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The temperature-jump problem in rarefied-gas dynamics

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An analytical version of the discrete-ordinates method is used here to solve the classical temperature-jump problem based on the BGK model in rarefied-gas dynamics. In addition to a complete development of the discrete-ordinates method for the application considered, the computational algorithm is implemented to yield very accurate results for the temperature jump and the complete temperature and density distributions in the gas. The algorithm is easy to use, and the developed code runs typically in less than a second on a 400 MHz Pentium-based PC.

1 Introduction

Following, for example, the basic books of Cercignani [5, 6] and Williams [21], we can consider that the diffusion of gas particles as they flow, say in a plane channel or in a cylindrical tube, can be described mathematically by the Boltzmann equation. Of course for the general case the gas particles interact with each other according to some inter-atomic force laws, and these same particles interact according to specified reflection laws with the surface or surfaces that confine the flow. So it is clear that, unless some special conditions are specified, the scattering term in the Boltzmann equation will depend upon the particle distribution function in a nonlinear way. While, for example, Monte Carlo methods and computationally intensive iterative methods are ways of attempting to extract some physical information from the nonlinear Boltzmann equation, another approach that can be used when the density of particles is small (rarefied-gas dynamics) is to replace the nonlinear Boltzmann equation by a so-called model equation. In regard to model equations for work with rarefied gases, we can say that the formulation introduced by Bhatnagar, Gross and Krook [4], and known in the classical literature as the BGK model, is the one that has most often been employed when exact or semi-analytical mathematical techniques are to be used to develop solutions with a (hoped for) high degree of rigour and accuracy.

As background material, we note that in a series of recent works [2, 3, 16] we have already used our newly developed analytical version [1] of the discrete-ordinates method [7] to solve most of the classical BGK problems, relevant to plane-parallel media, in the general area of rarefied-gas dynamics. To complete our work with these classical

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problems, we solve in this work, in a particularly concise and accurate way, the basic temperature-jump problem defined by Welander [20].

It is clear that the literature concerning the use of the BGK model [4] in rarefied-gas dynamics is very extensive, and so to keep this work to a modest length we do not attempt to review the many works already devoted to this subject. Instead we consider that the books by Cercignani [5, 6] and Williams [21] are available, and so we rely on these books, a paper by Kriese, Chang and Siewert [9] and a recent review paper by Williams [22] for the additional background material that could be of interest here.

2 The Boltzmann equation and boundary conditions

The temperature-jump problem defined by Welander [20] can, as mentioned by Williams [22], be thought of as the temperature version of Kramers' problem for flow over a flat plate. We therefore assume that the gas occupies the half space $x > 0$ and that there is a constant temperature gradient (normal to the plate) at infinity. We thus consider that the dimensionless temperature-jump problem for the BGK model can be formulated in terms of a linearized form of the Boltzmann equation written as

$$c_x \frac{\partial}{\partial x} h(x, \boldsymbol{c}) + h(x, \boldsymbol{c}) = \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} h(x, \boldsymbol{c}') K(\boldsymbol{c}' : \boldsymbol{c}) \mathrm{e}^{-c'^2} \, \mathrm{d}c'_x \, \mathrm{d}c'_y \, \mathrm{d}c'_z \tag{1}$$

for $x > 0$ and where the particle velocity vector, with magnitude c, is $\boldsymbol{c} = (c_x, c_y, c_z)$. We note that in equation (1)

$$h(x, \boldsymbol{c}) \Rightarrow h(x, c_x, c_y, c_z) \tag{2}$$

and

$$K(\boldsymbol{c}' : \boldsymbol{c}) = 1 + 2\boldsymbol{c}' \cdot \boldsymbol{c} + \frac{2}{3}\left(c'^2 - \frac{3}{2}\right)\left(c^2 - \frac{3}{2}\right). \tag{3}$$

