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ON THE TEMPERATURE-JUMP PROBLEM IN RAREFIED GAS DYNAMICS: THE EFFECT OF THE CERCIGNANI–LAMPIS BOUNDARY CONDITION*

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Abstract. An analytical version of the discrete-ordinates method (the ADO method) is used to establish a solution to the temperature-jump problem in the rarefied gas dynamics field. Kinetic models derived from the linearized Boltzmann equation are used to formulate the problem in the one gas case and for a binary gas mixture. The gas-surface interaction is described by the Cercignani–Lampis kernel, which is written in terms of two accommodation coefficients. The solution is found to be very accurate and fast. Numerical results are presented not only for the temperature-jump coefficient but also for the density and temperature profiles. In particular, the effect of both accommodation coefficients on the temperature-jump coefficient is analyzed.

Key words. rarefied gas dynamics, temperature-jump coefficient, binary gas mixture, Cercignani–Lampis kernel, discrete ordinates

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1. Introduction.

The increased interest in research fields related to the development of technologies associated with micro-electro-mechanical systems (MEMS) [1, 2] as well as other micro- and nanoflow applications [3] has brought attention to the rarefied gas dynamics field [4, 5, 6]. In fact, for these microsystems, where the characteristic length of the system is of the order of a mean-free path, and the gas flow is in the transition regime, the Boltzmann equation [7] has to be used in order to describe correctly the state of the gas. In this case the Knudsen number (Kn), defined as the ratio of the molecular mean-free path to a characteristic size, is close to the unity.

For a gas in a moderate state of rarefaction (Kn < 0.1), however, in order to take into account the rarefaction effects by using simpler models, it is usual to use the continuum mechanics equations to define the problem of interest, along with the velocity-slip and temperature-jump boundary conditions [3, 4, 5, 6, 7]. In particular, for the case of evaluating the temperature distribution in a rarefied gas restricted by a solid surface, the temperature-jump boundary condition is used to take into account the noted difference (proportional to the gradient of the temperature in the normal direction to the wall) between the temperature of the wall and the temperature of the gas near to the wall. In this way, the temperature-jump boundary condition is defined in terms of the temperature-jump coefficient [7, 8, 9].

Although the temperature-jump coefficient may be evaluated by solving either the Boltzmann equation or model equations (derived from the Bolztmann equation with simplified collision operators) [4, 10] it is usual to find its definition, as derived by Maxwell, written in terms of the accommodation coefficient of the gas [3]. This

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approach is, according to the literature [11], just an estimation, since it is based on the assumption that the distribution function does not vary in the Knudsen layer. In fact, such an approach has been shown [11] to underestimate the value of the temperature-jump coefficient.

On the other hand, surface effects play a very important role in the analysis of the temperature in microscales, and so particular attention has to be given to the definition of the boundary conditions and to the choice of appropriate kernels to describe the gas-surface interaction [12, 13, 14].

In this work, we present a complete derivation of the solution of the temperature-jump problem for the one gas case (based on the S-model [15]) and a binary gas mixture (based on the McCormack model [16]). The solution is developed in terms of an analytical version of the discrete-ordinates method (the ADO method) [17]. In fact, the temperature-jump problem has been studied over the years, and previous results on this problem, based on numerical approaches, can be found in the literature [4, 6, 18, 19, 20, 21, 22, 23, 24]. The ADO method, which has been successfully applied to derive unified solutions for a wide class of problems in the rarefied gas dynamics field [25, 26, 27, 28], has been also applied to evaluate the temperature-jump coefficient [29, 30, 31, 32]. In particular, the ADO solution has been shown to be accurate and fast, in comparison with numerical based approaches.

Here, in addition to complete the class of problems solved by the ADO method, based on the kinetic S-model of the linearized Boltzmann equation [28], and to establish the relation between this formulation and its extension to the binary mixture case based on the McCormack model [32], we include, for the temperature-jump problem, a special treatment for the gas-surface interaction: the Cercignani Lampis kernel [12]. In fact, considering the significance of the surface effect analysis on microflow applications and the good results obtained by the application of the ADO method to the solution of problems in this field, this kernel has been included in the treatment of channel problems by the ADO method [33, 34]. Differently from the commonly used Maxwell boundary condition [10], the Cercignani–Lampis kernel is defined in terms of two accommodation coefficients such that a better physical representation of the surface effects is allowed. In this work, a complete study of the dependence of the temperature-jump coefficient on different kinetic models as well as on the gas-surface interaction kernel is then carried out.

In this way, we develop in sections 2 and 3 the basic formulation for the one gas case, and we describe its ADO solution in section 4. We detail the McCormack model for a binary gas mixture in sections 5 and 6. In section 7 we present the discrete-ordinates solution for the mixture. We discuss computational aspects and numerical results in section 8 before presenting some concluding comments in section 9.

2. A model equation: The one gas case. To start this work, we follow Williams [10] and consider the steady-state nonlinear Boltzmann equation written, in a general form, as

$$\mathbf{v} \cdot \nabla_r f(\mathbf{r}, \mathbf{v}) = J(f', f), \tag{1}$$

where $f(\mathbf{r}, \mathbf{v})$ is the gas atom space and velocity distribution function (f and f' are associated with, respectively, before and after collision distributions) and J is the collision operator [10]. For the cases weakly far from the equilibrium, it is customary to write f as

$$f(\mathbf{r}, \mathbf{v}) = f_0(\mathbf{v})[1 + h(\mathbf{r}, \mathbf{v})], \tag{2}$$

where h is a perturbation caused, by the presence of the walls, to the absolute Maxwellian $f_0(\mathbf{v})$,

$$f_0(\mathbf{v}) = n_0(\lambda_0/\pi)^{3/2}\mathrm{e}^{-\lambda_0 v^2}, \quad \lambda_0 = m_0/(2kT_0). \tag{3}$$

Here k is the Boltzmann constant, T_0 is a reference temperature, m_0 is the mass, and n_0 is the equilibrium density of the gas. In this way, if we substitute (2) into (1) and use, along with properties of the collision operator [9], some physical considerations, we obtain, for the dimensionless velocity variable

$$\mathbf{c} = \mathbf{v}[(m/2kT_0)]^{1/2}, \tag{4}$$

the linearized Boltzmann equation written in terms of the perturbation function h as [10, 35]

$$c_y \frac{\partial}{\partial y} h(y,\mathbf{c}) + \varepsilon h(y,\mathbf{c}) = \varepsilon \pi^{-3/2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c'^2} h(y,\mathbf{c}')F(\mathbf{c}':\mathbf{c})\mathrm{d}c'_x\mathrm{d}c'_y\mathrm{d}c'_z. \tag{5}$$

Here, in addition to the three components of the velocity vector (c_x, c_y, c_z) which are expressed in dimensionless units, we consider the dimensionless (written in terms of a mean-free path l) spatial variable $y > 0$, and

$$\varepsilon = \sigma_0^2 n_0 \pi^{1/2} l, \tag{6}$$

where σ_0 is the collision diameter of the gas particles (in the rigid-sphere approximation).

For rigid spheres, the scattering kernel $F(\mathbf{c}':\mathbf{c})$ can be expanded in terms of Legendre functions [36]. However, even if we consider a truncated form of this expansion, the problem of solving the resulting approximation of the linearized Boltzmann equation is still difficult from a numerical point of view [35]. For this reason, keeping in mind mathematical properties [7], one seeks to approximate the true kernel by physically meaningful approximations that can be more easily handled by analytical tools and numerical algorithms. In this way, the resulting equations are known as "model (kinetic) equations." Here we follow Siewert [33] and express the kernel, in (5), such that two of the well-known constant collision frequency models of the rarefied gas dynamics are represented:

$$F(\mathbf{c}':\mathbf{c}) = 1 + 2(\mathbf{c}'.\mathbf{c}) + (2/3)(c'^2 - 3/2)(c^2 - 3/2) + \widehat{\beta} M(\mathbf{c}':\mathbf{c}) \tag{7a}$$

with

$$M(\mathbf{c}':\mathbf{c}) = (4/15)(\mathbf{c}'.\mathbf{c})(c'^2 - 5/2)(c^2 - 5/2), \tag{7b}$$

where the case $\widehat{\beta} = 0$ defines the well-known BGK model equation [37] and the case $\widehat{\beta} = 1$ defines the S-model equation [15]. We note that, for both constant collision frequency models we use in this work, if we choose a mean-free path based on the viscosity to evaluate (6), we obtain [28, 35]

$$\varepsilon = \varepsilon_p = 1. \tag{8}$$

On the other hand, if we use a mean-free path based on thermal conductivity to evaluate (6), we get, respectively, for the BGK and the S-model

$$\varepsilon = \varepsilon_t = 1 \quad \text{and} \quad \varepsilon = \varepsilon_t = 3/2. \tag{9}$$

Taking into account the values listed in (8) and (9) we see that the evaluation of $\varepsilon_p/\varepsilon_t$ for the case of the S-model leads to a correct value for the Prandtl number (equal to 2/3). This aspect is considered an advantage of that model in comparison with the BGK model.

To complete the formulation of the temperature-jump problem, we write the boundary condition in terms of the Cercignani–Lampis kernel [12, 33],

$$h(0, c_x, c_y, c_z) = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty h(0, c_x', -c_y', c_z') R(c_x', -c_y', c_z' : c_x, c_y, c_z) \mathrm{d}c_x' \mathrm{d}c_z' \mathrm{d}c_y', \tag{10a}$$

where

$$R(c_x', c_y', c_z' : c_x, c_y, c_z) = \frac{2c_y'}{\pi \alpha_n \alpha_t (2-\alpha_t)} T(c_x' : c_x) S(c_y' : c_y) T(c_z' : c_z) \tag{10b}$$

with

$$T(x : z) = \exp\left[-\frac{[(1-\alpha_t)z - x]^2}{\alpha_t(2-\alpha_t)}\right] \tag{10c}$$

and

$$S(x : z) = \exp\left[-\frac{[(1-\alpha_n)^{1/2} z - x]^2}{\alpha_n}\right] \widehat{I}_0\left[\frac{2(1-\alpha_n)^{1/2}|xz|}{\alpha_n}\right]. \tag{10d}$$

For computational purposes, we write

$$\widehat{I}_0(w) = I_0(w)\mathrm{e}^{-w}, \tag{11a}$$

where $I_0(w)$ is the modified Bessel function,

$$I_0(w) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{w \cos\phi} \mathrm{d}\phi. \tag{11b}$$

Differently from the usual case of Maxwell boundary condition [10] defined in terms of one accommodation coefficient α, where it is assumed that some fraction α of the particles are reflected diffusely and the rest $(1-\alpha)$ is reflected specularly, we can see in (10a) to (10d) that the Cercignani–Lampis kernel is defined in terms of two accommodation coefficients: $\alpha_t \in [0, 2)$ the accommodation coefficient of tangential momentum and $\alpha_n \in [0, 1)$ the accommodation coefficient of energy corresponding to the normal component of velocity. The use of more than one accommodation coefficient allows a better physical representation of the gas-surface interaction. In the case of the Cercignani Lampis kernel, that is the case, according to the literature, mainly for roughness surfaces [24].

Still, to complete the definition of the temperature-jump problem, we have to specify the behavior of the solution at infinity. We impose the Welander condition [8]

$$\lim_{y\to\infty} \frac{\mathrm{d}}{\mathrm{d}y} T(y) = K, \tag{12}$$

where K is known and here the temperature perturbation is given, in terms of h as

$$T(y) = \frac{2}{3}\pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c'^2} h(y, c_x, c_y, c_z)\left(c^2 - \frac{3}{2}\right)\mathrm{d}c_x\mathrm{d}c_y\mathrm{d}c_z. \tag{13}$$

In solving the temperature-jump problem, in addition to the temperature perturbation already defined, another quantity we seek to compute is the density perturbation

$$N(y) = \pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{e}^{-c'^2} h(y, c_x, c_y, c_z)\mathrm{d}c_x\mathrm{d}c_y\mathrm{d}c_z. \tag{14}$$

By looking at the above definitions, (13) and (14), we see that we do not need to obtain the complete distribution h, but only some related integrals (moments), to compute those quantities. In this way, in what follows, we develop a procedure in order to get simpler problems, in terms of those moments, for which we will develop a solution with the ADO method.

3. A vector formulation–the S-model. In order to develop simpler formulations to evaluate the quantities of interest, we multiply (5) first by

$$\phi_1(c_x, c_z) = \frac{1}{\pi}\mathrm{e}^{-(c_x^2+c_z^2)} \tag{15}$$

and, in a second step by

$$\phi_2(c_x, c_z) = \frac{1}{\pi}(c_x^2 + c_z^2 - 2)\mathrm{e}^{-(c_x^2+c_z^2)}, \tag{16}$$

and, in both cases, we integrate over all c_x and c_z, such that, if we define

$$h_1(y,\xi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_1(c_x, c_z)h(y, c_x, c_y, c_z)\mathrm{d}c_x\mathrm{d}c_z, \tag{17}$$

$$h_2(y,\xi) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_2(c_x, c_z)h(y, c_x, c_y, c_z)\mathrm{d}c_x\mathrm{d}c_z \tag{18}$$

and introduce the new notation $\xi = c_y$, we find that

$$\xi\frac{\partial}{\partial y}h_1(y,\xi) + \varepsilon h_1(y,\xi) = \varepsilon\int_{-\infty}^{\infty}\psi(\xi')\Big[\kappa_{11}(\xi',\xi)h_1(y,\xi') + \kappa_{12}(\xi',\xi)h_2(y,\xi')\Big]\mathrm{d}\xi' \tag{19}$$

and

$$\xi\frac{\partial}{\partial y}h_2(y,\xi) + \varepsilon h_2(y,\xi) = \varepsilon\int_{-\infty}^{\infty}\psi(\xi')\Big[\kappa_{21}(\xi',\xi)h_1(y,\xi') + \kappa_{22}(\xi',\xi)h_2(y,\xi')\Big]\mathrm{d}\xi', \tag{20}$$

with

$$\psi(\xi) = \pi^{-1/2}\mathrm{e}^{-\xi^2} \tag{21}$$

and

$$\kappa_{11}(\xi',\xi) = 1 + \frac{2}{3}\left(\xi^2 - \frac{1}{2}\right)\left(\xi'^2 - \frac{1}{2}\right) + \widehat{\beta}\left[2\xi'\xi + \frac{4}{15}\left(\xi'^2 - \frac{3}{2}\right)\left(\xi^2 - \frac{3}{2}\right)\xi'\xi\right], \tag{22}$$

$$\kappa_{12}(\xi',\xi) = \frac{2}{3}\left(\xi^2 - \frac{1}{2}\right) + \widehat{\beta}\left[\left(\frac{4}{15}\xi^2 - \frac{2}{5}\right)\xi\xi'\right], \tag{23}$$

$$\kappa_{21}(\xi',\xi) = \frac{2}{3}\left(\xi'^2 - \frac{1}{2}\right) + \widehat{\beta}\left[\left(\frac{4}{15}\xi'^2 - \frac{2}{5}\right)\xi\xi'\right], \tag{24}$$

$$\kappa_{22}(\xi',\xi) = \frac{2}{3} + \widehat{\beta}\frac{4}{15}\xi\xi'. \tag{25}$$

