PERGAMON

Journal of Quantitative Spectroscopy & Radiative Transfer 70 (2001) 321–332

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Couette flow for a binary gas mixture

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Received 11 September 2000; accepted 6 November 2000

Abstract

A recently developed analytical version of the discrete-ordinates method is used to establish a concise and particularly accurate solution to the problem of Couette flow of a binary gas mixture in a plane channel. The model kinetic equations used to describe the flow are based on the BGK theory of the linearized Boltzmann equation, and, in addition to the complete distribution functions for the two species of gas particles, numerical results are reported for the total sheer stress. The algorithm is considered especially easy to use, and the developed (FORTRAN) code runs typically in less than a second on a 400 MHz Pentium-based PC. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Rarefied gas dynamics; Discrete ordinates

1. Introduction

In a recent work [1], Onishi gives an extensive introduction to a general kinetic-theory description of flow problems relevant to a rarefied gas mixture made up of two species of gas particles. In addition to pointing out that a basic and often used model for binary gas mixtures was developed by Hamel [2], Onishi in that work [1] also solves the temperature–density problem for a binary mixture of gas particles. While we will not attempt to review the numerous works already published on the use of kinetic theory to describe binary gas mixtures, we must make note of the important contributions made by Onishi [1,3–5], Valougeorgis [6], Loyalka [7] and Cercignani and Lampis [8] to the general body of work that concerns us here.

In regard to the solution developed for the problem considered here, we note that our analytical version of Chandrasekhar's discrete-ordinates method [9] was first reported by Barichello and Siewert [10] in a work devoted to radiative transfer. Since that first work [10], the method has been used [11–15] to solve a collection of classical problems in the area of rarefied gas dynamics. And so here, we extend our earlier work for a single-species gas to the case of a binary gas mixture. Of course, the considered problem of Couette flow for a binary gas mixture in a plane channel has

PII: S0022-4073(00)00143-6

been solved previously, see for example Ref. [6], with what we might call "practical accuracy". However, we consider that the discrete-ordinates solution developed here yields especially accurate results. The developed discrete-ordinates method is also easy to use and, importantly, can very likely be extended for use with kinetic models more general than the one used here.

To define, in mathematical terms, the basic problem we intend to solve, we follow Hamel [2], Onishi [1,3–5] and Valougeorgis [6] and so consider the following system of coupled conservation equations and boundary conditions, the results of a linearization of the initial model equations, that define the Couette-flow problem:

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

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

$$\boldsymbol{Y}(0,\xi) = -\begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{2a}$$

and

$$\boldsymbol{Y}(d,-\xi) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{2b}$$

for $\xi \in (0,\infty)$. In Eq. (1) the elements $Y_1(x,\xi)$ and $Y_2(x,\xi)$ of the vector-valued function $\boldsymbol{Y}(x,\xi)$ are components of the particle distribution functions for the two gas species denoted by indices 1 and 2. In addition, x is the spatial variable, d is the normalized channel width, ξ is the x component (in different normalized units for each of the two species) of the particle velocities,

$$\boldsymbol{B} = \mathrm{diag}\{\beta_1, \beta_2\} \tag{3}$$

and

$$\boldsymbol{T} = \pi^{-1/2}\begin{bmatrix} \beta_1 - \alpha_1 & \alpha_1 \\ \alpha_2 & \beta_2 - \alpha_2 \end{bmatrix} \tag{4}$$

where from Valougeorgis [6]

$$\beta_1 = \left(\frac{m_1}{2kT_0}\right)^{1/2}(n_1 k_{11} + n_2 k_{12}), \tag{5a}$$

$$\beta_2 = \left(\frac{m_2}{2kT_0}\right)^{1/2}(n_2 k_{22} + n_1 k_{21}), \tag{5b}$$

$$\alpha_1 = \left(\frac{m_1}{2kT_0}\right)^{1/2} n_2 k_{12} \frac{m_2}{m_1 + m_2} \tag{6a}$$

and

$$\alpha_2 = \left(\frac{m_2}{2kT_0}\right)^{1/2} n_1 k_{21} \frac{m_1}{m_1 + m_2}. \tag{6b}$$

Continuing to follow Hamel [2], Onishi [1,3–5] and Valougeorgis [6], we note that m_1 and m_2 are the molecular masses of the two species of gas particles, k is the Boltzmann constant and T_0 is the equilibrium value of the temperature. Finally, the constants k_{11}, k_{22} and $k_{12} = k_{21}$ are [6] collision parameters, and the number densities of the two gas species are n_1 and n_2.