Here the basic unknown $h(x, \boldsymbol{c})$ is the perturbation from an initial Maxwellian distribution that, due to the presence of the wall, is a component of the particle distribution function. In addition to the defining form of the Boltzmann equation, we must specify how the particles interact with the wall. Here we consider that some fraction $1 - \alpha$ of the particles is reflected specularly and that the remaining fraction α is reflected diffusely. In other words, the wall acts somewhat like a mirror and at the same time appears to absorb some of the particles and then re-emit them isotropically. Because there is no loss or supply of particles due to the presence of the wall, the boundary condition can be thought of as conservative. This type of boundary condition can be expressed as

$$h(0, c_x, c_y, c_z) = (1 - \alpha) h(0, -c_x, c_y, c_z) + (\mathscr{I} h)(0) \tag{4}$$

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

$$(\mathscr{I} h)(0) = \frac{2\alpha}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{0}^{\infty} \mathrm{e}^{-c'^2} h(0, -c'_x, c'_y, c'_z) c'_x \, \mathrm{d}c'_x \, \mathrm{d}c'_y \, \mathrm{d}c'_z \,, \tag{5}$$

and $\alpha \in (0, 1]$ is the accommodation coefficient.

Should we wish to compute the complete solution $h(x, \boldsymbol{c})$ then we clearly would have to deal with equations (1) and (4) and some additional conditions imposed as x tends to

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infinity. However, since we seek only the temperature and density perturbations [22]

$$T(x) = \frac{2}{3}\pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2}(c^2 - 3/2)h(x,\boldsymbol{c})\,\mathrm{d}c_x\,\mathrm{d}c_y\,\mathrm{d}c_z \tag{6a}$$

and

$$N(x) = \pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2}h(x,\boldsymbol{c})\,\mathrm{d}c_x\,\mathrm{d}c_y\,\mathrm{d}c_z \tag{6b}$$

we can express the desired results in terms of some moments of $h(x,\boldsymbol{c})$. Defining the quantities

$$H_1(x,c_x) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-(c_y^2+c_z^2)}h(x,c_x,c_y,c_z)\,\mathrm{d}c_y\,\mathrm{d}c_z \tag{7}$$

and

$$H_2(x,c_x) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-(c_y^2+c_z^2)}(c_y^2 + c_z^2 - 1)h(x,c_x,c_y,c_z)\,\mathrm{d}c_y\,\mathrm{d}c_z, \tag{8}$$

we can rewrite equations (6) as

$$T(x) = \frac{2}{3}\pi^{-1/2}\int_{-\infty}^{\infty} \mathrm{e}^{-c_x^2}[(c_x^2 - 1/2)H_1(x,c_x) + H_2(x,c_x)]\,\mathrm{d}c_x \tag{9a}$$

and

$$N(x) = \pi^{-1/2}\int_{-\infty}^{\infty} \mathrm{e}^{-c_x^2}H_1(x,c_x)\,\mathrm{d}c_x\,. \tag{9b}$$

Now to find defining equations for $H_1(x,c_x)$ and $H_2(x,c_x)$ we first multiply equations (1) and (4) by

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

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

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

instead of $\phi_1(c_y,c_z)$. In this way we find, after making use of the condition of no net flow, i.e.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c^2}h(x,\boldsymbol{c})c_x\,\mathrm{d}c_x\,\mathrm{d}c_y\,\mathrm{d}c_z = 0, \tag{11}$$

and letting $c_x = \xi$,

$$\xi\frac{\partial}{\partial x}\boldsymbol{Y}(x,\xi) + \boldsymbol{Y}(x,\xi) = \pi^{-1/2}\boldsymbol{Q}(\xi)\int_{-\infty}^{\infty} \boldsymbol{Q}^{\mathrm{T}}(\xi')\boldsymbol{Y}(x,\xi')\mathrm{e}^{-\xi'^2}\,\mathrm{d}\xi', \tag{12}$$

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

$$\boldsymbol{Y}(0,\xi) - (1-\alpha)\boldsymbol{Y}(0,-\xi) - \mathrm{diag}\{2\alpha, 0\}\int_0^{\infty} \boldsymbol{Y}(0,-\xi')\mathrm{e}^{-\xi'^2}\xi'\,\mathrm{d}\xi' = \boldsymbol{0}, \tag{13}$$

for $\xi \in (0,\infty)$; here the upper and lower components of the vector $\boldsymbol{Y}(x,\xi)$ are $H_1(x,\xi)$ and $H_2(x,\xi)$, we use the superscript T to denote the transpose operation and

$$\boldsymbol{Q}(\xi) = \begin{bmatrix} (2/3)^{1/2}(\xi^2 - 1/2) & 1 \\ (2/3)^{1/2} & 0 \end{bmatrix}. \tag{14}$$