The same procedure, initiated in (15) and (16), is applied to the boundary condition, (10a), to define the components h_1 and h_2 at the boundary, which are written in the form

$$h_1(0,\xi) = \int_0^\infty h_1(0,-\xi')f(\xi',\xi)\mathrm{d}\xi' \tag{26}$$

and

$$h_2(0,\xi) = (1-\alpha_t)^2\int_0^\infty h_2(0,-\xi')f(\xi',\xi)\mathrm{d}\xi', \tag{27}$$

for $\xi, \xi' \in (0,\infty)$ and

$$f(\xi',\xi) = \frac{2\xi'}{\alpha_n}\exp\left[-\frac{[(1-\alpha_n)^{1/2}\xi - \xi']^2}{\alpha_n}\right]\widehat{I}_0\left[\frac{2(1-\alpha_n)^{1/2}\xi'\xi}{\alpha_n}\right]. \tag{28}$$

In this way, we let $\mathbf{H}(y,\xi)$ be the vector with components $h_1(y,\xi)$ and $h_2(y,\xi)$ and rewrite (19) to (28) in a more appropriate matrix form as

$$\xi\frac{\partial}{\partial y}\mathbf{H}(y,\xi) + \varepsilon\mathbf{H}(y,\xi) = \varepsilon\int_{-\infty}^\infty \psi(\xi')\boldsymbol{K}(\xi',\xi)\mathbf{H}(y,\xi')\mathrm{d}\xi', \tag{29}$$

for $y > 0$ and $\xi \in (-\infty,\infty)$. Here we note (21) to (25) and the definitions of

$$\mathbf{H}(y,\xi) = \begin{bmatrix} h_1(y,\xi) \\ h_2(y,\xi) \end{bmatrix} \tag{30}$$

and

$$\boldsymbol{K}(\xi',\xi) = \begin{bmatrix} \kappa_{11}(\xi',\xi) & \kappa_{12}(\xi',\xi) \\ \kappa_{21}(\xi',\xi) & \kappa_{22}(\xi',\xi \end{bmatrix}. \tag{31}$$

In regard to the boundary condition, we write

$$\mathbf{H}(0,\xi) = \mathbf{A}\int_0^\infty \mathbf{H}(0,-\xi')f(\xi',\xi)\mathrm{d}\xi', \tag{32}$$

with

$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & (1-\alpha_t)^2 \end{bmatrix}, \tag{33}$$

for $\xi, \xi' \in (0, \infty)$.

Finally, we also use the vector notation to express, respectively, the temperature and density perturbations, given in (13) and (14), in the form

$$T(y) = \frac{2}{3}\int_{-\infty}^{\infty} \begin{bmatrix} \xi^2 - 1/2 \\ 1 \end{bmatrix}^T \mathbf{H}(y,\xi)\psi(\xi)\mathrm{d}\xi \tag{34}$$

and

$$N(y) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}^T \int_{-\infty}^{\infty} \mathbf{H}(y,\xi)\psi(\xi)\mathrm{d}\xi. \tag{35}$$

We now proceed to develop a discrete-ordinates solution for the vector problem. In what follows we chose to assume the S-model case ($\widehat{\beta} = 1$), to which the expression for the kernel and the development of the solution are more general. Much simpler expressions can be found for the BGK model, and the work of Barichello and Siewert [29] can be used to follow that derivation.

4. A discrete-ordinates solution (I). We now seek for a discrete-ordinates solution of the problem defined by (29) and (32) and the condition given by (12). In this sense, the analytical discrete-ordinates method we use in this work, the ADO method [17], is based on a half-range quadrature scheme, and so as a first step we write (29) in the form

$$\xi\frac{\partial}{\partial y}\mathbf{H}(y,\xi) + \varepsilon\mathbf{H}(y,\xi) = \varepsilon\int_0^{\infty} \psi(\xi')[\boldsymbol{K}(\xi',\xi)\mathbf{H}(y,\xi') + \boldsymbol{K}(-\xi',\xi)\mathbf{H}(y,-\xi')]\mathrm{d}\xi', \tag{36}$$

and we seek solutions of (36) of the form

$$\mathbf{H}(y,\xi) = \mathbf{\Phi}(\nu,\xi)\,\mathrm{e}^{-y\varepsilon/\nu}, \tag{37}$$

where the separation constants ν and the elementary (2×1 vector) solutions $\mathbf{\Phi}$ are to be determined. Substituting (37) into (36) we find that

$$\varepsilon(\nu - \xi)\mathbf{\Phi}(\nu,\xi) = \varepsilon\nu\int_0^{\infty} \psi(\xi')[\boldsymbol{K}(\xi',\xi)\mathbf{\Phi}(\nu,\xi') + \boldsymbol{K}(-\xi',\xi)\mathbf{\Phi}(\nu,-\xi')]\mathrm{d}\xi' \tag{38}$$

and

$$\varepsilon(\nu + \xi)\mathbf{\Phi}(\nu,-\xi) = \varepsilon\nu\int_0^{\infty} \psi(\xi')[\boldsymbol{K}(\xi',-\xi)\mathbf{\Phi}(\nu,\xi') + \boldsymbol{K}(-\xi',-\xi)\mathbf{\Phi}(\nu,-\xi')]\mathrm{d}\xi'. \tag{39}$$

Here we note, since

$$\boldsymbol{K}(\xi',-\xi) = \boldsymbol{K}(-\xi',\xi), \tag{40}$$

that

$$\mathbf{\Phi}(\nu,\xi) = \mathbf{\Phi}(-\nu,-\xi). \tag{41}$$

Continuing our development, we add and subtract (38) and (39), one from the other, to find that

$$\frac{1}{\xi^2}\left[\mathbf{V}(\nu,\xi) - \int_0^\infty \psi(\xi')\mathbf{P}(\xi',\xi)\mathbf{V}(\nu,\xi')\mathrm{d}\xi'\right] = \lambda\mathbf{V}(\nu,\xi) \tag{42}$$

and

$$\mathbf{U}(\nu,\xi) = \frac{\nu}{\xi}\left[\mathbf{V}(\nu,\xi) - \int_0^\infty \psi(\xi')[\boldsymbol{K}(\xi',\xi)\mathbf{V}(\nu,\xi') - \boldsymbol{K}(-\xi',\xi)\mathbf{V}(\nu,\xi')]\mathrm{d}\xi'\right], \tag{43}$$

where

$$\mathbf{U}(\nu,\xi) = \mathbf{\Phi}(\nu,\xi) + \mathbf{\Phi}(\nu,-\xi), \tag{44}$$

$$\mathbf{V}(\nu,\xi) = \mathbf{\Phi}(\nu,\xi) - \mathbf{\Phi}(\nu,-\xi), \tag{45}$$

and

$$\lambda = 1/\nu^2. \tag{46}$$

Still, we note that the separation constants ν occur in $(\pm)$ pairs, and

$$\begin{aligned}\mathbf{P}(\xi',\xi) &= \frac{\xi}{\xi'}\Big[[\boldsymbol{K}(\xi',\xi) + \boldsymbol{K}(-\xi',\xi)] + [\boldsymbol{K}(\xi',\xi) - \boldsymbol{K}(-\xi',\xi)]\Big] \\ &- \int_0^\infty \psi(\xi'')\frac{\xi}{\xi''}[\boldsymbol{K}(\xi',\xi'') - \boldsymbol{K}(-\xi',\xi'')][\boldsymbol{K}(\xi'',\xi) + \boldsymbol{K}(-\xi'',\xi)]\mathrm{d}\xi''.\end{aligned} \tag{47}$$

At this point, we introduce a half-range quadrature scheme, in $[0,\infty)$, defined by N nodes $\{\xi_k\}$ and weights $\{\omega_k\}$, and rewrite (42) and (43) evaluated at the quadrature points as

$$\frac{1}{\xi_i^2}\left[\mathbf{V}(\nu_j,\xi_i) - \sum_{k=1}^N \omega_k\psi(\xi_k)\mathbf{P}(\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)\right] = \lambda_j\mathbf{V}(\nu_j,\xi_i) \tag{48}$$

and

$$\mathbf{U}(\nu_j,\xi_i) = \frac{\nu_j}{\xi_i}\left[\mathbf{V}(\nu_j,\xi_i) - \sum_{k=1}^N \omega_k\psi(\xi_k)[\mathbf{K}(\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k) - \mathbf{K}(-\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)]\right] \tag{49}$$

for $i = 1,2,\ldots,N$. Once we solve our eigenvalue problem, defined by (48), we have the elementary solutions from

$$\mathbf{\Phi}(\nu_j,\xi_i) = \frac{1}{2}\Big[\mathbf{U}(\nu_j,\xi_i) + \mathbf{V}(\nu_j,\xi_i)\Big] \tag{50}$$

and

$$\mathbf{\Phi}(\nu_j,-\xi_i) = \frac{1}{2}\Big[\mathbf{U}(\nu_j,\xi_i) - \mathbf{V}(\nu_j,\xi_i)\Big]. \tag{51}$$

In (48) to (51) we use the subscript j to label the eigenvalues. For each j, (50) and (51) express $2N \times 1$ vectors.

Here it may be important to make a comment in regard to the eigenvalue problem defined in (42). In applying the ADO method we have found, for different model equations and for different classes of problems, specific eigenvalue problems. In most of those cases the problem is much simpler and expressed in a much more concise form than in the case of this work. Even the case of diagonal + rank one type matrix can be mentioned [17, 38]. In fact, for the specific derivation presented above, some properties of the kernel can also be used to derive a simpler eigenvalue problem, as shown by Scherer [39]. We chose, however, to keep the derivation as it is, in order to establish more close connections and analogies with the mixtures case we will present later on in this text.

Continuing, we consider (50) and (51) along with (46), we take the positive root ν_j, and we write the general discrete-ordinates solution to (29) as

$$\mathbf{H}(y, \pm\xi_i) = \sum_{j=1}^{2N} [A_j \mathbf{\Phi}(\nu_j, \pm\xi_i) \mathrm{e}^{-y\varepsilon/\nu_j} + B_j \mathbf{\Phi}(\nu_j, \mp\xi_i) \mathrm{e}^{y\varepsilon/\nu_j}], \tag{52}$$

for $i = 1, 2, \ldots, N$. Here the arbitrary constants are to be determined from the boundary condition and the imposed condition at infinity. Before doing that, however, we note that the eigenvalue problem yields two separation constants, say ν_1 and ν_2, that become unbounded. Because of this, we rewrite the general solution as

$$\mathbf{H}(y, \pm\xi_i) = \mathbf{H}^*(y, \pm\xi_i) + \sum_{j=3}^{2N} [A_j \mathbf{\Phi}(\nu_j, \pm\xi_i) \mathrm{e}^{-y\varepsilon/\nu_j} + B_j \mathbf{\Phi}(\nu_j, \mp\xi_i) \mathrm{e}^{y\varepsilon/\nu_j}], \tag{53}$$

$i = 1, 2, \ldots, N$, where we then introduced, in (53), four linear independent exact solutions of (29). In other words,

$$\mathbf{H}^*(y, \xi) = A_1 \mathbf{H}_1 + A_2 \mathbf{H}_2(\xi) + B_1 \mathbf{H}_3(\xi) + B_2 \mathbf{H}_4(\xi), \tag{54}$$

where, for the S-model,

$$\mathbf{H}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{H}_2(\xi) = \begin{bmatrix} \xi^2 - 1/2 \\ 1 \end{bmatrix}, \quad \mathbf{H}_3(\xi) = \begin{bmatrix} \xi \\ 0 \end{bmatrix}, \tag{55}$$

and

$$\mathbf{H}_4(y, \xi) = y\mathbf{G}_1(\xi) + \mathbf{F}_1(\xi) \tag{56a}$$

with

$$\mathbf{G}_1(\xi) = \begin{bmatrix} \xi^2 - 3/2 \\ 1 \end{bmatrix} \tag{56b}$$

and

$$\mathbf{F}_1(\xi) = \frac{-3\xi}{2\varepsilon} \mathbf{G}_1(\xi). \tag{56c}$$

In fact, in the process of finding the $\mathbf{H}_4$ solution, once that (56b) is an exact solution of (29), we can follow analogous procedure as the one proposed by Siewert [32], and we substitute (56a) into (29) to find that

$$\mathbf{F}_1(\xi) = -\frac{1}{\varepsilon}\xi\mathbf{G}_1(\xi) + \int_{-\infty}^{\infty} \psi(\xi')\boldsymbol{K}(\xi',\xi)\mathbf{F}_1(\xi')\mathrm{d}\xi'. \tag{57}$$

The form of the inhomogeneous term, in (57), as well as the the form of $\boldsymbol{K}(\xi',\xi)$ suggest that we look for solutions of the form

$$\mathbf{F}_1(\xi) = \sum_{\alpha=0}^{3} P_\alpha(\xi)\mathbf{F}_{1,\alpha}, \tag{58}$$

where $\mathbf{F}_{1,\alpha}$ are constant vectors and $P_\alpha(\xi)$ are orthogonal polynomials given by

$$P_0(\xi) = 1\ ,\quad P_1(\xi) = \xi\ ,\quad P_2(\xi) = \xi^2 - 1/2, \quad \text{and} \quad P_3(\xi) = \xi(\xi^2 - 3/2). \tag{59}$$

Thus, if we first substitute (58) into (57), and then we multiply the equation by $\psi(\xi)P_k(\xi)$, for $k = 0,1,2,3$, to finally integrate over all ξ, we obtain an algebraic system (with 8 equations and rank 6)

$$\sum_{\alpha=0}^{3} P_\alpha(\xi)\mathbf{F}_{1,\alpha} = -\frac{1}{\varepsilon}\xi\mathbf{G}_1(\xi) + \int_{-\infty}^{\infty} \psi(\xi')\boldsymbol{K}(\xi',\xi)\sum_{\alpha=0}^{3} P_\alpha(\xi')\mathbf{F}_{1,\alpha}\mathrm{d}\xi', \tag{60}$$

for which a solution can be found explicitly, as the one given in (56a).