And so in this work, we consider that all the basic physical parameters are given and that our job is to solve (in a concise and accurate way) Eq. (1) subject to the boundary conditions given by Eqs. (2). However, before proceeding with our solution, we rewrite the defined problem in terms of dimensionless units. We divide Eq. (1) by β_1, define a new spatial variable $\tau = \beta_1 x$ and let

$$\boldsymbol{Y}(\tau/\beta_1, \xi) = \boldsymbol{Z}(\tau, \xi). \tag{7}$$

In this way we rewrite Eqs. (1) and (2) as

$$\xi \frac{\partial}{\partial \tau} \boldsymbol{Z}(\tau, \xi) + \boldsymbol{\Sigma} \boldsymbol{Z}(\tau, \xi) = \int_{-\infty}^{\infty} \boldsymbol{\Psi}(\xi') \boldsymbol{Z}(\tau, \xi') \, \mathrm{d}\xi' \tag{8}$$

for $\tau \in (0, \tau_0)$ and $\xi \in (-\infty, \infty)$, with

$$\boldsymbol{Z}(0, \xi) = -\begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{9a}$$

and

$$\boldsymbol{Z}(\tau_0, -\xi) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{9b}$$

for $\xi \in (0, \infty)$. Here we have defined $\tau_0 = \beta_1 d$,

$$\boldsymbol{\Sigma} = \mathrm{diag}\{1, \sigma\}, \tag{10}$$

with $\sigma = \beta_2/\beta_1$, and

$$\boldsymbol{\Psi}(\xi) = \boldsymbol{C} \mathrm{e}^{-\xi^2} \tag{11}$$

where

$$\boldsymbol{C} = \pi^{-1/2} \begin{bmatrix} 1 - \alpha_1/\beta_1 & \alpha_1/\beta_1 \\ \alpha_2/\beta_1 & \sigma - \alpha_2/\beta_1 \end{bmatrix}. \tag{12}$$

2. The discrete-ordinates method

In this section we develop, in general terms, the formalism of our discrete-ordinates method that we use in the following section to solve the specific problem of Couette flow in a plane channel. To start, we first rewrite Eq. (8) as

$$\xi \frac{\partial}{\partial \tau} \boldsymbol{Z}(\tau, \xi) + \boldsymbol{\Sigma} \boldsymbol{Z}(\tau, \xi) = \int_0^\infty \boldsymbol{\Psi}(\xi')[\boldsymbol{Z}(\tau, \xi') + \boldsymbol{Z}(\tau, -\xi')]\,\mathrm{d}\xi' \tag{13}$$

for $\tau \in (0, \tau_0)$ and $\xi \in (-\infty, \infty)$. We now let $\{w_k, \xi_k\}$, for $k = 1, 2, \ldots, N$, denote a collection of weights and nodes that defines a numerical quadrature scheme for evaluating integrals defined on the interval $[0, \infty)$. And so we use this quadrature scheme to approximate the integral term in Eq. (13) to obtain

$$\xi \frac{\partial}{\partial \tau} \boldsymbol{Z}(\tau, \xi) + \boldsymbol{\Sigma} \boldsymbol{Z}(\tau, \xi) = \sum_{k=1}^{N} w_k \boldsymbol{\Psi}(\xi_k)[\boldsymbol{Z}(\tau, \xi_k) + \boldsymbol{Z}(\tau, -\xi_k)] \tag{14}$$

for $\tau \in (0, \tau_0)$ and $\xi \in (-\infty, \infty)$. Assuming for the moment that

$$\boldsymbol{S}(\tau) = \sum_{k=1}^{N} w_k \boldsymbol{\Psi}(\xi_k)[\boldsymbol{Z}(\tau, \xi_k) + \boldsymbol{Z}(\tau, -\xi_k)] \tag{15}$$

is known, we can solve Eq. (14) to obtain

$$\boldsymbol{Z}(\tau, \xi) = \mathrm{e}^{-\Sigma\tau/\xi} \boldsymbol{Z}(0, \xi) + \int_0^\tau \mathrm{e}^{-\Sigma(\tau - x)/\xi} \boldsymbol{S}(x)\,\mathrm{d}x \tag{16a}$$

and

$$\boldsymbol{Z}(\tau, -\xi) = \mathrm{e}^{-\Sigma(\tau_0 - \tau)/\xi} \boldsymbol{Z}(\tau_0, -\xi) + \int_\tau^{\tau_0} \mathrm{e}^{-\Sigma(x - \tau)/\xi} \boldsymbol{S}(x)\,\mathrm{d}x \tag{16b}$$

for $\tau \in [0, \tau_0]$ and $\xi \in [0, \infty)$. Here

$$\mathrm{e}^{-\Sigma x} = \mathrm{diag}\{\mathrm{e}^{-x}, \mathrm{e}^{-\sigma x}\}. \tag{17}$$