Clearly, once we have found the desired $\boldsymbol{Y}(x,\xi)$ we can compute the desired temperature

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and density perturbations from equations (9) written as

$$T(x) = \frac{2}{3}\pi^{-1/2}\int_{-\infty}^{\infty}\begin{bmatrix}\xi^2 - 1/2\\ 1\end{bmatrix}^{\mathrm{T}} \boldsymbol{Y}(x,\xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi \tag{15}$$

and

$$N(x) = \pi^{-1/2}\begin{bmatrix}1\\ 0\end{bmatrix}^{\mathrm{T}}\int_{-\infty}^{\infty}\boldsymbol{Y}(x,\xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi. \tag{16}$$

As noted previously, it is assumed for this temperature-jump problem that there is a heat source at infinity that causes the temperature perturbation $T(x)$ to increase (with a constant gradient normal to the plate) as x tends to infinity. To be more precise, we follow the defining work [20] and two early papers [13, 17] and impose on the dimensionless temperature and density perturbations the conditions

$$\lim_{x\to\infty}\frac{\mathrm{d}}{\mathrm{d}x}T(x) = 1 \tag{17a}$$

and

$$\lim_{x\to\infty}\frac{\mathrm{d}}{\mathrm{d}x}N(x) = -1. \tag{17b}$$

It is clear that equations (17) define, once we note equations (15) and (16), conditions on $\boldsymbol{Y}(x,\xi)$ that we must consider in addition to the boundary condition given as equation (13). Thus we proceed to use our discrete-ordinates method to define a solution $\boldsymbol{Y}(x,\xi)$ of equation (12) such that the components of $\boldsymbol{Y}(x,\xi) \sim x$ as $x \to \infty$. In addition the required $\boldsymbol{Y}(x,\xi)$ must satisfy equation (13) and be such that the resulting $T(x)$ and $N(x)$, as computed from equations (15) and (16), satisfy equations (17).

3 The discrete-ordinates solution

Our version of the discrete-ordinates solution to equation (12) was developed and used to solve the classical heat-transfer problem for a plane channel [16], and so much of the material we require here is already available. However, to be complete we repeat (in modest detail) the material from Siewert [16] that we require here. To start we multiply equation (12) by $\boldsymbol{Q}^{-1}(\xi)$ and define

$$\boldsymbol{G}(x,\xi) = \boldsymbol{Q}^{-1}(\xi)\boldsymbol{Y}(x,\xi) \tag{18}$$

and

$$\boldsymbol{\Psi}(\xi) = \pi^{-1/2}\boldsymbol{Q}^{\mathrm{T}}(\xi)\boldsymbol{Q}(\xi)\mathrm{e}^{-\xi^2} \tag{19}$$

so we can obtain

$$\xi\frac{\partial}{\partial x}\boldsymbol{G}(x,\xi) + \boldsymbol{G}(x,\xi) = \int_{-\infty}^{\infty}\boldsymbol{\Psi}(\xi')\boldsymbol{G}(x,\xi')\,\mathrm{d}\xi'. \tag{20}$$

We note first of all that the characteristic matrix $\boldsymbol{\Psi}(\xi)$, as defined by equation (19), is symmetric. We note also that $\boldsymbol{\Psi}(\xi) = \boldsymbol{\Psi}(-\xi)$, and so we write our discrete-ordinates equations as

$$\pm\xi_i\frac{\mathrm{d}}{\mathrm{d}x}\boldsymbol{G}(x,\pm\xi_i) + \boldsymbol{G}(x,\pm\xi_i) = \sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\xi_k)[\boldsymbol{G}(x,\xi_k) + \boldsymbol{G}(x,-\xi_k)] \tag{21}$$