So, at this point we can go back to the issue of determining, in (53), the $4N$ arbitrary constants, such that our discrete-ordinates solution will be completely established. To start, if we consider the way that the solution is required to diverge at infinity, we take $B_j = 0$ for $j = 3,4,\ldots,2N$. In addition, when considering the Welander condition, given by (12) (and noting (34)), we find that

$$B_2 = K. \tag{61}$$

Still, we note that the solution $\mathbf{H}_1$, (55), satisfies the homogeneous boundary condition given by (32), and so the A_1 coefficient cannot be determined from that equation. However, following previous works [29, 40] we can impose on our solution an additional normalization condition

$$\lim_{y\to\infty}\left[N(y) + T(y)\right] = 0 \tag{62}$$

from where we get that

$$A_2 = -A_1. \tag{63}$$

In this way, we rewrite the general solution, (53), for $i = 1,2,\ldots,N$, as

$$\mathbf{H}(y,\pm\xi_i) = A_2\mathbf{G}_1(\pm\xi_i) + B_1\mathbf{H}_3(\pm\xi_i) + K\mathbf{H}_4(y,\pm\xi_i) + \sum_{j=3}^{2N} A_j\boldsymbol{\Phi}(\nu_j,\pm\xi_i)\mathrm{e}^{-y\varepsilon/\nu_j}. \tag{64}$$

To determine the remaining $2N$ arbitrary constants, we substitute (64) into the discrete-ordinates version of the boundary condition given by (32)

$$\mathbf{H}(0,\xi_i) = \mathbf{A}\sum_{k=1}^{N}\omega_k \mathrm{e}^{-\xi_k{}^2}\mathbf{H}(0,-\xi_k)f(\xi_k,\xi_i), \tag{65}$$

for $i = 1, 2, \ldots, N$. We then obtain the following $2N \times 2N$ linear algebraic system:

$$\begin{aligned} A_2\mathbf{C^1}(\xi_i) + B_1\mathbf{C^2}(\xi_i) + \sum_{j=3}^{2N} A_j\left\{\mathbf{\Phi}_+(\nu_j) - \sum_{k=1}^{N}\omega_k f(\xi_k,\xi_i)\mathbf{A}^*\mathbf{\Phi}_-(\nu_j)\right\} \\ = K\left\{\sum_{k=1}^{N}\omega_k f(\xi_k,\xi_i)\mathbf{A}^*\mathbf{B}^*(-\xi_k) - \mathbf{B}^*(\xi_i)\right\}, \end{aligned} \tag{66}$$

where the components of the vectors $\mathbf{\Phi}_+(\nu_j)$ and $\mathbf{\Phi}_-(\nu_j)$ are given by (50) and (51),

$$\mathbf{C^1}(\xi_i) = \sum_{k=1}^{N}\omega_k f(\xi_k,\xi_i)\mathbf{A}^*\mathbf{R}^*(-\xi_k) - \mathbf{R}^*(\xi_i), \tag{67}$$

and

$$\mathbf{C^2}(\xi_i) = \mathbf{H}_3^*(\xi_i) - \sum_{k=1}^{N}\omega_k f(\xi_k,\xi_i)\mathbf{A}^*\mathbf{H}_3^*(-\xi_k). \tag{68}$$

Here $\mathbf{R}^*(\xi)$ is a $2N \times 1$ vector where each 2×1 component is

$$\mathbf{R}(\xi) = -\mathbf{G}_1(\xi) \tag{69}$$

for $\mathbf{G}_1(\xi)$ defined in (56b); $\mathbf{A}^*$ is a $2N \times 2N$ block diagonal matrix

$$\mathbf{A}^* = \mathrm{diag}\Big\{\mathbf{A}, \mathbf{A}, \ldots, \mathbf{A}, \mathbf{A}\Big\} \tag{70}$$

with $\mathbf{A}$ given in (33); $\mathbf{H}_3^*(\xi)$ and $\mathbf{B}^*(\xi)$ are $2N \times 1$ vectors where each 2×1 component is, respectively, defined in (55) and (56c). In addition, $f(\xi_k,\xi_i)$ is defined in (28).

Considering now the quantities we want to evaluate, we substitute (53) into the discrete-ordinates version of (34) and (35) to write the temperature perturbation

$$T(y) = Ky + A_2 + 2/3\sum_{j=3}^{2N} A_j\ (\mathrm{e}^{-y\varepsilon/\nu_j})M_1(\nu_j) \tag{71}$$

and the density perturbation

$$N(y) = -Ky - A_2 + \sum_{j=3}^{2N} A_j\ (\mathrm{e}^{-y\varepsilon/\nu_j})M_2(\nu_j), \tag{72}$$

where M_1 and M_2 are, respectively, the components of the vector given by

$$\mathbf{M}^*(\nu_j) = \pi^{-1/2}\sum_{k=1}^{N}\omega_k e^{-\xi_k{}^2}\begin{bmatrix} \xi_k^2 - 1/2 & 1 \\ 1 & 0 \end{bmatrix}[\mathbf{\Phi}(\nu_j,\xi_k) + \mathbf{\Phi}(\nu_j,-\xi_k)]. \tag{73}$$

Still, if we look now at the linear component of the temperature perturbation expression

$$T^*(y) = Ky + A_2 \tag{74}$$

we can define another quantity of interest, which relates the temperature perturbation at the wall with the gradient of the temperature, the temperature-jump coefficient ζ, as

$$T^*(0) = \zeta \frac{\mathrm{d}}{\mathrm{d}y} T^*(y)\Big|_{y=0} \tag{75}$$

such that

$$\zeta = A_2/K. \tag{76}$$

To be clear, we note that the normalization constant introduced in (62) does not affect the temperature-jump coefficient or the temperature perturbation. In fact, another choice of that constant would change only the density perturbation by the addition of a constant factor [30].

5. The McCormack model and a mixture of gases. In regard to a binary gas mixture, in this work we base our discussion on the McCormack model, as introduced by McCormack [16], following an appropriate notation proposed by Siewert [32]. In this way, to derive the balance equation, we consider the functions $h_\alpha(x, \mathbf{v})$ for the two types of particles ($\alpha = 1$ and 2) which denote perturbations from Maxwellian distributions for each species,

$$f_\alpha(y^*, \mathbf{v}) = f_{\alpha,0}(\mathbf{v})[1 + h_\alpha(y^*, \mathbf{v})], \tag{77}$$

where

$$f_{\alpha,0}(\mathbf{v}) = n_\alpha(\lambda_\alpha/\pi)^{3/2}\mathrm{e}^{-\lambda_\alpha v^2}, \quad \lambda_\alpha = m_\alpha/(2kT_0). \tag{78}$$

Here, again, k is the Boltzmann constant, m_α is the mass, n_α is the equilibrium density of the αth species, T_0 is a reference temperature, y^* is the spatial variable, and the vector $\mathbf{v}$, with magnitude v, is the particle velocity with components v_x, v_y, and v_z. It is found [16] that the balance equation is of the form

$$c_y \frac{\partial}{\partial y^*} h_\alpha(y^*, \mathbf{c}) + w_\alpha \gamma_\alpha h_\alpha(y^*, \mathbf{c}) = w_\alpha \gamma_\alpha \mathcal{L}_\alpha\{h_1, h_2\}(y^*, \mathbf{c}), \quad \alpha = 1, 2, \tag{79}$$

where $\mathbf{c}$, with magnitude c and components c_x, c_y, and c_z, is now a dimensionless velocity variable. In obtaining (79), we followed Siewert [32] and expressed the dimensionless variable $\mathbf{c}$ differently in the two equations: for the case $\alpha = 1$ we defined $\mathbf{c} = w_1\mathbf{v}$, and, analogously, for the case $\alpha = 2$ we defined $\mathbf{c} = w_2\mathbf{v}$, where

$$w_\alpha = [m_\alpha/(2kT_0)]^{1/2}, \quad \alpha = 1, 2. \tag{80}$$

Still, in (79), the γ_α are to be defined later, and the collision operator is written as

(81)

$$\mathcal{L}_\alpha\{h_1, h_2\}(y^*, \mathbf{c}) = \frac{1}{\pi^{3/2}} \sum_{\beta=1}^{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-c'^2} h_\beta(y^*, \mathbf{c}') \mathbf{K}_{\beta,\alpha}(\mathbf{c}', \mathbf{c}) \mathrm{d}c'_x \mathrm{d}c'_y \mathrm{d}c'_z,$$

with the kernels expressed, in a general form, as [32]

(82)
$$\boldsymbol{K}_{\beta,\alpha} = \boldsymbol{K}^{(1)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) + \boldsymbol{K}^{(2)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) + \boldsymbol{K}^{(3)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}) + \boldsymbol{K}^{(4)}_{\beta,\alpha}(\mathbf{c}',\mathbf{c}), \quad \alpha,\beta = 1,2.$$

To avoid a heavy notation in the middle of the text, explicit expressions for each of the components in (82) are listed in Appendix A.

As in the one gas case, in (5), we introduce a dimensionless spatial variable $y = y^*/l_0$, where now l_0 is the mean-free path suggested by Sharipov and Kalempa [41], based on viscosity, defined as

$$l_0 = \frac{\mu v_0}{P_0}, \tag{83}$$

for

$$v_0 = \left(\frac{2kT_0}{m}\right)^{1/2} \tag{84}$$

and

$$m = \frac{n_1 m_1 + n_2 m_2}{n_1 + n_2}. \tag{85}$$

In regard to (81), we continue to follow Sharipov and Kalempa [41] and Siewert [32] and express the viscosity of the mixture in terms of the pressures P_α and the collision frequencies γ_α as

$$\mu = \frac{P_1}{\gamma_1} + \frac{P_2}{\gamma_2}, \tag{86}$$

where

$$\frac{P_\alpha}{P_0} = \frac{n_\alpha}{n_1 + n_2}, \tag{87}$$

$$\gamma_1 = \frac{\Psi_1\Psi_2 - \nu^{(4)}_{1,2}\nu^{(4)}_{2,1}}{\Psi_2 + \nu^{(4)}_{1,2}}, \tag{88a}$$

and

$$\gamma_2 = \frac{\Psi_1\Psi_2 - \nu^{(4)}_{1,2}\nu^{(4)}_{2,1}}{\Psi_1 + \nu^{(4)}_{2,1}}. \tag{88b}$$

In addition,

$$\Psi_1 = \nu^{(3)}_{1,1} - \nu^{(4)}_{1,1} + \nu^{(3)}_{1,2}, \tag{89a}$$

$$\Psi_2 = \nu^{(3)}_{2,2} - \nu^{(4)}_{2,2} + \nu^{(3)}_{2,1}. \tag{89b}$$

Again, we used above some definitions listed in Appendix A.

At this point, we introduce [32]

$$\sigma_\alpha = \gamma_\alpha \omega_\alpha l_0 \tag{90}$$

or, more explicitly,

$$\sigma_\alpha = \gamma_\alpha \frac{n_1/\gamma_1 + n_2/\gamma_2}{n_1 + n_2} \left(\frac{m_\alpha}{m}\right)^{1/2}, \tag{91}$$

such that, in the next section, we rewrite (79), in order to specifically define the temperature-jump problem based on the McCormack model, that we want to solve in this work, including the Cercignani Lampis kernel.

6. A binary gas mixture. Taking into account the development presented in the previous section, our starting point is now, analogously to the one gas case, (5), the kinetic equation for the McCormack model written as

$$c_y \frac{\partial}{\partial y} h_\alpha(y, \mathbf{c}) + \sigma_\alpha h_\alpha(y, \mathbf{c}) = \sigma_\alpha \mathcal{L}_\alpha\{h_1, h_2\}(y, \mathbf{c}) \tag{92}$$

for $y > 0$, the dimensionless variable (measured in terms of the mean-free path l_0), σ_α given in (90), and the collision operator defined in (82) and in Appendix A. For defining the temperature-jump problem, we supplement (92) with boundary condition, written in terms of the Cercignani–Lampis kernel as

$$h_\alpha(0, c_x, -c_y, c_z) = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty h_\alpha(0, c'_x, c'_y, c'_z) R_\alpha(c'_x, c'_y, c'_z : c_x, -c_y, c_z) \mathrm{d}c'_x \mathrm{d}c'_z \mathrm{d}c'_y, \tag{93}$$

for $c_y > 0$, all c_x, c_z, and $\alpha = 1, 2$. Here

$$R_\alpha(c'_x, c'_y, c'_z : c_x, c_y, c_z) = \frac{2c'_y}{\pi a_{n\alpha} a_{t\alpha}(2 - a_{t\alpha})} T_\alpha(c'_x : c_x) S_\alpha(c'_y : c_y) T_\alpha(c'_z : c_z), \tag{94a}$$

$$T_\alpha(x : z) = \exp\left[-\frac{[(1 - a_{t\alpha})z - x]^2}{a_{t\alpha}(2 - a_{t\alpha})}\right], \tag{94b}$$

$$S_\alpha(x : z) = \exp\left[-\frac{[(1 - a_{n\alpha})^{1/2} z - x]^2}{a_{n\alpha}}\right] \widehat{I}_0\left[\frac{2(1 - a_{n\alpha})^{1/2}|xz|}{a_{n\alpha}}\right], \tag{94c}$$

and $\widehat{I}_0(z)$ is defined as in (11a). In addition, $a_{t\alpha}$ are the tangential momentum accommodation coefficients for each species α ($\alpha = 1, 2$), and $a_{n\alpha}$ are the normal accommodation coefficients for each species α ($\alpha = 1, 2$). The formulation of the temperature-jump problem will be complete with the use of the condition, at infinity, on the temperature perturbation, as we show later on in this text.