Clearly, we can use Eqs. (9) to rewrite Eqs. (16) as

$$\boldsymbol{Z}(\tau, \xi) = -\mathrm{e}^{-\Sigma\tau/\xi} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \int_0^\tau \mathrm{e}^{-\Sigma(\tau - x)/\xi} \boldsymbol{S}(x)\,\mathrm{d}x \tag{18a}$$

and

$$\boldsymbol{Z}(\tau, -\xi) = \mathrm{e}^{-\Sigma(\tau_0 - \tau)/\xi} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \int_\tau^{\tau_0} \mathrm{e}^{-\Sigma(x - \tau)/\xi} \boldsymbol{S}(x)\,\mathrm{d}x \tag{18b}$$

for $\tau \in [0, \tau_0]$ and $\xi \in [0, \infty)$. At this point, we see that Eqs. (18) define, once $\boldsymbol{S}(\tau)$ is determined, the complete solution for the particle distribution functions.

Now to find the required $\boldsymbol{S}(\tau)$ we evaluate Eq. (14) at $\xi = \pm\xi_i$ to obtain the system of differential equations

$$\pm \xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} \boldsymbol{Z}(\tau, \pm\xi_i) + \boldsymbol{\Sigma} \boldsymbol{Z}(\tau, \pm\xi_i) = \sum_{k=1}^{N} w_k \boldsymbol{\Psi}(\xi_k)[\boldsymbol{Z}(\tau, \xi_k) + \boldsymbol{Z}(\tau, -\xi_k)] \tag{19}$$

for $i = 1,2,\ldots,N$. Seeking exponential solutions, we substitute

$$\boldsymbol{Z}(\tau, \pm\xi_i) = \boldsymbol{\Phi}(\nu, \pm\xi_i)\mathrm{e}^{-\tau/\nu} \tag{20}$$

into Eq. (19) to obtain

$$(\nu\boldsymbol{\Sigma} \mp \xi_i\boldsymbol{I})\boldsymbol{\Phi}(\nu, \pm\xi_i) = \nu\sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\xi_k)[\boldsymbol{\Phi}(\nu, \xi_k) + \boldsymbol{\Phi}(\nu, -\xi_k)] \tag{21}$$

where $\boldsymbol{I}$ is the 2×2 identity matrix. If we now introduce

$$\boldsymbol{\Phi}_{\pm}(\nu) = [\boldsymbol{\Phi}^{\mathrm{T}}(\nu, \pm\xi_1) \quad \boldsymbol{\Phi}^{\mathrm{T}}(\nu, \pm\xi_2) \quad \cdots \quad \boldsymbol{\Phi}^{\mathrm{T}}(\nu, \pm\xi_N)]^{\mathrm{T}} \tag{22}$$

where the superscript T is used to denote the transpose operation, then we can follow our previous work [10–15] and rewrite the two versions of Eq. (21) as

$$\boldsymbol{S}\boldsymbol{\Phi}_{+}(\nu) - \frac{1}{\nu}\boldsymbol{M}\boldsymbol{\Phi}_{+}(\nu) = \boldsymbol{W}[\boldsymbol{\Phi}_{+}(\nu) + \boldsymbol{\Phi}_{-}(\nu)] \tag{23a}$$

and

$$\boldsymbol{S}\boldsymbol{\Phi}_{-}(\nu) + \frac{1}{\nu}\boldsymbol{M}\boldsymbol{\Phi}_{-}(\nu) = \boldsymbol{W}[\boldsymbol{\Phi}_{+}(\nu) + \boldsymbol{\Phi}_{-}(\nu)] \tag{23b}$$

where

$$\boldsymbol{S} = \mathrm{diag}\{\boldsymbol{\Sigma}, \boldsymbol{\Sigma}, \ldots, \boldsymbol{\Sigma}\} \tag{24}$$

and

$$\boldsymbol{M} = \mathrm{diag}\{\xi_1\boldsymbol{I}, \xi_2\boldsymbol{I}, \ldots, \xi_N\boldsymbol{I}\}. \tag{25}$$