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for $i = 1, 2, \ldots, N$. In writing equations (21) as we have, we clearly are 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. Continuing, we substitute

$$\boldsymbol{G}(x, \pm\xi_i) = \boldsymbol{\Phi}(v, \pm\xi_i)\mathrm{e}^{-x/v} \tag{22}$$

into equations (21) to find

$$(v \mp \xi_i)\boldsymbol{\Phi}(v, \pm\xi_i) = v\sum_{k=1}^{N} w_k \boldsymbol{\Psi}(\xi_k)[\boldsymbol{\Phi}(v, \xi_k) + \boldsymbol{\Phi}(v, -\xi_k)] \tag{23}$$

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

$$\boldsymbol{\Phi}_{1\pm} = \left[\Phi_1(v, \pm\xi_1), \Phi_1(v, \pm\xi_2), \ldots, \Phi_1(v, \pm\xi_N)\right]^{\mathrm{T}} \tag{24a}$$

and

$$\boldsymbol{\Phi}_{2\pm} = \left[\Phi_2(v, \pm\xi_1), \Phi_2(v, \pm\xi_2), \ldots, \Phi_2(v, \pm\xi_N)\right]^{\mathrm{T}} \tag{24b}$$

then we can rewrite equations (23) as

$$\frac{1}{v}\boldsymbol{M}\boldsymbol{\Phi}_+ = (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{\Phi}_+ - \boldsymbol{W}\boldsymbol{\Phi}_- \tag{25a}$$

and

$$-\frac{1}{v}\boldsymbol{M}\boldsymbol{\Phi}_- = (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{\Phi}_- - \boldsymbol{W}\boldsymbol{\Phi}_+. \tag{25b}$$

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

$$(\boldsymbol{W}_{m,n})_{i,j} = w_j \psi_{m,n}(\xi_j) \tag{26}$$

for $i, j = 1, 2, \ldots, N$. Here $\psi_{m,n}(\xi)$, $m, n = 1, 2$, are the elements of $\boldsymbol{\Psi}(\xi)$ and

$$\boldsymbol{M} = \mathrm{diag}\{\xi_1, \xi_2, \ldots, \xi_N, \xi_1, \xi_2, \ldots, \xi_N\}. \tag{27}$$

Continuing, we now let

$$\boldsymbol{U} = \boldsymbol{\Phi}_+ + \boldsymbol{\Phi}_- \tag{28a}$$

and

$$\boldsymbol{V} = \boldsymbol{\Phi}_+ - \boldsymbol{\Phi}_- \tag{28b}$$

so that we can eliminate between the sum and the difference of equations (25) to find

$$\left(\boldsymbol{D} - 2\boldsymbol{M}^{-1}\boldsymbol{W}\boldsymbol{M}^{-1}\right)\boldsymbol{M}\boldsymbol{U} = \lambda\boldsymbol{M}\boldsymbol{U} \tag{29}$$

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

$$\boldsymbol{D} = \mathrm{diag}\{\xi_1^{-2}, \xi_2^{-2}, \ldots, \xi_N^{-2}, \xi_1^{-2}, \xi_2^{-2}, \ldots, \xi_N^{-2}\}. \tag{30}$$

Considering that we have found the required separation constants $\{\pm v_j\}$, where $v_j > 0$, from the eigenvalues defined by equation (29), we go back to equations (23) to find

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$\boldsymbol{\Phi}(\nu_j, \pm\xi_i)$, and so we write our general solution to equations (21) as

$$\boldsymbol{G}(x, \pm\xi_i) = \sum_{j=1}^{2N} \left[A_j \frac{\nu_j}{\nu_j \mp \xi_i} \mathrm{e}^{-x/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \xi_i} \mathrm{e}^{x/\nu_j} \right] \boldsymbol{F}(\nu_j). \tag{31}$$

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

$$\boldsymbol{\Omega}(\nu_j) = \boldsymbol{I} - 2{\nu_j}^2 \sum_{\alpha=1}^{N} w_\alpha \boldsymbol{\Psi}(\xi_\alpha) \frac{1}{{\nu_j}^2 - {\xi_\alpha}^2}\,, \tag{32}$$