In addition to the temperature perturbation

$$T_\alpha(y) = \frac{2}{3}\pi^{-3/2} \int_{-\infty}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \mathrm{e}^{-c'^2} h_\alpha(y, c_x, c_y, c_z) \left(\mathbf{c}^2 - \frac{3}{2}\right) \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z \tag{95}$$

we seek to compute also the density perturbation

$$N_\alpha(y) = \pi^{-3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-c'^2} h_\alpha(y, c_x, c_y, c_z) \mathrm{d}c_x \mathrm{d}c_y \mathrm{d}c_z. \tag{96}$$

Since we do not have to compute the complete distribution h, as we did for the one gas case, we develop a simpler formulation, by multiplying successively (92) by (15) and (16) and defining

$$g_{2\alpha-1}(y,\xi) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_1(c_x, c_z) h_\alpha(y, c_x, \xi, c_z) \mathrm{d}c_x \mathrm{d}c_z \tag{97}$$

and

$$g_{2\alpha}(y,\xi) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_2(c_x, c_z) h_\alpha(y, c_x, \xi, c_z) \mathrm{d}c_x \mathrm{d}c_z, \tag{98}$$

for $\alpha = 1, 2$. We then obtain four coupled equations, which we write in a matrix form, for the components of $\mathbf{G}(y,\xi)$ given by (97) and (98),

$$\xi \frac{\partial}{\partial y} \mathbf{G}(y,\xi) + \mathbf{\Sigma} \mathbf{G}(y,\xi) = \mathbf{\Sigma} \int_{-\infty}^{\infty} \psi(\xi') \boldsymbol{K}_M(\xi', \xi) \mathbf{G}(y, \xi') \mathrm{d}\xi', \tag{99}$$

with

$$\mathbf{\Sigma} = \mathrm{diag}\{\sigma_1, \sigma_1, \sigma_2, \sigma_2\} \tag{100}$$

and $\psi(\xi)$ given in (21). In regard to (99), we list the elements $k_{i,j}(\xi', \xi)$ of the (matrix) kernel $\boldsymbol{K}_M(\xi', \xi)$ in Appendix B.

To establish the matrix form of the boundary condition, once more, we use the projections defined by (15) and (16) along with (97) and (98) to obtain, from (93),

$$\mathbf{G}(0,\xi) = \mathbf{D} \int_0^{\infty} \mathbf{F}(\xi', \xi) \mathbf{G}(0, -\xi) \mathrm{d}\xi', \quad \xi > 0, \tag{101}$$

where

$$\mathbf{D} = \mathrm{diag}\ \{1, (1 - a_{t1})^2, 1, (1 - a_{t2})^2\} \tag{102}$$

and

$$\mathbf{F}(\xi', \xi) = \mathrm{diag}\ \{f_1(\xi', \xi), f_1(\xi', \xi), f_2(\xi', \xi), f_2(\xi', \xi)\}. \tag{103}$$

Here

$$f_1(\xi', \xi) = \frac{2\xi'}{a_{n1}} \exp\left[-\frac{[(1 - a_{n1})^{1/2}\xi - \xi']^2}{a_{n1}}\right] \widehat{I}_0 \left[\frac{2(1 - a_{n1})^{1/2} \xi' \xi}{a_{n1}}\right] \tag{104}$$

and

$$f_2(\xi', \xi) = \frac{2\xi'}{a_{n2}} \exp\left[-\frac{[(1 - a_{n2})^{1/2}\xi - \xi']^2}{a_{n2}}\right] \widehat{I}_0 \left[\frac{2(1 - a_{n2})^{1/2} \xi' \xi}{a_{n2}}\right], \tag{105}$$

for $\xi, \xi' \in (0, \infty)$.

Once we solve the vector problem, we can compute the density and the temperature perturbations, respectively, given by

$$N_\alpha(y) = \int_{-\infty}^{\infty} \psi(\xi) g_{2\alpha-1}(y,\xi)\mathrm{d}\xi, \quad \alpha = 1,2, \tag{106}$$

and

$$T_\alpha(y) = \frac{2}{3}\int_{-\infty}^{\infty} \psi(\xi)\left[\left(\xi^2 - \frac{1}{2}\right) g_{2\alpha-1}(y,\xi) + g_{2\alpha}(y,\xi)\right]\mathrm{d}\xi, \quad \alpha = 1,2, \tag{107}$$

and we write, in this new notation, the condition imposed to the behavior of the solution at infinity [32]

$$\lim_{y\to\infty} \frac{\mathrm{d}}{\mathrm{dy}}\mathbf{T}(y) = K\begin{bmatrix} 1 \\ 1 \end{bmatrix}. \tag{108}$$

Here K is considered known and $T_\alpha(y)$ are the components of the vector $\mathbf{T}(y)$.

In the next section we develop a discrete-ordinates solution for the problem defined by (99) to (108).

7. A discrete-ordinates solution (II). When seeking (4×1) solutions of (99) in the form

$$\mathbf{G}(y,\xi) = \mathbf{\Phi}(\nu,\xi)\,\mathrm{e}^{-y/\nu} \tag{109}$$

we follow the same steps described in section 4, when dealing with the one gas case. Then we do not repeat it here, but we write the eigenvalue problem relevant to this case:

$$(1/\xi_i^2)\left[\mathbf{\Sigma}^2\mathbf{V}(\nu_j,\xi_i) - \sum_{k=1}^{N}\omega_k\psi(\xi_k)\mathbf{P}(\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)\right] = \lambda_j\mathbf{V}(\nu_j,\xi_i) \tag{110}$$

with

$$\begin{aligned}\mathbf{U}(\nu_j,\xi_i) = (\nu_j/\xi_i)\mathbf{\Sigma}\Bigg[\mathbf{V}(\nu_j,\xi_i) - \sum_{k=1}^{N}\omega_k\psi(\xi_k)[\boldsymbol{K}_M(\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)\\ -\boldsymbol{K}_M(-\xi_k,\xi_i)\mathbf{V}(\nu_j,\xi_k)]\Bigg]\end{aligned} \tag{111}$$

for $i = 1,2,\ldots,N$. Here

$$\begin{aligned}\mathbf{P}(\xi',\xi) &= (\xi/\xi')\mathbf{\Sigma}[\boldsymbol{K}_M(\xi',\xi) + \boldsymbol{K}_M(-\xi',\xi)]\mathbf{\Sigma} + \mathbf{\Sigma}^2[\boldsymbol{K}_M(\xi',\xi) - \boldsymbol{K}_M(-\xi',\xi)]\\ &- \int_0^\infty \psi(\xi'')(\xi/\xi'')\mathbf{\Sigma}[\boldsymbol{K}_M(\xi'',\xi) + \boldsymbol{K}_M(-\xi'',\xi)]\mathbf{\Sigma}[\boldsymbol{K}_M(\xi',\xi'') - \boldsymbol{K}_M(-\xi',\xi'')]\mathrm{d}\xi''.\end{aligned} \tag{112}$$

We are also able to get the elementary solutions

$$\mathbf{\Phi}(\nu_j,\xi_i) = (1/2)\Big[\mathbf{U}(\nu_j,\xi_i) + \mathbf{V}(\nu_j,\xi_i)\Big] \tag{113}$$

and

$$\mathbf{\Phi}(\nu_j,-\xi_i) = (1/2)\Big[\mathbf{U}(\nu_j,\xi_i) - \mathbf{V}(\nu_j,\xi_i)\Big] \tag{114}$$

to write the general solution of the problem given by (99) as

$$\mathbf{G}(y,\pm\xi_i)=\sum_{j=1}^{4N}[A_j\mathbf{\Phi}(\nu_j,\pm\xi_i)\mathrm{e}^{-y/\nu_j}+B_j\mathbf{\Phi}(\nu_j,\mp\xi_i)\mathrm{e}^{y/\nu_j}] \tag{115}$$

for $i=1,2,\ldots,N$.

As noted in the one gas case, and as usual for conservative problems as these in the rarefied gas dynamics, we find again some unbounded separation constants: in this case the number is three. So, we rewrite the previous equation as

$$\mathbf{G}(y,\pm\xi_i)=\mathbf{G}^*(y,\pm\xi_i)+\sum_{j=4}^{4N}[A_j\mathbf{\Phi}(\nu_j,\pm\xi_i)\mathrm{e}^{-y/\nu_j}+B_j\mathbf{\Phi}(\nu_j,\mp\xi_i)\mathrm{e}^{y/\nu_j}] \tag{116}$$

for $i=1,2,\ldots,N$, where

$$\begin{aligned}\mathbf{G}^*(y,\xi)=&\,A_1\mathbf{G}_1+A_2\mathbf{G}_2+A_3\mathbf{G}_3+B_1\mathbf{G}_4(\xi)\\&+B_2[y\mathbf{H}_1(\xi)+\mathbf{F}_1(\xi)]+B_3[y\mathbf{H}_2(\xi)+\mathbf{F}_2(\xi)]\end{aligned} \tag{117}$$

with the exact solutions of (99) given by [32]

$$\mathbf{G}_1=\begin{bmatrix}1\\0\\0\\0\end{bmatrix},\qquad \mathbf{G}_2=\begin{bmatrix}0\\0\\1\\0\end{bmatrix}, \tag{118}$$

$$\mathbf{G}_3(\xi)=\begin{bmatrix}\xi^2-1/2\\1\\\xi^2-1/2\\1\end{bmatrix}\quad\text{and}\quad \mathbf{G}_4(\xi)=\begin{bmatrix}r\xi\\0\\\xi\\0\end{bmatrix}. \tag{119}$$

Considering, in addition, the functions

$$\mathbf{H}_1(\xi)=\begin{bmatrix}-1+c_1(\xi^2-1/2)\\c_1\\c_1(\xi^2-1/2)\\c_1\end{bmatrix}\quad\text{and}\quad \mathbf{H}_2(\xi)=\begin{bmatrix}c_2(\xi^2-1/2)\\c_2\\-1+c_2(\xi^2-1/2)\\c_2\end{bmatrix} \tag{120}$$

with

$$r=(m_1/m_2)^{1/2},\quad c_1=(n_1/n),\quad c_2=(n_2/n),\quad\text{and}\quad n=n_1+n_2, \tag{121}$$

we can then find functions $\mathbf{F}_1(\xi)$ and $\mathbf{F}_2(\xi)$ such that

$$\mathbf{G}_5(y,\xi)=y\mathbf{H}_1(\xi)+\mathbf{F}_1(\xi)\quad\text{and}\quad \mathbf{G}_6(y,\xi)=y\mathbf{H}_2(\xi)+\mathbf{F}_2(\xi) \tag{122}$$

complete the set of exact solutions we are looking for. In general,

$$\mathbf{F}_\beta(\xi)=-\xi\mathbf{\Sigma}^{-1}\mathbf{H}_\beta(\xi)+\int_{-\infty}^{\infty}\psi(\xi')\mathbf{K}(\xi',\xi)\mathbf{F}_\beta(\xi')\mathrm{d}\xi', \tag{123}$$

and, as we did previously in section 4, we write

$$\mathbf{F}_\beta(\xi) = \sum_{\alpha=0}^{3} P_\alpha(\xi)\mathbf{F}_{\beta,\alpha} \tag{124}$$

to find the components of the vectors $\mathbf{F}_{\beta,\alpha}$ required in (124). Here the linear algebraic system with 16 equations, defined to find those components, is rank deficient (rank 12). Since equations (120) are solutions of (99), we can write [32]

$$\mathbf{F}_\beta(\xi) = \mathbf{U}_\beta P_1(\xi) + \mathbf{V}_\beta P_3(\xi), \tag{125}$$

where now the constant vectors $\mathbf{U}_\beta$ and $\mathbf{V}_\beta$ are solutions of the (rank 8) linear systems

$$(\mathbf{I} - \mathbf{A}_1^*)\mathbf{U}_1 - \mathbf{C}_1^*\mathbf{V}_1 = \begin{bmatrix}(c_2/\sigma_1) & -(c_1/\sigma_1) & -(c_1/\sigma_2) & -(c_1/\sigma_2)\end{bmatrix}^T, \tag{126}$$

$$(\mathbf{I} - \mathbf{D}_1^*)\mathbf{V}_1 - \mathbf{B}_1^*\mathbf{U}_1 = \begin{bmatrix}-(c_1/\sigma_1) & 0 & -(c_1/\sigma_2) & 0\end{bmatrix}^T \tag{127}$$

and

$$\begin{bmatrix}0 & 0 & 1 & 0\end{bmatrix}\mathbf{U}_1 = 0, \tag{128}$$

for $\beta = 1$. In addition,

$$(\mathbf{I} - \mathbf{A}_1^*)\mathbf{U}_2 - \mathbf{C}_1^*\mathbf{V}_2 = \begin{bmatrix}-(c_2/\sigma_1) & -(c_2/\sigma_1) & (c_1/\sigma_2) & -(c_2/\sigma_2)\end{bmatrix}^T, \tag{129}$$

$$(\mathbf{I} - \mathbf{D}_1^*)\mathbf{V}_2 - \mathbf{B}_1^*\mathbf{U}_2 = \begin{bmatrix}-(c_2/\sigma_1) & 0 & -(c_2/\sigma_2) & 0\end{bmatrix}^T \tag{130}$$

and

$$\begin{bmatrix}0 & 0 & 1 & 0\end{bmatrix}\mathbf{U}_2 = 0, \tag{131}$$

for $\beta = 2$. Here (128) and (131) were made part of the linear system to guarantee a unique solution. Still, in the above expressions $\mathbf{I}$ is the identity matrix, the superscript T denotes transpose operation, and

$$\mathbf{A}_1^* = 2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}_M(\xi',\xi)P_1(\xi')P_1(\xi)\mathrm{d}\xi'\mathrm{d}\xi, \tag{132}$$

$$\mathbf{B}_1^* = (4/3)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}_M(\xi',\xi)P_1(\xi')P_3(\xi)\mathrm{d}\xi'\mathrm{d}\xi, \tag{133}$$

$$\mathbf{C}_1^* = 2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}_M(\xi',\xi)P_3(\xi')P_1(\xi)\mathrm{d}\xi'\mathrm{d}\xi \tag{134}$$

and

$$\mathbf{D}_1^* = (4/3)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi(\xi')\psi(\xi)\boldsymbol{K}_M(\xi',\xi)P_3(\xi')P_3(\xi)\mathrm{d}\xi'\mathrm{d}\xi. \tag{135}$$

However, (132) to (135) can be evaluated, by means of the quadrature scheme, such that we rewrite them (using notation listed in the appendix) in a final form

$$\mathbf{A}_1^* = \begin{bmatrix} 1-\eta_{1,2}^{(1)} & -(1/2)\eta_{1,2}^{(2)} & r\eta_{1,2}^{(1)} & (r^3/2)\eta_{1,2}^{(2)} \\ -(1/2)\eta_{1,2}^{(2)} & (2/5)\beta_1 & (r/2)\eta_{1,2}^{(2)} & (2/5)\eta_{1,2}^{(6)} \\ s\eta_{2,1}^{(1)} & (s^3/2)\eta_{2,1}^{(2)} & 1-\eta_{2,1}^{(1)} & -(1/2)\eta_{2,1}^{(2)} \\ (s/2)\eta_{2,1}^{(2)} & (2/5)\eta_{2,1}^{(6)} & -(1/2)\eta_{2,1}^{(2)} & (2/5)\beta_2 \end{bmatrix}, \tag{136}$$

$$\mathbf{B}_1^* = \begin{bmatrix} -(1/2)\eta_{1,2}^{(2)} & (2/5)\beta_1 & (r/2)\eta_{1,2}^{(2)} & (2/5)\eta_{1,2}^{(6)} \\ 0 & 0 & 0 & 0 \\ (s/2)\eta_{2,1}^{(2)} & (2/5)\eta_{2,1}^{(6)} & -(1/2)\eta_{2,1}^{(2)} & (2/5)\beta_2 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{137}$$

$$\mathbf{C}_1^* = \begin{bmatrix} -(3/4)\eta_{1,2}^{(2)} & 0 & (3r^3/4)\eta_{1,2}^{(2)} & 0 \\ (3/5)\beta_1 & 0 & (3/5)\eta_{1,2}^{(6)} & 0 \\ (3s^3/4)\eta_{2,1}^{(2)} & 0 & -(3/4)\eta_{2,1}^{(2)} & 0 \\ (3/5)\eta_{2,1}^{(6)} & 0 & (3/5)\beta_2 & 0 \end{bmatrix} \tag{138}$$

and

$$\mathbf{D}_1^* = \begin{bmatrix} (3/5)\beta_1 & 0 & (3/5)\eta_{1,2}^{(6)} & 0 \\ 0 & 0 & 0 & 0 \\ (3/5)\eta_{2,1}^{(6)} & 0 & (3/5)\beta_2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{139}$$

Thus, looking back to (116), the general discrete-ordinates solution for (99) can be written as

$$\mathbf{G}(y, \pm\xi_i) = \mathbf{G}^*(y, \pm\xi_i) + \sum_{j=4}^{4N} A_j \mathbf{\Phi}(\nu_j, \pm\xi_i)\mathrm{e}^{-y/\nu_j}, \tag{140}$$

taking into account that it is not allowed to diverge exponentially as y tends to infinity.