In addition, the 2×2 block elements of each row of blocks of the $2N\times 2N$ matrix $\boldsymbol{W}$ are given by

$$\{\boldsymbol{W}\}_k = w_k\boldsymbol{\Psi}(\xi_k) \tag{26}$$

for $k = 1,2,\ldots,N$. We now let

$$\boldsymbol{U}(\nu) = \boldsymbol{\Phi}_{+}(\nu) + \boldsymbol{\Phi}_{-}(\nu) \tag{27}$$

and

$$\boldsymbol{\Upsilon}(\nu) = \boldsymbol{\Phi}_{+}(\nu) - \boldsymbol{\Phi}_{-}(\nu) \tag{28}$$

and then add Eqs. (23) to obtain

$$\frac{1}{\nu}\boldsymbol{M}\boldsymbol{\Upsilon}(\nu) = (\boldsymbol{S} - 2\boldsymbol{W})\boldsymbol{U}(\nu). \tag{29}$$

We can also subtract Eqs. (23b) from (23a) to find

$$\frac{1}{\nu}\boldsymbol{M}\boldsymbol{U}(\nu) = \boldsymbol{S}\boldsymbol{\Upsilon}(\nu). \tag{30}$$

At this point, we can eliminate $\boldsymbol{\Upsilon}(v)$ between Eqs. (29) and (30) to arrive at an eigenvalue problem which we write as

$$(\boldsymbol{D} - 2\boldsymbol{B})\boldsymbol{X}(v) = \lambda \boldsymbol{X}(v) \tag{31}$$

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

$$\boldsymbol{X}(v) = \boldsymbol{M}\boldsymbol{U}(v). \tag{32}$$

In addition,

$$\boldsymbol{D} = \mathrm{diag}\{\boldsymbol{\Sigma}^2/\xi_1^2, \boldsymbol{\Sigma}^2/\xi_2^2, \dots, \boldsymbol{\Sigma}^2/\xi_N^2\} \tag{33}$$

and the 2×2 block elements of the $2N \times 2N$ matrix $\boldsymbol{B}$ are given by

$$(\boldsymbol{B})_{i,j} = \frac{w_j}{\xi_i \xi_j} \boldsymbol{\Sigma}\boldsymbol{\Psi}(\xi_j) \tag{34}$$

for $i, j = 1, 2, \dots, N$. Assuming that we have found the $2N$ eigenvalues λ_j defined by Eq. (31), we now have the $4N$ separation constants $v_j = \pm \lambda_j^{-1/2}$ available, and so we return to Eq. (21) to obtain

$$\boldsymbol{\Phi}(v_j, \pm \xi_i) = v_j (v_j \boldsymbol{\Sigma} \mp \xi_i \boldsymbol{I})^{-1} \boldsymbol{M}(v_j) \tag{35}$$

where

$$\boldsymbol{M}(v_j) = \sum_{k=1}^{N} w_k \boldsymbol{\Psi}(\xi_k)[\boldsymbol{\Phi}(v_j, \xi_k) + \boldsymbol{\Phi}(v_j, -\xi_k)]. \tag{36}$$

At this point, we can multiply each of the two versions of Eqs. (35) by $w_i \boldsymbol{\Psi}(\xi_i)$, sum over i and add the two resulting equations to obtain

$$\boldsymbol{\Omega}(v_j)\boldsymbol{M}(v_j) = \boldsymbol{0} \tag{37}$$

where

$$\boldsymbol{\Omega}(v_j) = \boldsymbol{I} + 2v_j^2 \sum_{k=1}^{N} w_k \boldsymbol{\Psi}(\xi_k) \mathrm{diag}\left\{ \frac{1}{\xi_k^2 - v_j^2}, \frac{\sigma}{\xi_k^2 - (\sigma v_j)^2} \right\}. \tag{38}$$