$\boldsymbol{I}$ is now the 2×2 identity matrix and the constants $\{A_j\}$ and $\{B_j\}$ are, at this point, arbitrary. Of course, we cannot allow $\nu_j = \xi_i$ in equation (31). Having obtained equation (31), we go back and use equation (18) to write a first version of our discrete-ordinates solution for $\boldsymbol{Y}(x, \xi)$ as

$$\boldsymbol{Y}(x, \pm\xi_i) = \boldsymbol{Q}(\xi_i) \sum_{j=1}^{2N} \left[A_j \frac{\nu_j}{\nu_j \mp \xi_i} \mathrm{e}^{-x/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \xi_i} \mathrm{e}^{x/\nu_j} \right] \boldsymbol{F}(\nu_j) \tag{33}$$

where the arbitrary constants $\{A_j, B_j\}$ are to be determined from the conditions of the problem to be solved. At this point we wish to introduce a modification to equation (33) that is important for the problem considered in this work. First of all, it was shown in Kriese *et al.* [9] that $\det \boldsymbol{\Omega}(z)$, where

$$\boldsymbol{\Omega}(z) = \boldsymbol{I} - 2z^2 \int_0^\infty \boldsymbol{\Psi}(\xi) \frac{\mathrm{d}\xi}{z^2 - \xi^2}\,, \tag{34}$$

has a fourth-order zero at infinity, and so we ignore the contributions in equation (33) from the two largest eigenvalues, say ν_1 and ν_2, and, instead, include the exact solutions

$$\boldsymbol{F}_1(x, \xi) = \boldsymbol{F}_1(\xi) = (2/3)^{1/2} \begin{bmatrix} \xi^2 - 1/2 \\ 1 \end{bmatrix}, \tag{35a}$$

$$\boldsymbol{F}_2(x, \xi) = \boldsymbol{F}_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{35b}$$

$$\boldsymbol{F}_3(x, \xi) = (\xi - x)\boldsymbol{F}_1(\xi) \tag{35c}$$

and

$$\boldsymbol{F}_4(x, \xi) = (\xi - x)\boldsymbol{F}_2 \tag{35d}$$

that Kriese, Chang and Siewert [9] found as a result of the four-fold eigenvalue at infinity. And so, we rewrite equation (33) as

$$\boldsymbol{Y}(x, \pm\xi_i) = \boldsymbol{Y}_*(x, \pm\xi_i) + \boldsymbol{Q}(\xi_i) \sum_{j=3}^{2N} \left[A_j \frac{\nu_j}{\nu_j \mp \xi_i} \mathrm{e}^{-x/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm \xi_i} \mathrm{e}^{x/\nu_j} \right] \boldsymbol{F}(\nu_j) \tag{36}$$

where

$$\boldsymbol{Y}_*(x, \xi) = [A_1 + B_1(x - \xi)]\boldsymbol{F}_1(\xi) + [A_2 + B_2(x - \xi)]\boldsymbol{F}_2. \tag{37}$$

We note that we still have $4N$ arbitrary constants to determine from the imposed conditions of our problem.

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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 § 2, we seek an unbounded (as x tends to infinity) solution to

$$\xi \frac{\partial}{\partial x} \boldsymbol{Y}(x,\xi) + \boldsymbol{Y}(x,\xi) = \pi^{-1/2} \boldsymbol{Q}(\xi) \int_{-\infty}^{\infty} \boldsymbol{Q}^{\mathrm{T}}(\xi') \boldsymbol{Y}(x,\xi') \mathrm{e}^{-\xi'^2} \, \mathrm{d}\xi', \tag{38}$$

for $x > 0$ and $\xi \in (-\infty, \infty)$, subject to the boundary condition

$$\boldsymbol{Y}(0,\xi) - (1-\alpha)\boldsymbol{Y}(0,-\xi) - \mathrm{diag}\{2\alpha, 0\} \int_0^{\infty} \boldsymbol{Y}(0,-\xi')\mathrm{e}^{-\xi'^2}\xi' \, \mathrm{d}\xi' = \mathbf{0}, \tag{39}$$

for $\xi \in (0, \infty)$, and the conditions at infinity

$$\lim_{x\to\infty} \frac{\mathrm{d}}{\mathrm{d}x} \left\{ \frac{2}{3} \pi^{-1/2} \int_{-\infty}^{\infty} \begin{bmatrix} \xi^2 - 1/2 \\ 1 \end{bmatrix}^{\mathrm{T}} \boldsymbol{Y}(x,\xi) \mathrm{e}^{-\xi^2} \, \mathrm{d}\xi \right\} = 1 \tag{40}$$

and

$$\lim_{x\to\infty} \frac{\mathrm{d}}{\mathrm{d}x} \left\{ \pi^{-1/2} \begin{bmatrix} 1 \\ 0 \end{bmatrix}^{\mathrm{T}} \int_{-\infty}^{\infty} \boldsymbol{Y}(x,\xi) \mathrm{e}^{-\xi^2} \, \mathrm{d}\xi \right\} = -1. \tag{41}$$