If we use (140) to evaluate (the discrete-ordinates version) (106) and (107) and we take the asymptotic part (the exponential terms were ignored) of the resulting expressions, we can write

$$N_1^*(y) = A_1 - B_2 y, \tag{141}$$

$$N_2^*(y) = A_2 - B_3 y, \tag{142}$$

$$T_1^*(y) = A_3 + (c_1 B_2 + c_2 B_3) y \tag{143}$$

and

$$T_2^*(y) = A_3 + (c_1 B_2 + c_2 B_3) y. \tag{144}$$

But again, as in the one gas case, two of the exact solutions, (118), satisfy the boundary condition, (101), such that the constants A_1 and A_2 cannot be determined from that boundary condition (density perturbations are not uniquely defined). As we did in the one gas case we make use of the condition given by (108) along with a normalization condition, similar to (62), to write

$$A_1 = -A_3, \tag{145}$$

$$A_2 = -A_3 \tag{146}$$

and

$$c_1 B_2 + c_2 B_3 = K. \tag{147}$$

In (147) we choose to write B_3 in terms of B_2 such that the general solution of the problem given by (99) is finally written as in (140) with

$$\begin{aligned}\mathbf{G}_*(y,\xi) = A_3\mathbf{R}(\xi) + B_1\mathbf{G}_4(\xi) + B_2\Big[[y\mathbf{H}_1(\xi) + \mathbf{F}_1(\xi)] - (c_1/c_2)[y\mathbf{H}_2(\xi) + \mathbf{F}_2(\xi)]\Big] \\ + (K/c_2)[y\mathbf{H}_2(\xi) + \mathbf{F}_2(\xi)].\end{aligned} \tag{148}$$

Here

$$\mathbf{R}(\xi) = \begin{bmatrix} \xi^2 - 3/2 \\ 1 \\ \xi^2 - 3/2 \\ 1 \end{bmatrix}. \tag{149}$$

The application of (140) in the discrete ordinates version of the boundary condition

$$\mathbf{G}(0,\xi_i) = \mathbf{D}\sum_{k=1}^{N}\omega_k\mathbf{F}(\xi_k,\xi_i)\mathbf{G}(0,-\xi_k) \tag{150}$$

results in the following linear system:

$$\begin{aligned}A_3\mathbf{C^3}(\xi_i) + B_1\mathbf{C^4}(\xi_i) + B_2\mathbf{C^5}(\xi_i) + \sum_{j=4}^{4N} A_j\left\{\mathbf{\Phi}_+(\nu_j) - \mathbf{D}^*\sum_{k=1}^{N}\omega_k\mathbf{F}^*(\xi_k,\xi_i)\mathbf{\Phi}_-(\nu_j)\right\} \\ = K\left\{-\mathbf{J}_1^*(\xi_i) + \mathbf{D}^*\sum_{k=1}^{N}\omega_k\mathbf{F}^*(\xi_k,\xi_i)\mathbf{J}_1^*(-\xi_k)\right\},\end{aligned} \tag{151}$$

where the components of the vectors $\mathbf{\Phi}_+(\nu_j)$ and $\mathbf{\Phi}_-(\nu_j)$ are given by (113) and (114),

$$\mathbf{C^3}(\xi_i) = \mathbf{R}^*(\xi_i) - \mathbf{D}^*\sum_{k=1}^{N}\omega_k\mathbf{F}^*(\xi_k,\xi_i)\mathbf{R}^*(-\xi_k), \tag{152}$$

$$\mathbf{C^4}(\xi_i) = \mathbf{G}_4^*(\xi_i) - \mathbf{D}^*\sum_{k=1}^{N}\omega_k\mathbf{F}^*(\xi_k,\xi_i)\mathbf{G}_4^*(-\xi_k) \tag{153}$$

and

$$\mathbf{C}^5(\xi_i) = \mathbf{K}_1^*(\xi_i) - \mathbf{D}^* \sum_{k=1}^{N} \omega_k \mathbf{F}^*(\xi_k, \xi_i) \mathbf{K}_1^*(-\xi_k). \tag{154}$$

Here $\mathbf{R}^*(\xi)$ is a $4N \times 1$ vector where each N component is of the type of (149); $\mathbf{K}_1^*(\xi)$ is a $4N \times 1$ vector defined by N components of the type

$$\mathbf{K}_1(\xi) = \mathbf{F}_1(\xi) - (c_1/c_2)\mathbf{F}_2(\xi), \tag{155}$$

and $\mathbf{J}_1^*(\xi)$ is a $4N \times 1$ vector where each N component is of the type

$$\mathbf{J}_1(\xi) = (1/c_2)\mathbf{F}_2(\xi). \tag{156}$$

In addition $\mathbf{D}^*$ and $\mathbf{F}^*(\xi_k, \xi)$ are $4N \times 4N$ diagonal matrices defined, looking back to (102) and (103), by

$$\mathbf{D}^* = \operatorname{diag}\Big\{\mathbf{D}, \mathbf{D}, \ldots, \mathbf{D}\Big\} \tag{157}$$

and

$$\mathbf{F}^*(\xi_k, \xi) = \operatorname{diag}\Big\{\mathbf{F}(\xi_1, \xi), \mathbf{F}(\xi_2, \xi), \ldots, \mathbf{F}(\xi_N, \xi)\Big\}. \tag{158}$$

Based on the derivation above we can write the density perturbation vector (two species) as

$$\mathbf{N}(y) = -\begin{bmatrix} A_3 + B_2 y \\ A_3 + \big(K/c_2 - (c_1/c_2)B_2\big)y \end{bmatrix} + \sum_{j=4}^{4N} A_j \, \mathrm{e}^{-y/\nu_j} \, \mathbf{M}_1(\nu_j), \tag{159}$$

where

$$\mathbf{M}_1(\nu_j) = \pi^{-1/2} \sum_{k=1}^{N} \omega_k \mathrm{e}^{-\xi_k{}^2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} [\mathbf{\Phi}(\nu_j, \xi_k) + \mathbf{\Phi}(\nu_j, -\xi_k)]. \tag{160}$$

The components $T_\alpha(y)$, $\alpha = 1, 2$, define the temperature perturbation vector

$$\mathbf{T}(y) = (A_3 + Ky) \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{2}{3} \sum_{j=4}^{4N} A_j \, \mathrm{e}^{-y/\nu_j} \, \mathbf{M}_2(\nu_j), \tag{161}$$

where

(162)

$$\mathbf{M}_2(\nu_j) = \pi^{-1/2} \sum_{k=1}^{N} \omega_k \mathrm{e}^{-\xi_k{}^2} \begin{bmatrix} \xi_k^2 - 1/2 & 1 & 0 & 0 \\ 0 & 0 & \xi_k^2 - 1/2 & 1 \end{bmatrix} [\mathbf{\Phi}(\nu_j, \xi_k) + \mathbf{\Phi}(\nu_j, -\xi_k)].$$

From (161), and taking into account (143) and (144), along with definitions (for each species) analogous to (75), we define the temperature-jump coefficient

$$\zeta = A_3/K, \tag{163}$$

which we found to be the same for both species of the gas.

8. Computational aspects and numerical results. To implement the ADO solution, in order to define the quantities of interest, the first step is to define the associated quadrature scheme. In this sense, for most of the problems in the rarefied gas dynamics field that have been solved by this method [25, 26, 27, 28, 29, 30] the following approach has been shown to be adequate: to map the interval of integration into the interval $[0,1]$ and then map the Gauss–Legendre points linearly to this interval. In general, the expression

$$u(\xi) = \mathrm{e}^{-\xi} \tag{164}$$

is the one used to map the interval $[0,\infty)$ into $[0,1]$. After that, the eigenvalue problem which defines the separation constants and the elementary solutions can be formulated and solved. Next, the linear systems which define the exact solutions have to be considered. Continuing, the linear algebraic system for the arbitrary constants of the general solution is solved and then the quantities of interest are evaluated. In this way, the algorithm is fast and easy to implement.

The results presented in Tables 1 to 14 (which we believe to be correct for all digits listed, plus or minus one in the last digit) were obtained with $N = 60$ quadrature points for the one gas case and $N = 80$ quadrature points for the mixtures case (except for $\alpha_n = 0.01$, where $N = 120$). For both cases we consider $K = 1$. The developed (and not particularly optimized) Fortran code requires around four seconds to yield, on a 3.0 GHz Pentium 4 machine, all quantities of interest for a general mixture case.

For the one gas case we used $\varepsilon = \varepsilon_t$ (according to (8) and (9)), in general, in order to obtain the numerical results shown (otherwise we added the statement $\varepsilon = \varepsilon_p$ in the table). We also note the notation DS and CL for referring to the use of, respectively, diffuse-specular and Cercignani–Lampis boundary condition. In fact, as we have worked on trying to establish a very general and complete comparison on results for different problems, provided by different model equations, we list in this work some results we obtained by the ADO method, for the temperature-jump problem, based on the BGK and S-models with diffuse-specular and Cercignani Lampis boundary condition, which were not available.

Continuing, we note that, in Tables 8 to 11, and in the text below, we use the notation $a_{n\alpha}$ and $a_{t\alpha}$, for the species $\alpha = 1,2$, to refer to the accommodation coefficients, respectively, of energy and tangential momentum.

In order to generate numerical results, we consider three mixtures cases related to the following gases: (i) Ne-Ar, (ii) He-Xe and (iii) He-Ar, as follow:

- Ne-Ar: $m_1 = 20.183$, $m_2 = 39.948$, and $d_2/d_1 = 1.406$
  - case I $a_{t1} = 0.849$, $a_{t2} = 0.916$, $a_{n1} = 0.1$, $a_{n2} = 0.4$
  - case II $a_{t1} = 0.31$, $a_{t2} = 0.67$, $a_{n1} = 0.1$, $a_{n2} = 0.4$
  - case III $a_{t1} = 0.849$, $a_{t2} = 0.916$, $a_{n1} = 0.082$, $a_{n2} = 0.222$
- He-Xe: $m_1 = 4.0026$, $m_2 = 131.30$, and $d_2/d_1 = 2.226$
  - case IV $a_{t1} = 0.20$, $a_{t2} = 0.95$, $a_{n1} = 0.01$, $a_{n2} = 0.7$
  - case V $a_{t1} = 0.20$, $a_{t2} = 0.95$, $a_{n1} = 0.05$, $a_{n2} = 0.4$
  - case VI $a_{t1} = 0.882$, $a_{t2} = 1.014$, $a_{n1} = 0.01$, $a_{n2} = 0.7$
- He-Ar: $m_1 = 4.0026$, $m_2 = 39.948$, and $d_2/d_1 = 1.665$
  - case VII $a_{t1} = 0.20$, $a_{t2} = 0.916$, $a_{n1} = 0.01$, $a_{n2} = 0.4$
  - case VIII $a_{t1} = 0.882$, $a_{t2} = 0.91$, $a_{n1} = 0.01$, $a_{n2} = 0.4$
  - case IX $a_{t1} = 0.20$, $a_{t2} = 0.916$, $a_{n1} = 0.01$, $a_{n2} = 0.222$

The data set used, and listed above, regarding the mass and diameter of the particles, was reproduced from [32, 41, 42].

In addition, we used experimental data for defining the values of the tangential momentum accommodation coefficient: cases II, IV, and V were formulated in terms of data provided by Lord [43]; in cases I, III, and VI, the value of that coefficient was reproduced from [11], which followed the experimental work of Porodnov et al. [44]. Cases VII to IX were formulated based on the previous cases.

Since, to the best of our knowledge, experimental results for the (normal) energy accommodation coefficient are not available, we chose numerical values based (order of magnitude) on the thermal accommodation coefficient of the gases listed above. We used, in this way, the works of Thomas [45] and Thomas and Lord [46].

The results were tabulated, for the three mixtures, in terms of the molar concentration defined in terms of the first particle as

$$C = \frac{n_1/n_2}{1 + n_1/n_2}. \tag{165}$$

In addition to provide results, which we believe were not available in the literature, for this problem, based on a more general law for describing the gas-surface interaction, we have been able to perform many simulations from which we try to point out some aspects, commented below.

First of all, we think that an important aspect of providing results, based on models related to the normal energy accommodation coefficient, which may not be measured, is the possibility of using quantities we are able to evaluate, in connection with a procedure for estimating parameters [47], in order to estimate that coefficient numerically. In this sense, we include in Tables 1 to 14, in addition to the temperature-jump coefficient, results for temperature and density perturbations, for several values of accommodation coefficients, and for different values of concentration, in the mixture cases.

In regard to the one gas case, based on the experience with previous analysis for other classes of problems [28], the fact of getting results for the BGK and S-model in agreement, in general, in one or two digits (for a choice of the mean-free path), was, in fact, used as a way of having some confidence in our program. In addition, we confirm previous observation [32] that both models lead to the same value for the temperature-jump coefficient but slightly different values for the temperature and density perturbation; we also simulate (considering $n_1 = 0$, $n_2 = 0$ or $m_1 = m_2$ and $d_1 = d_2$) the one gas case, from the McCormack model, and the results agree perfectly with the S-model, as observed previously [32].

