−1) | −5.78738(−1) |
| 0.1 | 6.75739(−1) | −4.37145(−1) |
| 0.2 | 5.58061(−1) | −3.23881(−1) |
| 0.3 | 4.46818(−1) | −2.15527(−1) |
| 0.4 | 3.38031(−1) | −1.08983(−1) |
| 0.5 | 2.29936(−1) | −2.94476(−3) |
| 0.6 | 1.21266(−1) | 1.03501(−1) |
| 0.7 | 1.05785(−2) | 2.11399(−1) |
| 0.8 | −1.04578(−1) | 3.22577(−1) |
| 0.9 | −2.30311(−1) | 4.41826(−1) |
| 1.0 | −4.10298(−1) | 6.07501(−1) |

heat-flux results quoted as exact in Ref. [9] for $\alpha_1 = 0.7$ and $\alpha_1 = 0.3$ and various values of $a \in [0.0005, 50]$. We have also used our solution, again with $N = 60$, and the relations given by Eqs. (51b) and (51c) to confirm to all six figures given the temperature and density perturbations reported by Valougeorgis and Thomas [9] for the case $\alpha_1 = 0.7$ and $\alpha_2 = 0.3$ with $a = 1.0$ and the case $\alpha_1 = 1.0$ and $\alpha_2 = 0.5$ with $a = 2.5$. So having found such good agreement with Refs. [7–9], we feel justified in having confidence that our solution and the FORTRAN implementation of the solution are good.

Finally, we wish to report some numerical results that we have found with the solution developed, and so in Tables I and II we list the temperature perturbations and the density perturbations as computed (with $N = 60$) from Eqs. (47), (49), and (50). We note also that we found (in perfect agreement with the heat fluxes given in Ref. [9]) $q = 0.772293$ for the case defined in Table I and $q = 0.447227$ for the case defined in Table II.

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