Looking at equations (36), (37), (40) and (41), we see that we must take $B_j = 0$ for $j = 3, 4, \ldots, 2N$. Continuing to consider that equation (36) defines the solution we seek, we note

$$\boldsymbol{Y}(x,\xi) \sim \boldsymbol{Y}_*(x,\xi) \tag{42}$$

as $x \to \infty$. In writing equation (42) in terms of continuous values of ξ we are making use of a basic feature we have made a part of our discrete-ordinates solution. To be clear on this point, we note that while equation (36) is defined only at the quadrature points $\{\xi_i\}$ the first part of that solution is, by way of equation (37), defined for all values of ξ. Thus our strategy, when a relevant integration of the solution is required, is to integrate the first component of equation (36), *viz.* $\boldsymbol{Y}_*(x,\xi)$, analytically and to use the defined quadrature scheme to integrate the second component. Now, substituting equation (37) into equations (40) and (41), we conclude that we must take

$$B_1 = (3/2)^{1/2} \tag{43 a}$$

and

$$B_2 = -1, \tag{43 b}$$

and so we can express our solution as

$$\boldsymbol{Y}(x, \pm\xi_i) = \boldsymbol{Y}_*(x, \pm\xi_i) + \boldsymbol{Q}(\xi_i) \sum_{j=3}^{2N} A_j \frac{\nu_j}{\nu_j \mp \xi_i} \mathrm{e}^{-x/\nu_j} \boldsymbol{F}(\nu_j) \tag{44}$$

where

$$\boldsymbol{Y}_*(x,\xi) = (2/3)^{1/2} A_1 \boldsymbol{R}(\xi) + (x-\xi)\boldsymbol{R}(\xi) + \gamma \boldsymbol{F}_2. \tag{45}$$

Here we have introduced a new constant,

$$\gamma = (2/3)^{1/2} A_1 + A_2, \tag{46}$$

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and

$$\boldsymbol{R}(\xi) = \begin{bmatrix} \xi^2 - 3/2 \\ 1 \end{bmatrix}. \tag{47}$$

To complete the solution we let

$$\boldsymbol{Y}_0(\pm\xi_i) = (2/3)^{1/2} A_1 \boldsymbol{R}(\xi_i) + \boldsymbol{Q}(\xi_i) \sum_{j=3}^{2N} A_j \frac{\nu_j}{\nu_j \mp \xi_i} \boldsymbol{F}(\nu_j) \tag{48}$$

and then substitute equation (44) into a discrete-ordinates version of equation (39) to find

$$\boldsymbol{Y}_0(\xi_i) - (1-\alpha)\boldsymbol{Y}_0(-\xi_i) - \mathrm{diag}\{2\alpha, 0\} \int_0^\infty \boldsymbol{Y}_0(-\xi')\mathrm{e}^{-\xi'^2}\xi'\,\mathrm{d}\xi' = (2-\alpha)\xi_i \boldsymbol{R}(\xi_i), \tag{49}$$

for $i = 1, 2, \ldots, N$. To be very clear, we repeat what we have already mentioned and note that when the first term in equation (48) is used in the integral term in equation (49), the integration is done exactly; on the other hand, we use our quadrature scheme to evaluate that integral term when the second part of equation (48) is used in equation (49). We note that the term $\gamma \boldsymbol{F}_2$ that appears in equation (45) satisfies equation (39) exactly and so makes no contribution to our linear system. The collection of equations defined by equation (49) consists of $2N$ linear equations for the $2N-1$ unknowns A_1 and A_j, for $j = 3, 4, \ldots 2N$, and so the linear system is over-determined. While we could follow what was done in Siewert [16] and use a projection technique to obtain a 'square' system, we solve the system in a 'least-squares' sense. And so our solution is complete. Of course, having defined the vector-valued function $\boldsymbol{Y}(x, \xi)$, we can find the dimensionless temperature and density perturbations from equations (15) and (16). It follows that