Having used the ADO method, which is an analytical approach to the spatial variable, to deal with the temperature-jump problem for a wide class of model equations, in the one gas case, with Cercignani Lampis and Maxwell boundary condition, and having compared with available results [48] based on the linearized Boltzmann equation (LBE), we can say that in general the evaluation of this coefficient is not sensitive to the model equation to be used (see Table 7); comparisons between results (see Tables 1 to 5) obtained by the S-model and the LBE show agreement in one to two digits.

We generate results, showed in Tables 2 to 4, for a small value of α_n, which is, in general, hard to obtain accurately or even very much time consuming, from numerical approaches, but is consistent, in order of magnitude, with experimental values available for the total energy accommodation coefficient. It is noted that the

TABLE 1
The temperature-jump coefficient ζ.

α	BGK-DS	S-DS($\varepsilon = \varepsilon_p$)	S-DS	LBE-DS[31]
0.1	2.145012(1)	3.21752(1)	2.14501(1)	2.1349(1)
0.2	1.034747(1)	1.55212(1)	1.03475(1)	1.0251(1)
0.3	6.630514	9.94577	6.63051	6.5396
0.4	4.760333	7.14050	4.76033	4.6745
0.5	3.629125	5.44369	3.62912	3.5485
0.6	2.867615	4.30142	2.86761	2.7922
0.7	2.317534	3.47630	2.31753	2.2474
0.8	1.899741	2.84961	1.89974	1.8349
0.9	1.570264	2.35540	1.57026	1.5108
1.0	1.302716	1.95407	1.30272	1.2486

TABLE 2
The temperature-jump coefficient ζ, $\alpha_t = 0.25$.

α_n	BGK-CL	S-CL($\varepsilon = \varepsilon_p$)	S-CL	S-CL[24]	LBE-CL[48]
0.01	9.75601	1.46340(1)	9.75601	—	—
0.25	5.78950	8.68426	5.78950	8.684	5.7318
0.5	3.84176	5.76263	3.84176	5.763	3.7707
0.75	2.72408	4.08612	2.72408	4.087	2.6655
1.0	2.00553	3.00830	2.00553	3.009	1.9609

temperature-jump coefficient is very sensitive to the normal energy accommodation coefficient. In fact, from the cases shown in Figures 1 and 2, it is clear that the temperature-jump coefficient depends on both accommodation coefficients (the same is observed for the mixtures cases later on) and the significant variation occurs mainly when α_n and α_t are lower than 0.5. In these cases, in comparison with the results shown in Table 1 based on the Maxwell boundary condition, we see great increase in the jump values.

In Tables 12 to 14, we present results for the temperature-jump coefficient for the mixtures cases I to IX described previously in this section. We included the cases of concentration equal to one ($n_1 = 1$ and $n_2 = 0$) and equal to zero ($n_1 = 0$ and $n_2 = 1$), which reproduce exactly the results obtained for the one gas case (respectively, gas 1 and gas 2) and that may show how mixing a very small quantity of a different species can produce significant change in the jump coefficient. In fact, as observed for the case of Maxwell boundary conditions [32, 42], in Table 13, we note a small decrease on the value of the coefficient when we simulate the one gas case (species one). It seems that the (bigger) molecular mass ratio can be a reason for noticing this behavior; however, the same (decreasing) behavior is observed in Table 14, for the case VIII, and then, based on comparisons with cases VII and IX, one can also see for the same mixture the influence of the accommodation coefficients. However, one has to remember that the real values for α_n are unknown, and it has to be considered as a limitation for more specific conclusions.

Finally, in Figures 3 to 6, we tried to analyze the influence of each one of the accommodation coefficients, for the mixtures cases, based on cases I to VI. It really shows that the temperature-jump coefficient depends on both accommodation coefficients and mainly on the value of α_n. In addition, from Figures 4 and 6, the influence of the mass ratio in the magnitude order of the jump coefficient can be seen.

TABLE 3
The temperature-jump coefficient ζ, $\alpha_t = 0.5$.

α_n	BGK-CL	S-CL($\varepsilon = \varepsilon_p$)	S-CL	S-CL[24]	LBE-CL[48]
0.01	5.66914	8.50371	5.66914	—	—
0.25	3.88593	5.82890	3.88593	5.828	3.8696
0.5	2.78041	4.17061	2.78041	4.170	2.7282
0.75	2.05839	3.08759	2.05839	3.088	2.0010
1.0	1.55658	2.33487	1.55658	2.335	1.5015

TABLE 4
The temperature-jump coefficient ζ, $\alpha_t = 1.0$.

α_n	BGK-CL	S-CL($\varepsilon = \varepsilon_p$)	S-CL	S-CL[24]	LBE-CL[48]
0.01	4.20852	6.31278	4.20852	—	—
0.25	3.04475	4.56713	3.04475	4.567	3.0524
0.5	2.25090	3.37635	2.25090	3.376	2.2161
0.75	1.70032	2.55048	1.70032	2.551	1.6514
1.0	1.30272	1.95407	1.30272	1.954	1.2486

TABLE 5
Temperature $T(y)$ and density $N(y)$ perturbations, $\alpha = 0.5$.

	S-DS($\varepsilon = \varepsilon_p$)		S-DS		BGK-DS[30]		LBE-DS[31]	
y	$T(y)$	$N(y)$	$T(y)$	$N(y)$	$T(y)$	$N(y)$	$T(y)$	$N(y)$
0.0	4.37396	–4.61156	2.91597	–3.07437	2.91597	–3.07437	2.9250	–3.1153
0.1	4.72063	–4.92495	3.22570	–3.35355	3.18042	–3.31664	3.2342	–3.3647
0.2	4.94416	–5.12484	3.42167	–3.52947	3.36278	–3.48323	3.4238	–3.5257
0.3	5.13250	–5.29421	3.58709	–3.67966	3.52167	–3.62947	3.5831	–3.6654
0.4	5.30131	–5.44717	3.73615	–3.81653	3.66754	–3.76478	3.7268	–3.7944
0.5	5.45733	–5.58965	3.87478	–3.94514	3.80489	–3.89310	3.8605	–3.9167
0.6	5.60422	–5.72479	4.00614	–4.06814	3.93615	–4.01653	3.9874	–4.0345
0.7	5.74424	–5.85449	4.13216	–4.18706	4.06283	–4.13633	4.1093	–4.1491
0.8	5.87889	–5.98001	4.25410	–4.30291	4.18593	–4.25334	4.2275	–4.2612
0.9	6.00921	–6.10220	4.37281	–4.41637	4.30614	–4.36814	4.3428	–4.3715
1.0	6.13600	–6.22170	4.48894	–4.52793	4.42400	–4.48113	4.4558	–4.4802
2.0	7.29393	–7.33511	5.57466	–5.58912	5.52928	–5.55674	5.5196	–5.5251
3.0	8.36200	–8.38367	6.60474	–6.61081	6.57466	–6.58912	–	–
4.0	9.39637	–9.40840	7.61737	–7.62010	7.59758	–7.60560	–	–
5.0	1.04152(1)	–1.04221(1)	8.62318	–8.62448	8.61013	–8.61476	–	–
6.0	1.14260(1)	–1.14302(1)	9.62601	–9.62665	9.61737	–9.62011	–	–
7.0	1.24325(1)	–1.24350(1)	1.06274(1)	–1.06278(1)	1.06217(1)	–1.06234(1)	–	–
8.0	1.34365(1)	–1.34380(1)	1.16282(1)	–1.16284(1)	1.16243(1)	–1.16254(1)	–	–
9.0	1.44390(1)	–1.44400(1)	1.26286(1)	–1.26287(1)	1.26260(1)	–1.26267(1)	–	–
10.0	1.54406(1)	–1.54412(1)	1.36288(1)	–1.36289(1)	1.36271(1)	–1.36275(1)	–	–
20.0	2.54436(1)	–2.54436(1)	2.36291(1)	–2.36291(1)	2.36291(1)	–2.36291(1)	–	–

TABLE 6
Temperature $T(y)$ and density $N(y)$ perturbations, $\alpha_t = 0.5$, $\alpha_n = 0.5$.

	BGK-CL		S-CL($\varepsilon = \varepsilon_p$)		S-CL	
y	$T(y)$	$N(y)$	$T(y)$	$N(y)$	$T(y)$	$N(y)$
0.0	2.10157	−2.56938	3.15236	−3.85407	2.10157	−2.56938
0.1	2.34143	−2.71400	3.46214	−4.02100	2.38212	−2.72494
0.2	2.51598	−2.83371	3.67398	−4.15056	2.57076	−2.84749
0.3	2.67076	−2.94749	3.85614	−4.27124	2.73298	−2.96295
0.4	2.81423	−3.05829	4.02135	−4.38743	2.88054	−3.07492
0.5	2.95014	−3.16724	4.17520	−4.50085	3.01854	−3.18477
0.6	3.08054	−3.27492	4.32081	−4.61238	3.14976	−3.29315
0.7	3.20674	−3.38167	4.46011	−4.72251	3.27590	−3.40045
0.8	3.32960	−3.48770	4.59441	−4.83155	3.39810	−3.50691
0.9	3.44976	−3.59315	4.72464	−4.93973	3.51717	−3.61267
1.0	3.56767	−3.69812	4.85151	−5.04718	3.63369	−3.71786
2.0	4.67538	−4.73195	6.01307	−6.09793	4.72288	−4.75046
3.0	5.72288	−5.75046	7.08432	−7.12570	5.75467	−5.76525
4.0	6.74708	−6.76147	8.12062	−8.14220	6.76804	−6.77248
5.0	7.76037	−7.76823	9.14056	−9.15235	7.77418	−7.77617
6.0	8.76804	−8.77248	1.01520(1)	−1.01587(1)	8.77716	−8.77810
7.0	9.77261	−9.77519	1.11589(1)	−1.11628(1)	9.77867	−9.77912
8.0	1.07754(1)	−1.07769(1)	1.21631(1)	−1.21654(1)	1.07795(1)	−1.07797(1)
9.0	1.17772(1)	−1.17781(1)	1.31657(1)	−1.31671(1)	1.17799(1)	−1.17800(1)
10.0	1.27783(1)	−1.27788(1)	1.41674(1)	−1.41683(1)	1.27801(1)	−1.27802(1)
20.0	2.27804(1)	−2.27804(1)	2.41705(1)	−2.41705(1)	2.27804(1)	−2.27804(1)

TABLE 7
The temperature-jump coefficient ζ, $\alpha = 0.5$ with Maxwell boundary condition.

Model	ζ
BGK	3.629125[30]
Williams	3.435960[30]
Rigid-sphere	3.476180[30]
S ($\varepsilon = \varepsilon_p$)	5.443688
S ($\varepsilon = \varepsilon_t$)	3.629125
LBE	3.5485[31]

TABLE 8

Density and temperature perturbations for the mixture Ne-Ar, $C = 0.3$, $a_{t1} = 0.31$, $a_{n1} = 0.10$, $a_{t2} = 0.67$, $a_{n2} = 0.40$, $\zeta = 5.609842$.

y	$N_1(y)$	$N_2(y)$	$T_1(y)$	$T_2(y)$
0.0	−6.094582	−5.020045	5.003068	3.628826
0.1	−6.093327	−5.196696	5.221407	4.100402
0.2	−6.114674	−5.343053	5.381062	4.408179
0.3	−6.147316	−5.482370	5.524230	4.664051
0.4	−6.187790	−5.617862	5.658380	4.889534
0.5	−6.234186	−5.750740	5.786684	5.094294
0.6	−6.285266	−5.881609	5.910838	5.283771
0.7	−6.340156	−6.010827	6.031871	5.461415
0.8	−6.398206	−6.138629	6.150460	5.629586
0.9	−6.458912	−6.265184	6.267077	5.789991
1.0	−6.521875	−6.390621	6.382064	5.943908
2.0	−7.225736	−7.600364	7.479400	7.273053
3.0	−7.990690	−8.758942	8.529533	8.421366
4.0	−8.775655	−9.889628	9.558614	9.498200
5.0	−9.567645	−1.100422(1)	1.057641(1)	1.054113(1)
6.0	−1.036200(1)	−1.210921(1)	1.158764(1)	1.156635(1)
7.0	−1.115696(1)	−1.320832(1)	1.259490(1)	1.258170(1)
8.0	−1.195190(1)	−1.430375(1)	1.359967(1)	1.359130(1)
9.0	−1.274662(1)	−1.539684(1)	1.460285(1)	1.459745(1)
10.0	−1.354108(1)	−1.648842(1)	1.560499(1)	1.560145(1)
20.0	−2.147838(1)	−2.738018(1)	2.560967(1)	2.560958(1)

TABLE 9

Density and temperature perturbations for the mixture Ne-Ar, $C = 0.8$, $a_{t1} = 0.31$, $a_{n1} = 0.10$, $a_{t2} = 0.67$, $a_{n2} = 0.40$, $\zeta = 8.594219$.

y	$N_1(y)$	$N_2(y)$	$T_1(y)$	$T_2(y)$
0.0	−8.750733	−7.120369	7.090958	5.242827
0.1	−8.783852	−7.506333	7.459928	6.084367
0.2	−8.835794	−7.786932	7.709797	6.587750
0.3	−8.897839	−8.033746	7.922874	6.982114
0.4	−8.966726	−8.260064	8.114582	7.312956
0.5	−9.040610	−8.471952	8.291754	7.600955
0.6	−9.118298	−8.672914	8.458194	7.857802
0.7	−9.198955	−8.865234	8.616298	8.090910
0.8	−9.281972	−9.050521	8.767701	8.305339
0.9	−9.366890	−9.229963	8.913578	8.504716
1.0	−9.453352	−9.404472	9.054812	8.691742
2.0	−1.036126(1)	−1.098707(1)	1.031358(1)	1.018410(1)
3.0	−1.129379(1)	−1.242872(1)	1.143514(1)	1.138000(1)
4.0	−1.222722(1)	−1.381496(1)	1.249962(1)	1.247343(1)
5.0	−1.315743(1)	−1.517507(1)	1.353609(1)	1.352266(1)
6.0	−1.408435(1)	−1.652151(1)	1.455762(1)	1.455032(1)
7.0	−1.500869(1)	−1.786030(1)	1.557073(1)	1.556658(1)
8.0	−1.593117(1)	−1.919461(1)	1.657891(1)	1.657646(1)
9.0	−1.685235(1)	−2.052622(1)	1.758410(1)	1.758262(1)
10.0	−1.777263(1)	−2.185615(1)	1.858746(1)	1.858654(1)
20.0	−2.695996(1)	−3.513052(1)	2.859404(1)	2.859402(1)