Considering Eq. (37), we let $\Omega_{ij}(v_j)$ denote the elements of $\boldsymbol{\Omega}(v_j)$ and choose to write

$$\boldsymbol{M}(v_j) = \begin{bmatrix} -\Omega_{12}(v_j) \\ \Omega_{11}(v_j) \end{bmatrix}, \tag{39}$$

and so Eq. (35) is now completely defined. Since our separation constants occur in plus–minus pairs we, from here onward, let v_j denote the positive value of $\lambda_j^{-1/2}$, and so we write

$$\boldsymbol{Z}(\tau, \pm \xi_i) = \sum_{j=1}^{2N} [A_j \boldsymbol{\Phi}(v_j, \pm \xi_i) \mathrm{e}^{-\tau/v_j} + B_j \boldsymbol{\Phi}(v_j, \mp \xi_i) \mathrm{e}^{-(\tau_0 - \tau)/v_j}] \tag{40}$$

where the constants $\{A_j, B_j\}$ are to be determined from the boundary conditions of a considered problem. However, before constraining the solution given by Eq. (40) to meet discrete-ordinates versions of the boundary conditions, we make a modification to our solution that is required since our problem is conservative. While the term conservative has numerous implications, we use it here to mean that one of the separation constants, say ν_1, from the collection $\{\nu_j\}$ becomes unbounded as N increases without bound. We choose to take this fact into account by ignoring the largest of the computed separation constants and by replacing the subsequently ignored solutions by easily deduced exact solutions. And so we write our modified form of Eq. (40) as

$$\boldsymbol{Z}(\tau, \pm\xi_i) = \boldsymbol{Z}_0(\tau, \pm\xi_i) + \sum_{j=2}^{2N} [A_j \boldsymbol{\Phi}(\nu_j, \pm\xi_i) \mathrm{e}^{-\tau/\nu_j} + B_j \boldsymbol{\Phi}(\nu_j, \mp\xi_i) \mathrm{e}^{-(\tau_0 - \tau)/\nu_j}]. \tag{41}$$

Here

$$\boldsymbol{Z}_0(\tau, \xi) = A_1(\tau \boldsymbol{I} - \xi \boldsymbol{\Sigma}^{-1}) \boldsymbol{K} + B_1[(\tau_0 - \tau)\boldsymbol{I} + \xi \boldsymbol{\Sigma}^{-1}] \boldsymbol{K} \tag{42}$$

where we use

$$\boldsymbol{K} = \begin{bmatrix} \sigma + \pi^{1/2}(c_{12} - c_{22}) \\ 1 + \pi^{1/2}(c_{21} - c_{11}) \end{bmatrix} \tag{43}$$

and where c_{ij} is used to denote an element of the matrix $\boldsymbol{C}$.

3. Boundary conditions and macroscopic quantities

To start, we note from Eqs. (8) and (9) that the solution to the problem of Couette flow (as formulated here) has the (anti) symmetry property

$$\boldsymbol{Z}(\tau_0 - \tau, -\xi) = -\boldsymbol{Z}(\tau, \xi) \tag{44}$$

and so we set $B_j = -A_j$ in Eqs. (41) and (42) to obtain

$$\boldsymbol{Z}(\tau, \pm\xi_i) = \boldsymbol{Z}_0(\tau, \pm\xi_i) + \sum_{j=2}^{2N} A_j [\boldsymbol{\Phi}(\nu_j, \pm\xi_i) \mathrm{e}^{-\tau/\nu_j} - \boldsymbol{\Phi}(\nu_j, \mp\xi_i) \mathrm{e}^{-(\tau_0 - \tau)/\nu_j}] \tag{45}$$

where now

$$\boldsymbol{Z}_0(\tau, \xi) = A_1[(2\tau - \tau_0)\boldsymbol{I} - 2\xi \boldsymbol{\Sigma}^{-1}] \boldsymbol{K}. \tag{46}$$

At this point, we can substitute Eq. (45) into our discrete-ordinates version of Eq. (9a), viz.,

$$\boldsymbol{Z}(0, \xi_i) = -\begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{47}$$

for $i = 1, 2, \ldots, N$, to obtain a system of $2N$ linear algebraic equations we can solve to obtain the required constants $\{A_j\}$.

We note that out final complete solution for $\boldsymbol{Z}(\tau, \xi)$ is continuous in all variables and is given by Eqs. (18) once $\boldsymbol{S}(x)$ is available. And so we now substitute Eq. (45) into Eq. (15) to find

$$\boldsymbol{S}(x) = \boldsymbol{S}_0(x) + \sum_{j=2}^{2N} A_j [\mathrm{e}^{-x/\nu_j} - \mathrm{e}^{-(\tau_0 - x)/\nu_j}] \boldsymbol{M}(\nu_j) \tag{48}$$

where we have used Eq. (36) to integrate the discrete-ordinates terms and where we have used exact integration to find

$$\boldsymbol{S}_0(x) = A_1(2x - \tau_0)\boldsymbol{CK}. \tag{49}$$

Of course the integrals in Eqs. (18) can be evaluated immediately once Eq. (48) has been used there.