$$T(x) = x + (2/3)^{1/2} A_1 + (2/3)^{1/2} \sum_{j=3}^{2N} A_j f_1(\nu_j) \mathrm{e}^{-x/\nu_j} \tag{50}$$

and

$$N(x) = -x + \gamma - (2/3)^{1/2} A_1 + \sum_{j=3}^{2N} A_j f_2(\nu_j) \mathrm{e}^{-x/\nu_j} \tag{51}$$

where $f_1(\nu_j)$ and $f_2(\nu_j)$ are the upper and lower components of $\boldsymbol{F}(\nu_j)$. We now let

$$T_{\mathrm{asy}}(x) = x + (2/3)^{1/2} A_1, \tag{52}$$

and so we can readily see that the temperature jump ζ defined [9, 20, 22] by

$$T_{\mathrm{asy}}(0) = \zeta \frac{\mathrm{d}}{\mathrm{d}x} T_{\mathrm{asy}}(x)\big|_{x=0} \tag{53}$$

is available from equation (52) as

$$\zeta = (2/3)^{1/2} A_1. \tag{54}$$

Finally, we rewrite equations (50) and (51) as

$$T(x) = x + \zeta + (2/3)^{1/2} \sum_{j=3}^{2N} A_j f_1(\nu_j) \mathrm{e}^{-x/\nu_j} \tag{55}$$

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and

$$N(x) = -x + \gamma - \zeta + \sum_{j=3}^{2N} A_j f_2(\nu_j) \mathrm{e}^{-x/\nu_j}. \tag{56}$$

At this point we note that our solution satisfies all of the imposed conditions, and yet the constant γ is still arbitrary; however, it is clear that the value of γ does not affect the temperature jump ζ nor the dimensionless temperature perturbation $T(x)$. On the other hand, we will see when we compare our results to previous works that different choices of γ have been used in previous computations of the dimensionless density perturbation.

Having formulated our results we are ready to discuss a few of the computational details concerning the numerical implementation of the solution. We note that 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 [2]. First of all, we have used both the transformations

$$u(\xi) = \frac{1}{1+\xi} \tag{57 a}$$

and

$$u(\xi) = \mathrm{e}^{-\xi} \tag{57 b}$$

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 $[0, 1]$. 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 $\{\nu_j\}$ by using the driver program RG from the EISPACK collection [18] to find the eigenvalues defined by equation (29), and so, after using the subroutines DQRDC and DQRSL from the LINPACK package [8] to solve, in a least-squares sense, the linear system derived from equation (49) to find the constants A_1, A_j, for $j = 3, 4, \ldots, 2N$, we consider our solution complete.

Finally, but importantly, we note that since the matrix-valued function $\boldsymbol{\Psi}(\xi)$ as defined by equation (19) can be zero, from a computational point-of-view, we can have some, say a total of N_0, of the quadrature points $\{\xi_i\}$ equal to some of the separation constants $\{\nu_j\}$. Of course this is not allowed in our solution, and so, since the quadrature points where $\boldsymbol{\Psi}(\xi_i)$ is effectively zero make no contribution to the right-hand side of equation (23), we can simply omit these quadrature points from our calculation. Of course, in omitting these N_0 quadrature points we must be sure to eliminate exactly $2N_0$ appropriate separation constants, and so we have effectively changed N to $N - N_0$ in some aspects of our final calculation.

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 ζ and the dimensionless temperature and density perturbations, $T(x)$ and $N(x)$. 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

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Table 1. *The temperature jump* ζ