TABLE 10

Density and temperature perturbations for the mixture He-Xe, $C = 0.3$, $a_{t1} = 0.20$, $a_{n1} = 0.05$, $a_{t2} = 0.95$, $a_{n2} = 0.40$, $\zeta = 9.208216$.

y	$N_1(y)$	$N_2(y)$	$T_1(y)$	$T_2(y)$
0.0	−9.859661	−6.752228	8.842905	4.550386
0.1	−9.879711	−6.953128	9.108078	5.171764
0.2	−9.907475	−7.131582	9.294006	5.587051
0.3	−9.940046	−7.306519	9.454962	5.936198
0.4	−9.976171	−7.479783	9.601494	6.246081
0.5	−1.001510(1)	−7.651818	9.738338	6.528768
0.6	−1.005634(1)	−7.822732	9.868148	6.791054
0.7	−1.009952(1)	−7.992533	9.992600	7.037259
0.8	−1.014435(1)	−8.161199	1.011283(1)	7.270349
0.9	−1.019063(1)	−8.328707	1.022967(1)	7.492473
1.0	−1.023817(1)	−8.495034	1.034371(1)	7.705251
2.0	−1.075993(1)	−1.009326(1)	1.139936(1)	9.508343
3.0	−1.132934(1)	−1.158524(1)	1.239185(1)	1.099113(1)
4.0	−1.192301(1)	−1.299418(1)	1.336773(1)	1.231344(1)
5.0	−1.253117(1)	−1.434063(1)	1.434089(1)	1.353987(1)
6.0	−1.314884(1)	−1.564032(1)	1.531607(1)	1.470376(1)
7.0	−1.377312(1)	−1.690495(1)	1.629469(1)	1.582465(1)
8.0	−1.440213(1)	−1.814319(1)	1.727694(1)	1.691501(1)
9.0	−1.503463(1)	−1.936146(1)	1.826251(1)	1.798316(1)
10.0	−1.566972(1)	−2.056457(1)	1.925092(1)	1.903493(1)
20.0	−2.207846(1)	−3.225069(1)	2.921173(1)	2.919434(1)

TABLE 11

Density and temperature perturbations for the mixture He-Xe, $C = 0.8$, $a_{t1} = 0.20$, $a_{n1} = 0.05$, $a_{t2} = 0.95$, $a_{n2} = 0.40$, $\zeta = 16.699401$.

y	$N_1(y)$	$N_2(y)$	$T_1(y)$	$T_2(y)$
0.0	−1.683016(1)	−1.227521(1)	1.458384(1)	8.714419
0.1	−1.686467(1)	−1.286386(1)	1.500194(1)	9.979183
0.2	−1.690923(1)	−1.332670(1)	1.528673(1)	1.079195(1)
0.3	−1.696028(1)	−1.374765(1)	1.552854(1)	1.145073(1)
0.4	−1.701606(1)	−1.414201(1)	1.574502(1)	1.201558(1)
0.5	−1.707549(1)	−1.451664(1)	1.594411(1)	1.251425(1)
0.6	−1.713784(1)	−1.487549(1)	1.613030(1)	1.296271(1)
0.7	−1.720259(1)	−1.522113(1)	1.630641(1)	1.337133(1)
0.8	−1.726932(1)	−1.555540(1)	1.647441(1)	1.374735(1)
0.9	−1.733772(1)	−1.587970(1)	1.663570(1)	1.409609(1)
1.0	−1.740755(1)	−1.619513(1)	1.679132(1)	1.442160(1)
2.0	−1.815177(1)	−1.900579(1)	1.815832(1)	1.688453(1)
3.0	−1.893156(1)	−2.143660(1)	1.935084(1)	1.861137(1)
4.0	−1.972025(1)	−2.366427(1)	2.046522(1)	2.001624(1)
5.0	−2.050975(1)	−2.577354(1)	2.153768(1)	2.125641(1)
6.0	−2.129757(1)	−2.781055(1)	2.258546(1)	2.240502(1)
7.0	−2.208315(1)	−2.980205(1)	2.361789(1)	2.349988(1)
8.0	−2.286658(1)	−3.176423(1)	2.464036(1)	2.456193(1)
9.0	−2.364816(1)	−3.370713(1)	2.565619(1)	2.560336(1)
10.0	−2.442825(1)	−3.563718(1)	2.666750(1)	2.663148(1)
20.0	−3.219264(1)	−5.471661(1)	3.669732(1)	3.669609(1)

TABLE 12
The temperature-jump coefficient ζ for the mixture Ne-Ar with CL boundary condition.

C	case I	case II	case III
0.00	3.819923	4.165162	4.763477
0.10	4.026792	4.624545	4.884249
0.20	4.229354	5.105370	5.001942
0.30	4.427408	5.609842	5.116410
0.40	4.620807	6.140509	5.227559
0.50	4.809467	6.700354	5.335369
0.60	4.993409	7.292911	5.439917
0.70	5.172797	7.922448	5.541419
0.80	5.348012	8.594219	5.640298
0.90	5.519769	9.314559	5.737289
0.94	5.587756	9.560220	5.775806
1.00	5.689301	1.009305(1)	5.833604

TABLE 13
The temperature-jump coefficient ζ for the mixture He-Xe with CL boundary condition.

C	case IV	case V	case VI
0.00	2.699092	3.805644	2.694548
0.10	4.980593	5.930889	3.592355
0.20	6.918308	7.665855	4.242706
0.30	8.703196	9.208216	4.776130
0.40	1.043710(1)	1.066110(1)	5.253175
0.50	1.218908(1)	1.209149(1)	5.708463
0.60	1.401600(1)	1.355138(1)	6.165612
0.70	1.596817(1)	1.508366(1)	6.641839
0.80	1.806406(1)	1.669940(1)	7.139433
0.90	2.004926(1)	1.816252(1)	7.558874
0.94	2.041581(1)	1.835065(1)	7.560751
1.00	1.775163(1)	1.577430(1)	6.407679

TABLE 14
The temperature-jump coefficient ζ for the mixture He-Ar with CL boundary condition.

C	case VII	case VIII	case IX
0.00	3.819923	3.823209	4.763477
0.10	4.830295	4.049216	5.771355
0.20	5.902419	4.287304	6.829256
0.30	7.054171	4.539984	7.953144
0.40	8.305739	4.811649	1.031862(1)
0.50	9.680309	5.101938	1.047218(1)
0.60	1.120361(1)	5.418278	1.188326(1)
0.70	1.286814(1)	5.760482	1.348900(1)
0.80	1.476387(1)	6.118533	1.520249(1)
0.90	1.666506(1)	6.434606	1.690730(1)
0.94	1.731059(1)	6.503639	1.746042(1)
1.00	1.775163(1)	6.407678	1.775163(1)

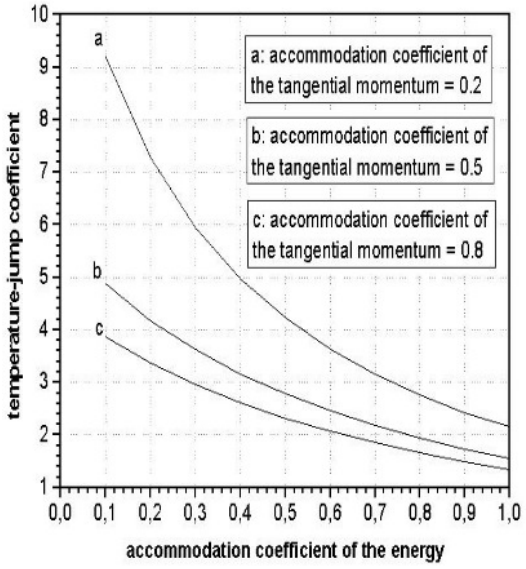

FIG. 1. *The temperature-jump coefficient: one gas case.*

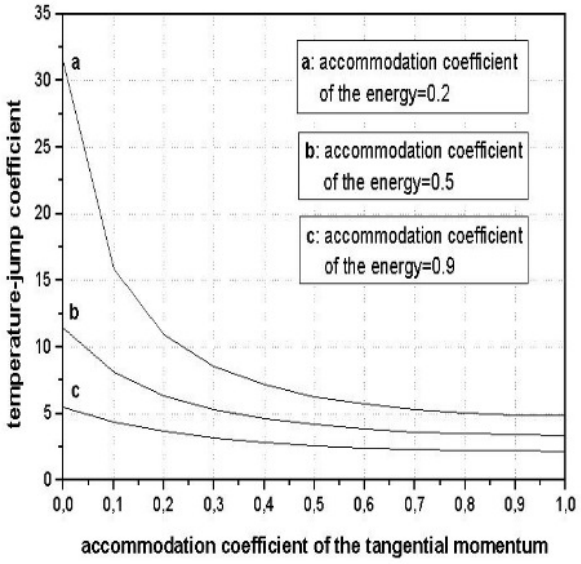

FIG. 2. *The temperature-jump coefficient: one gas case.*

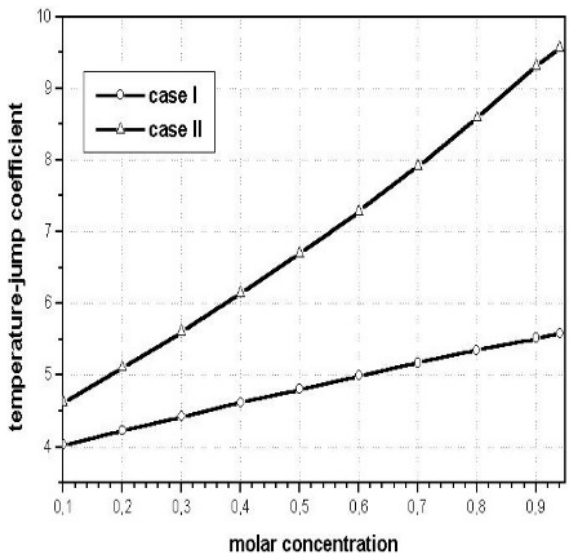

FIG. 3. *The temperature-jump coefficient: mixture Ne-Ar.*

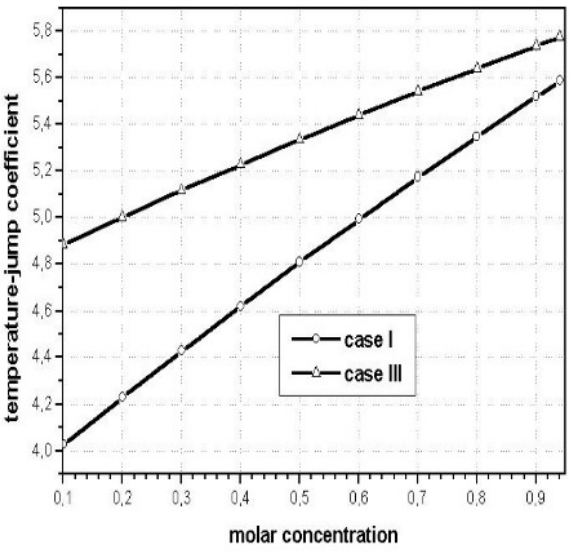

FIG. 4. *The temperature-jump coefficient: mixture Ne-Ar.*

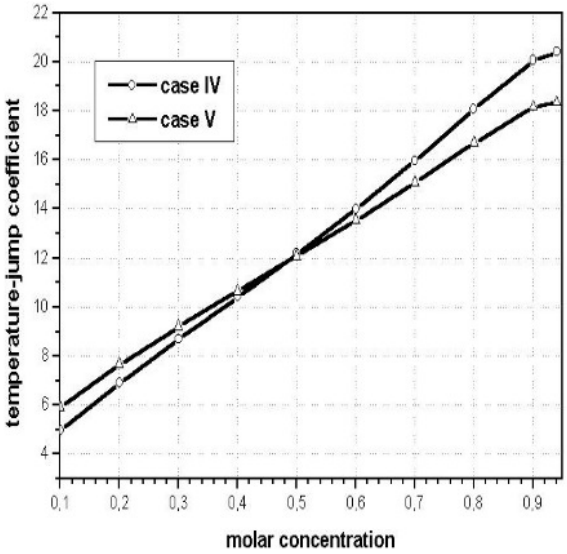

FIG. 5. *The temperature-jump coefficient: mixture He-Xe.*

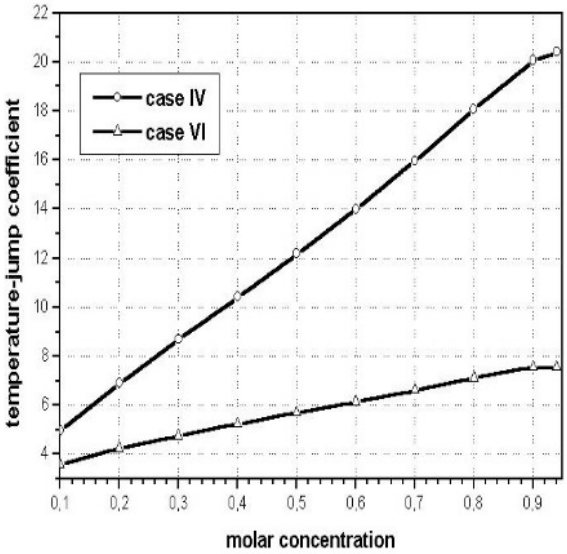

FIG. 6. *The temperature-jump coefficient: mixture He-Xe.*

9. Concluding comments. An analytical version of the discrete-ordinates method was used to develop a solution for the temperature-jump problem in rarefied gas dynamics, modeled by the S-model and the McCormack model, for the one gas and binary gas mixture cases, respectively. The gas-surface interaction was described by the Cercignani–Lampis boundary condition. The dependence of jump coefficient on both accommodation coefficients was shown, which points out the importance of special attention to the description of the gas-surface interaction. The evaluation of the jump coefficient for a binary mixture of gases shows more significant difference from the one gas case for a great mass ratio. Once more the discrete-ordinates solution was found to be very precise.

Appendix A. Basic definitions.