Since $\boldsymbol{Z}(\tau, \xi)$ can now be considered known, any quantity defined in terms of that basic result is also readily available. For example, the normal total stress

$$P = -\frac{1}{\zeta + 1}\begin{bmatrix} \zeta \\ 1 \end{bmatrix}^{\mathrm{T}} \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2}\boldsymbol{Z}(\tau, \xi)\xi\,\mathrm{d}\xi \tag{50}$$

where

$$\zeta = \frac{n_1}{n_2}\left(\frac{m_1}{m_2}\right)^{1/2}, \tag{51}$$

as defined by Valougeorgis [6] is a constant of physical interest that we can easily compute. If we go back and multiply Eq. (21) by $w_i\boldsymbol{\Psi}(\xi_i)$, sum over i and add the two versions of the resulting equation, we find, after noting Eq. (36),

$$v_j\boldsymbol{\Delta}\boldsymbol{M}(v_j) = \sum_{k=1}^{N} w_k\xi_k\boldsymbol{\Psi}(\xi_k)[\boldsymbol{\Phi}(v_j, \xi_k) - \boldsymbol{\Phi}(v_j, -\xi_k)] \tag{52}$$

where

$$\boldsymbol{\Delta} = \boldsymbol{\Sigma} - 2\sum_{k=1}^{N} w_k\boldsymbol{\Psi}(\xi_k). \tag{53}$$

We note that Eq. (53) is a quadrature approximation to the exact value

$$\boldsymbol{\Delta} = \boldsymbol{\Sigma} - \pi^{1/2}\boldsymbol{C}. \tag{54}$$

Now if we use our quadrature scheme to rewrite the integral in Eq. (50), make use of Eq. (45) and note that

$$\begin{bmatrix} \zeta \\ 1 \end{bmatrix}^{\mathrm{T}}\boldsymbol{\Delta} = \boldsymbol{0}, \tag{55}$$

then we find

$$P = \frac{A_1\pi^{1/2}}{\zeta + 1}\begin{bmatrix} \zeta \\ 1 \end{bmatrix}^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}\boldsymbol{K} \tag{56}$$

where $\boldsymbol{K}$ is given by Eq. (43).

To conclude this section, we list our results for some other quantities of physical interest. First of all, we note that the normalized macroscopic velocities defined [6] by

$$\boldsymbol{V}(\tau) = \pi^{-1/2}\int_{-\infty}^{\infty}\boldsymbol{Z}(\tau, \xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi \tag{57}$$

are available, in this work, from

$$\boldsymbol{V}(\tau) = \pi^{-1/2}\boldsymbol{C}^{-1}\int_{-\infty}^{\infty} \boldsymbol{\Psi}(\xi)\boldsymbol{Z}(\tau,\xi)\,\mathrm{d}\xi \tag{58}$$

or

$$\boldsymbol{V}(\tau) = \pi^{-1/2}\boldsymbol{C}^{-1}\boldsymbol{S}(\tau) \tag{59}$$

where $\boldsymbol{S}(\tau)$ is available from Eqs. (48) and (49). In a similar way, we find here that the stress vector

$$\boldsymbol{P}(\tau) = -\int_{-\infty}^{\infty} \boldsymbol{\Psi}(\xi)\boldsymbol{Z}(\tau,\xi)\xi\,\mathrm{d}\xi \tag{60}$$

can be expressed as

$$\boldsymbol{P}(\tau) = A_1\pi^{1/2}\boldsymbol{\Sigma}^{-1}\boldsymbol{K} - \boldsymbol{\Delta}\sum_{j=2}^{2N} A_j \nu_j[\mathrm{e}^{-\tau/\nu_j} + \mathrm{e}^{-(\tau_0-\tau)/\nu_j}]\boldsymbol{M}(\nu_j). \tag{61}$$

Having defined our solution, we now turn to some of the computational details and our numerical results.