$\alpha = 0.1$	$\alpha = 0.3$	$\alpha = 0.5$	$\alpha = 0.6$	$\alpha = 0.7$	$\alpha = 0.9$	$\alpha = 1$
21.45012	6.630514	3.629125	2.867615	2.317534	1.570264	1.302716

equations (57) to obtain the same results as given in our tables. In regard to published results, we have confirmed all six of the significant figures for the temperature jump reported for the case $\alpha = 1$ in Kriese *et al.* [9]. We have also confirmed to five or six significant figures and for selected values of $\alpha \in [0, 1]$ the results for the temperature jump given in Loyalka *et al.* [10]. We list in Table 1 some typical results for the temperature jump ζ as defined by equation (53). In Table 2 we report our results, as computed from equations (55) and (56), for the temperature and density perturbations. We note that here we have chosen to use $\gamma = 0$ in order to be consistent with recent work by Onishi [12]. In comparing our results with two known computations, we first can say that we have confirmed the six-figure results given [17, 19] for $T(x)$ for the case $\alpha = 1$. In regard to the results for $N(x)$ given in Siewert & Thomas [17] and Thomas & Valougeorgis [19], we see that our results reported here differ by an additive constant to those older results. This difference can, however, be accommodated simply by redefining the constant γ. We note, for example, that from equations (55) and (56) we have the general result

$$\lim_{x \to \infty} [T(x) + N(x)] = \gamma. \tag{58}$$

Some authors, see for example Kriese *et al.* [9] and Onishi [12], have elected to normalize the density perturbation by taking $\gamma = 0$ in equation (58), and others [13, 17, 19] have normalized the problem in such a way that the integral term in equation (13) is taken to be zero. Finally, we note that we have confirmed Onishi's numerical results [11] for the temperature jump and the qualitative results (given in graphical form) for the temperature perturbation.

We note that we have typically used $N = 50$ to generate the results listed in our tables. To comment on the computational time required to solve a typical problem, we note 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 second on a 400 MHz Pentium-based 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 $\epsilon = 10^{-14}$ 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 equation (57*b*) were used.

5 Concluding remarks

Having successfully implemented our version of the discrete-ordinates method to complete our collection of solutions to the classical plane-parallel problems based on the BGK model, we believe the ease of use and the particularly 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. In fact we are confident, because of the simplicity

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Table 2. *The temperature and density perturbations*

	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 1.0$	
x	$T(x)$	$N(x)$	$T(x)$	$N(x)$	$T(x)$	$N(x)$
0.0	20.5027	–20.7100	2.91597	–3.07437	8.53515(–1)	–9.55009(–1)
0.1	20.8260	–21.0044	3.18042	–3.31664	1.05430	–1.14151
0.2	21.0362	–21.1940	3.36278	–3.48323	1.20568	–1.28284
0.3	21.2147	–21.3558	3.52167	–3.62947	1.34266	–1.41176
0.4	21.3756	–21.5028	3.66754	–3.76478	1.47158	–1.53394
0.5	21.5250	–21.6404	3.80489	–3.89310	1.59520	–1.65180
0.6	21.6663	–21.7714	3.93615	–4.01653	1.71501	–1.76661
0.7	21.8015	–21.8976	4.06283	–4.13633	1.83196	–1.87916
0.8	21.9320	–22.0200	4.18593	–4.25334	1.94665	–1.98996
0.9	22.0586	–22.1395	4.30614	–4.36814	2.05952	–2.09937
1.0	22.1821	–22.2567	4.42400	–4.48113	2.17091	–2.20764
2.0	23.3201	–23.3559	5.52928	–5.55674	3.23831	–3.25601
3.0	24.3793	–24.3981	6.57466	–6.58912	4.26751	–4.27684
4.0	25.4092	–25.4196	7.59758	–7.60560	5.28229	–5.28748
5.0	26.4255	–26.4315	8.61013	–8.61476	6.29041	–6.29340
6.0	27.4349	–27.4384	9.61737	–9.62011	7.29509	–7.29686
7.0	28.4405	–28.4426	10.6217	–10.6234	8.29789	–8.29897
8.0	29.4439	–29.4453	11.6243	–11.6254	9.29961	–9.30028
9.0	30.4461	–30.4469	12.6260	–12.6267	10.3007	–10.3011
10.0	31.4475	–31.4480	13.6271	–13.6275	11.3014	–11.3016
20.0	41.4501	–41.4501	23.6291	–23.6291	21.3027	–21.3027

of the numerical-analytical methods reported here, that a class of basic problems based on linear models more general than the BGK model, for example the so-called ‘S model’ of Shakhov [14], as quoted by Sharipov & Seleznev [15], will soon be solved with a high degree of rigour and accuracy.

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