In (82),

$$\boldsymbol{K}_{1,1}^{(1)}(\mathbf{c}',\mathbf{c}) = 1 + \{2[1-\eta_{1,2}^{(1)}] - \eta_{1,2}^{(2)}(c'^2 - 5/2)\}\mathbf{c}'\cdot\mathbf{c}, \tag{A.1}$$

$$\boldsymbol{K}_{1,1}^{(2)}(\mathbf{c}',\mathbf{c}) = (2/3)[1-2r^*\eta_{1,2}^{(1)}](c'^2 - 3/2)(c^2 - 3/2), \tag{A.2}$$

$$\boldsymbol{K}_{1,1}^{(3)}(\mathbf{c}',\mathbf{c}) = 2\varpi_1[(\mathbf{c}'\cdot\mathbf{c})^2 - (1/3)c'^2c^2], \tag{A.3}$$

$$\boldsymbol{K}_{1,1}^{(4)}(\mathbf{c}',\mathbf{c}) = [(4/5)\beta_1(c'^2 - 5/2) - \eta_{1,2}^{(2)}](c^2 - 5/2)\mathbf{c}'\cdot\mathbf{c}, \tag{A.4}$$

$$\boldsymbol{K}_{2,1}^{(1)}(\mathbf{c}',\mathbf{c}) = r\{2\eta_{1,2}^{(1)} + \eta_{1,2}^{(2)}[r^2(c'^2 - 5/2) + c^2 - 5/2]\}\mathbf{c}'\cdot\mathbf{c}, \tag{A.5}$$

$$\boldsymbol{K}_{2,1}^{(2)}(\mathbf{c}',\mathbf{c}) = (4/3)r^*\eta_{1,2}^{(1)}(c'^2 - 3/2)(c^2 - 3/2), \tag{A.6}$$

$$\boldsymbol{K}_{2,1}^{(3)}(\mathbf{c}',\mathbf{c}) = 2\eta_{1,2}^{(4)}[(\mathbf{c}'\cdot\mathbf{c})^2 - (1/3)c'^2c^2], \tag{A.7}$$

$$\boldsymbol{K}_{2,1}^{(4)}(\mathbf{c}',\mathbf{c}) = (4/5)\eta_{1,2}^{(6)}(c'^2 - 5/2)(c^2 - 5/2)\mathbf{c}'\cdot\mathbf{c}, \tag{A.8}$$

$$\boldsymbol{K}_{2,2}^{(1)}(\mathbf{c}',\mathbf{c}) = 1 + \{2[1-\eta_{2,1}^{(1)}] - \eta_{2,1}^{(2)}(c'^2 - 5/2)\}\mathbf{c}'\cdot\mathbf{c}, \tag{A.9}$$

$$\boldsymbol{K}_{2,2}^{(2)}(\mathbf{c}',\mathbf{c}) = (2/3)[1-2s^*\eta_{2,1}^{(1)}](c'^2 - 3/2)(c^2 - 3/2), \tag{A.10}$$

$$\boldsymbol{K}_{2,2}^{(3)}(\mathbf{c}',\mathbf{c}) = 2\varpi_2[(\mathbf{c}'\cdot\mathbf{c})^2 - (1/3)c'^2c^2], \tag{A.11}$$

$$\boldsymbol{K}_{2,2}^{(4)}(\mathbf{c}',\mathbf{c}) = [(4/5)\beta_2(c'^2 - 5/2) - \eta_{2,1}^{(2)}](c^2 - 5/2)\mathbf{c}'\cdot\mathbf{c}, \tag{A.12}$$

$$\boldsymbol{K}_{1,2}^{(1)}(\mathbf{c}',\mathbf{c}) = s\{2\eta_{2,1}^{(1)} + \eta_{2,1}^{(2)}[s^2(c'^2 - 5/2) + c^2 - 5/2]\}\mathbf{c}'\cdot\mathbf{c}, \tag{A.13}$$

$$\boldsymbol{K}_{1,2}^{(2)}(\mathbf{c}',\mathbf{c}) = (4/3)s^*\eta_{2,1}^{(1)}({c'}^2 - 3/2)(c^2 - 3/2), \tag{A.14}$$

$$\boldsymbol{K}_{1,2}^{(3)}(\mathbf{c}',\mathbf{c}) = 2\eta_{2,1}^{(4)}[(\mathbf{c}'\cdot\mathbf{c})^2 - (1/3){c'}^2c^2] \tag{A.15}$$

and

$$\boldsymbol{K}_{1,2}^{(4)}(\mathbf{c}',\mathbf{c}) = (4/5)\eta_{2,1}^{(6)}({c'}^2 - 5/2)(c^2 - 5/2)\mathbf{c}'\cdot\mathbf{c}. \tag{A.16}$$

In the definitions above it is used that

$$r = (m_1/m_2)^{1/2} \quad \text{and} \quad s = (m_2/m_1)^{1/2} \tag{A.17}$$

and

$$r^* = \frac{r^2}{1+r^2} \quad \text{and} \quad s^* = \frac{s^2}{1+s^2}. \tag{A.18}$$

In addition,

$$\varpi_1 = 1 + \eta_{1,1}^{(4)} - \eta_{1,1}^{(3)} - \eta_{1,2}^{(3)}, \tag{A.19}$$

$$\varpi_2 = 1 + \eta_{2,2}^{(4)} - \eta_{2,2}^{(3)} - \eta_{2,1}^{(3)}, \tag{A.20}$$

$$\beta_1 = 1 + \eta_{1,1}^{(6)} - \eta_{1,1}^{(5)} - \eta_{1,2}^{(5)}, \tag{A.21}$$

$$\beta_2 = 1 + \eta_{2,2}^{(6)} - \eta_{2,2}^{(5)} - \eta_{2,1}^{(5)}, \tag{A.22}$$

with

$$\eta_{i,j}^{(k)} = \frac{\nu_{i,j}^{(k)}}{\gamma_i}. \tag{A.23}$$

Continuing, following McCormack and Siewert's works [16, 32], we write

$$\nu_{\alpha,\beta}^{(1)} = \frac{16}{3}\frac{m_{\alpha,\beta}}{m_\alpha}n_\beta\Omega_{\alpha,\beta}^{11}, \tag{A.24}$$

$$\nu_{\alpha,\beta}^{(2)} = \frac{64}{15}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^2 n_\beta\Big(\Omega_{\alpha,\beta}^{12} - \frac{5}{2}\Omega_{\alpha,\beta}^{11}\Big), \tag{A.25}$$

$$\nu_{\alpha,\beta}^{(3)} = \frac{16}{5}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^2\frac{m_\alpha}{m_\beta}n_\beta\Big(\frac{10}{3}\Omega_{\alpha,\beta}^{11} + \frac{m_\beta}{m_\alpha}\Omega_{\alpha,\beta}^{22}\Big), \tag{A.26}$$

$$\nu_{\alpha,\beta}^{(4)} = \frac{16}{5}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^2\frac{m_\alpha}{m_\beta}n_\beta\Big(\frac{10}{3}\Omega_{\alpha,\beta}^{11} - \Omega_{\alpha,\beta}^{22}\Big), \tag{A.27}$$

(A.28)
$$\nu^{(5)}_{\alpha,\beta} = \frac{64}{15}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^3 \frac{m_\alpha}{m_\beta} n_\beta \Big[\Omega^{22}_{\alpha,\beta} + \Big(\frac{15m_\alpha}{4m_\beta} + \frac{25m_\beta}{8m_\alpha}\Big)\Omega^{11}_{\alpha,\beta} - \Big(\frac{m_\beta}{2m_\alpha}\Big)\Big(5\Omega^{12}_{\alpha,\beta} - \Omega^{13}_{\alpha,\beta}\Big)\Big]$$

and

(A.29)
$$\nu^{(6)}_{\alpha,\beta} = \frac{64}{15}\Big(\frac{m_{\alpha,\beta}}{m_\alpha}\Big)^3 \Big(\frac{m_\alpha}{m_\beta}\Big)^{3/2} n_\beta \Big[-\Omega^{22}_{\alpha,\beta} + \frac{55}{8}\Omega^{11}_{\alpha,\beta} - \frac{5}{2}\Omega^{12}_{\alpha,\beta} + \frac{1}{2}\Omega^{13}_{\alpha,\beta}\Big].$$

Here

(A.30)
$$m_{\alpha,\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}.$$

Finally, the Ω functions are the Chapman–Cowling integrals [49, 50]

(A.31)
$$\Omega^{ij}_{\alpha,\beta} = \frac{(j+1)!}{8}\left[1 - \frac{1+(-1)^i}{2(i+1)}\right]\left(\frac{\pi kT}{2m_{\alpha,\beta}}\right)^{1/2}(d_\alpha + d_\beta)^2.$$

We note that here d_1 and d_2 are the diameters of the two types of particles and, as defined in the text, k is the Boltzmann constant and T_0 is a reference temperature.

Appendix B. The elements of the kernel.

We follow Siewert [32] and express the components of the matrix $\boldsymbol{K}_M(\xi',\xi)$ in (99) as

(B.1)
$$k_{1,1}(\xi',\xi) = 1 + f_{1,1}(\xi',\xi)\xi'\xi + (2/3)[1 - 2r^*\eta^{(1)}_{1,2} + 2\varpi_1]({\xi'}^2 - 1/2)(\xi^2 - 1/2),$$

(B.2)
$$k_{1,2}(\xi',\xi) = [(4/5)\beta_1(\xi^2 - 3/2) - \eta^{(2)}_{1,2}]\xi'\xi + (2/3)[1 - 2r^*\eta^{(1)}_{1,2} - \varpi_1](\xi^2 - 1/2),$$

(B.3)
$$k_{1,3}(\xi',\xi) = f_{1,3}(\xi',\xi)\xi'\xi + (4/3)[r^*\eta^{(1)}_{1,2} + \eta^{(4)}_{1,2}]({\xi'}^2 - 1/2)(\xi^2 - 1/2),$$

(B.4)
$$k_{1,4}(\xi',\xi) = [r^3\eta^{(2)}_{1,2} + (4/5)\eta^{(6)}_{1,2}(\xi^2 - 3/2)]\xi'\xi + (2/3)[2r^*\eta^{(1)}_{1,2} - \eta^{(4)}_{1,2}](\xi^2 - 1/2),$$

(B.5)
$$k_{2,1}(\xi',\xi) = [(4/5)\beta_1({\xi'}^2 - 3/2) - \eta^{(2)}_{1,2}]\xi'\xi + (2/3)[1 - 2r^*\eta^{(1)}_{1,2} - \varpi_1]({\xi'}^2 - 1/2),$$

(B.6)
$$k_{2,2}(\xi',\xi) = (2/3)[1 - 2r^*\eta^{(1)}_{1,2}] + (1/3)\varpi_1 + (4/5)\beta_1\xi'\xi,$$

(B.7)
$$k_{2,3}(\xi',\xi) = [r\eta^{(2)}_{1,2} + (4/5)\eta^{(6)}_{1,2}({\xi'}^2 - 3/2)]\xi'\xi + (2/3)[2r^*\eta^{(1)}_{1,2} - \eta^{(4)}_{1,2}]({\xi'}^2 - 1/2),$$

$$k_{2,4}(\xi',\xi) = (4/5)\eta_{1,2}^{(6)}\xi'\xi + (1/3)[4r^*\eta_{1,2}^{(1)} + \eta_{1,2}^{(4)}], \tag{B.8}$$

$$k_{3,1}(\xi',\xi) = f_{3,1}(\xi',\xi)\xi'\xi + (4/3)[s^*\eta_{2,1}^{(1)} + \eta_{2,1}^{(4)}](\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B.9}$$

$$k_{3,2}(\xi',\xi) = [s^3\eta_{2,1}^{(2)} + (4/5)\eta_{2,1}^{(6)}(\xi^2 - 3/2)]\xi'\xi + (2/3)[2s^*\eta_{2,1}^{(1)} - \eta_{2,1}^{(4)}](\xi^2 - 1/2), \tag{B.10}$$

$$k_{3,3}(\xi',\xi) = 1 + f_{3,3}(\xi',\xi)\xi'\xi + (2/3)[1 - 2s^*\eta_{2,1}^{(1)} + 2\varpi_2](\xi'^2 - 1/2)(\xi^2 - 1/2), \tag{B.11}$$

$$k_{3,4}(\xi',\xi) = [(4/5)\beta_2(\xi^2 - 3/2) - \eta_{2,1}^{(2)}]\xi'\xi + (2/3)[1 - 2s^*\eta_{2,1}^{(1)} - \varpi_2](\xi^2 - 1/2), \tag{B.12}$$

$$k_{4,1}(\xi',\xi) = [s\eta_{2,1}^{(2)} + (4/5)\eta_{2,1}^{(6)}(\xi'^2 - 3/2)]\xi'\xi + (2/3)[2s^*\eta_{2,1}^{(1)} - \eta_{2,1}^{(4)}](\xi'^2 - 1/2), \tag{B.13}$$

$$k_{4,2}(\xi',\xi) = (4/5)\eta_{2,1}^{(6)}\xi'\xi + (1/3)[4s^*\eta_{2,1}^{(1)} + \eta_{2,1}^{(4)}], \tag{B.14}$$

$$k_{4,3}(\xi',\xi) = [(4/5)\beta_2(\xi'^2 - 3/2) - \eta_{2,1}^{(2)}]\xi'\xi + (2/3)[1 - 2s^*\eta_{2,1}^{(1)} - \varpi_2](\xi'^2 - 1/2), \tag{B.15}$$

and

$$k_{4,4}(\xi',\xi) = (2/3)[1 - 2s^*\eta_{2,1}^{(1)}] + (1/3)\varpi_2 + (4/5)\beta_2\xi'\xi \tag{B.16}$$

with

$$f_{1,1}(\xi',\xi) = 2[1 - \eta_{1,2}^{(1)}] - \eta_{1,2}^{(2)}(\xi'^2 + \xi^2 - 3) + (4/5)\beta_1(\xi'^2 - 3/2)(\xi^2 - 3/2), \tag{B.17}$$

$$f_{3,3}(\xi',\xi) = 2[1 - \eta_{2,1}^{(1)}] - \eta_{2,1}^{(2)}(\xi'^2 + \xi^2 - 3) + (4/5)\beta_2(\xi'^2 - 3/2)(\xi^2 - 3/2), \tag{B.18}$$

$$\begin{aligned} f_{1,3}(\xi',\xi) = {} & 2r\eta_{1,2}^{(1)} + r\eta_{1,2}^{(2)}[r^2(\xi'^2 - 3/2) + \xi^2 - 3/2] \\ & + (4/5)\eta_{1,2}^{(6)}(\xi'^2 - 3/2)(\xi^2 - 3/2) \end{aligned} \tag{B.19}$$

$$\begin{aligned} f_{3,1}(\xi',\xi) = {} & 2s\eta_{2,1}^{(1)} + s\eta_{2,1}^{(2)}[s^2(\xi'^2 - 3/2) + \xi^2 - 3/2] \\ & + (4/5)\eta_{2,1}^{(6)}(\xi'^2 - 3/2)(\xi^2 - 3/2). \end{aligned} \tag{B.20}$$

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