4. Computational details and numerical results

Much of this section follows directly from Refs. [10,11]. 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 [11]. First of all we have used either the transformation

$$u(\xi) = \frac{1}{1+\xi} \tag{62a}$$

or the transformation

$$u(\xi) = \mathrm{e}^{-\xi} \tag{62b}$$

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. In fact, we note that a recent work by Garcia [16] has 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

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

seems a natural choice for this work. However, we have found the use of a mapping defined by either of Eqs. (62) followed by the use of the Gauss–Legendre integration formulas to be so effective that we have not tried other integration techniques. 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 [17] to find the eigenvalues defined by Eq. (31), and so, after using the subroutines DGECO and DGESL from the LINPACK package [18] to solve the linear system, defined by Eq. (47), to find the constants $\{A_j\}$ we consider our solution complete.

Finally, but importantly, we note that since the matrix-valued function $\mathbf{\Psi}(\xi)$ as defined by Eq. (11) 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 $\{\nu_j\}$ or equal to some of the elements of $\{\sigma\nu_j\}$. Of course, this is not allowed in our solution, and so, since the quadrature points where $\mathbf{\Psi}(\xi)$ is effectively zero make no contribution to the right-hand side of Eq. (35), we have seen that we can simply omit these quadrature points from parts of 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 solution.

To complete this work, we use Table 1 to list our results, which we believe to be correct to all digits given, of the normalized sheer as computed from Eq. (56). While we have found general agreement with the numerical results reported in Ref. [6], we do not accept as correct all of the digits in the tabulation given there. Of course, we have no proof of the accuracy of our results, but we have done various things to establish the confidence we have. For example, 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. (62) to obtain the same results as given in our table.

We note that we have typically used $N = 80$ to generate the results listed in Table 1. To have an idea of 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 solutions (with $N = 80$) runs in less than a second on a 400 MHz Pentium-based PC.

Table 1
Normalized total sheer stress for the case $k_{11} = k_{12} = k_{22}$ with $\beta_1 = 1$

	$m_1/m_2 = 0.5$		$m_1/m_2 = 2.0$	
d	$n_1/n_2 = 0.1$	$n_1/n_2 = 10.0$	$n_1/n_2 = 0.1$	$n_1/n_2 = 10.0$
1.0 (− 1)	9.01866 (− 1)	9.22624 (− 1)	9.42970 (− 1)	9.27092 (− 1)
5.0 (− 1)	6.77688 (− 1)	7.30472 (− 1)	7.87836 (− 1)	7.42247 (− 1)
1.0	5.28222 (− 1)	5.91160 (− 1)	6.64405 (− 1)	6.05554 (− 1)
2.0	3.71401 (− 1)	4.34140 (− 1)	5.13286 (− 1)	4.48941 (− 1)
3.0	2.87588 (− 1)	3.44869 (− 1)	4.20830 (− 1)	3.58660 (− 1)
4.0	2.34896 (− 1)	2.86516 (− 1)	3.57411 (− 1)	2.99130 (− 1)
5.0	1.98594 (− 1)	2.45203 (− 1)	3.10912 (− 1)	2.56723 (− 1)
7.0	1.51749 (− 1)	1.90428 (− 1)	2.46991 (− 1)	2.00147 (− 1)
1.0 (1)	1.12106 (− 1)	1.42684 (− 1)	1.88930 (− 1)	1.50488 (− 1)
2.0 (1)	5.99282 (− 2)	7.77418 (− 2)	1.06003 (− 1)	8.23915 (− 2)

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 $\varepsilon = 10^{-13}$ to decide if an eigenvalue and a quadrature point were the same "computationally", we found $N_0 = 3$ when $N = 80$ and the map defined by Eq. (62b) were used.

5. Concluding remarks

In developing (what we can call) an analytical version of the discrete-ordinates method to solve the considered problem of Couette flow for a binary gas mixture, we have found that the method can be used efficiently to obtain high-quality results with very little computational effort. In addition, we believe it is clear that the method can readily be extended for use with other, more challenging models in the general area of rarefied gas dynamics. In fact, recent work [19] with the so-called variable collision frequency model has shown this observation to be valid. Finally, we note that while some experience with numerical linear algebra is helpful, the method is especially easy to implement.

Acknowledgements

The author wishes to take this opportunity to thank L.B. Barichello, M. Camargo, R.D.M. Garcia, S.K. Loyalka, Y. Onishi, P. Rodrigues, D. Valougeorgis and M.M.R. Williams for some helpful discussions concerning this (and other) work.

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