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ON THE TEMPERATURE-JUMP PROBLEM IN RAREFIED GAS DYNAMICS

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Abstract. *Recent results on the temperature-jump problem in the rarefied gas dynamics field are presented. In particular, results obtained from different kinetic equations with two different types of surface-gas interaction law, are analyzed. Analytical and computational aspects on the discrete-ordinates method, used to develop the solution, are reported.*

keywords: *temperature-jump problem, rarefied gas dynamics, gas-surface interaction law*

1. Introduction

In analyzing the temperature distribution of a rarefied gas near to the gas-solid interface, a difference between the temperature of the gas near to the wall and the temperature of the wall is noted (Welander, 1954). This analysis, which can be also seen as the analysis of the heat exchange in the region, depending on the gas species, can be associated with the evaluation of the *temperature-jump coefficient* of the gas. Over the years, starting from a basic paper by Welander (Welander, 1954), a long list of papers on this subject can be referenced (Loyalka, 1989; Onishi, 1997; Barichello and Siewert, 2000; Williams, 2001; Barichello et al., 2002; Sharipov, 2003; Sharipov, 2004; Siewert, 2003a). Of course, in dealing with a gas of arbitrary rarefaction, a modeling based on the Boltzmann equation or kinetic (model) equations must be considered. Since the recent interest on the microsystems field renew the interest on the rarefied gas dynamics (RGD) theory, analytical, numerical and computational tools have been studied, and, investigations have been sought for improvements in regard to previous results. In particular, a recent analytical version of the discrete-ordinates method (Barichello and Siewert, 1999) has been used to solve a wide class of problems in the RGD field (Barichello et al., 2001; Barichello et al., 2002;Siewert, 2003b), including the temperature-jump problem (Barichello and Siewert, 2000; Barichello et al., 2002; Siewert, 2003a). This approach has been shown adequate to deal with several kinetic equations and the linearized Boltzmann equation (LBE), along with different types of gas-surface interaction laws. An advantage that has been noted in using this approach, is exactly the fact of looking the results of a wide class of models under the same basic methodology and having, then, good conditions for a more general analysis of modeling $\times$ accurate results $\times$ computational efforts, when trying to solve problems of practical interest.

In this work, in addition to show some recent results on the temperature-jump problem for different models, in order to analyse the dependence on the model equation as well the gas-surface interaction law, we present basic steps involved in applying the ADO (analytical discrete ordinates) methodology to solve the temperature-jump problem, using for this, the BGK model equation. In addition to the use a different approach regarding to the elementary functions in terms of which the general solution is written, differently of the previous paper on this subject (Barichello and Siewert, 2000), we present here results based on the use of the Cercignani-Lampis boundary condition.

2. General Formulation

We consider as a starting point, the kinetic equation written in terms of a perturbation $h(\tau, \mathbf{c})$, to the distribution function from the absolute Maxwellian, as

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

with

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

where σ_0 is the collision diameter of the gas particles (in the rigid-sphere approximation), n_0 is the (constant) density of gas particles and l is a mean-free-path, which, at this point, we leave arbitrary. Still, we note that, in Eq. (1), the three components (c_x, c_y, c_z) of the velocity vector (with magnitude c) are expressed in dimensionless units and we use the dimensionless spatial variable $y \geq 0$ to measure the distance from the wall.

2.1. The scattering kernel and the mean-free-path

In regard to the scattering kernel $\boldsymbol{K}(\mathbf{c}' : \mathbf{c})$, in order to represent all the cases we want to describe in this work, we write it, in a general form, as

$$\boldsymbol{K}(\mathbf{c}', \mathbf{c}) = \frac{1}{4\pi} \eta(c') \eta(c) \Big[\gamma_{01} + 3\gamma_{11} (\mathbf{c}' \cdot \mathbf{c}) + \gamma_{02} (c'^2 - \omega)(c^2 - \omega) \Big] + \beta \boldsymbol{M}(\mathbf{c}', \mathbf{c}), \tag{3}$$

where $\eta(c)$ is the collision frequency, and

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

Here

$$\gamma_{01} = \frac{1}{V_0}, \qquad \gamma_{11} = \frac{1}{V_2}, \qquad \gamma_{02} = \frac{V_0}{V_0 V_4 - V_2^2} \quad \text{and} \quad \omega = \frac{V_2}{V_0} \tag{5a,b,c,d}$$

and

$$V_n = \int_0^{\infty} \eta(c) c^n e^{-c^2} \mathrm{d}c. \tag{6}$$

In writing the scattering kernel as in Eq. (3), we can define three kinetic equations:

The CLF Model ($\beta = 0$)

The CLF model of Cercignani (Cercignani, 1966) and Loyalka and Ferziger (Loyalka and Ferziger, 1968) is a variable collision frequency model, obtained, from Eq. (3), for the case $\beta = 0$. Since, for this model, the collision frequency is arbitrary (Barichello and Siewert, 2003), we have studied variants of this model (Barichello et al., 2002; Camargo, 2003), defined by the *rigid-sphere case*, where

$$\eta(c) = \big(c + \frac{1}{2c}\big) \pi^{1/2} \mathrm{erf}(c) + \mathrm{e}^{-c^2} \tag{7}$$

and the *Williams model*

$$\eta(c) = c. \tag{8}$$

The BGK model ($\beta = 0$ and $\eta(c) = 1$)

The well known and commonly used BGK model (Bhatnagar et al., 1954), which is a constant collision frequency model, can be seen, in fact, as a particular case of the CLF model for what, the scattering kernel results as

$$\boldsymbol{K}(\mathbf{c}', \mathbf{c}) = 1 + 2\mathbf{c}' \cdot \mathbf{c} + (2/3)(c'^2 - 3/2)(c^2 - 3/2). \tag{9}$$

The S model ($\beta = 1$ and $\eta(c) = 1$)

For this constant collision frequency model (Sharipov and Seleznev, 1998), we consider Eq. (4) and write

$$\boldsymbol{K}(\mathbf{c}', \mathbf{c}) = 1 + 2\mathbf{c}' \cdot \mathbf{c} + (2/3)(c'^2 - 3/2)(c^2 - 3/2) + \boldsymbol{M}(\mathbf{c}', \mathbf{c}). \tag{10}$$

Having defined the three different kinetic equations we want to refer in this work, we note that we can evaluate the mean-free-path, based on viscosity (l_p) or thermal conductivity (l_t), via each one of those models (Barichello and Siewert, 2003). In consequence, we obtain, from Eq. (2), for the CLF model, rigid-sphere case,

$$\varepsilon_p = 0.2788040528277 \quad \text{and} \quad \varepsilon_t = 0.2753345876233, \tag{11a,b}$$

for the Williams model

$$\varepsilon_p = \frac{16}{15}\pi^{-1/2} \quad \text{and} \quad \varepsilon_t = \frac{6}{5}\pi^{-1/2}, \tag{12a,b}$$

for the BGK model

$$\varepsilon_p = 1 \quad \text{and} \quad \varepsilon_t = 1, \tag{13a,b}$$

and, for the S model

$$\varepsilon_p = 1 \quad \text{and} \quad \varepsilon_t = \frac{3}{2}. \tag{14a,b}$$

In evaluating the ratio $\varepsilon_p/\varepsilon_t$ one can see that while the CLF model (including the particular case of the BGK model) yields poor results for the Prandtl number, from the S model one obtains $2/3$.

2.2. The gas-surface interaction and the boundary-conditions

We supplement Eq. (1) with a boundary condition. In this work, we use, to describe the surface-gas interaction, two different boundary-conditions law. The classical *diffuse-specular* approach, where some fraction $(1 - \alpha)$ of the particles is reflected specularly and the remaining fraction α is reflected diffusely

$$h(0, c_x, c_y, c_z) = (1 - \alpha)h(0, c_x, -c_y, c_z) + \frac{2\alpha}{\pi}\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-c'^2} h(0, c_x', -c_y', c_z')c_y' \mathrm{d}c_x' \mathrm{d}c_z' \mathrm{d}c_y', \tag{15}$$

for $c_y \in (0, \infty)$ and all c_x e c_z. Here $\alpha \in (0, 1]$ is the accommodation coefficient.

As a second choice, to describe the interaction with the surface, we use the Cercignani-Lampis (Cercignani, 1988; Siewert, 2003a) boundary condition, which is defined in terms of two accommodation coefficients: $\alpha_t \in (0, 2]$ the tangential momentum accommodation coefficient and $\alpha_n \in (0, 1]$ the energy accommodation coefficient. Since α_t can be greater than unity, this type of law allow us to consider the back scattering, which can be useful for dealing with rough surfaces (Sharipov, 2003). Following this approach, Eq. (1) is supplemented by a boundary condition written as

$$h(0, c_x, c_y, c_z) = \int_{-\infty}^\infty \int_{-\infty}^\infty \int_0^\infty h(0, c_x', -c_y', c_z')R(\mathbf{c}' : \mathbf{c})dc_y' dc_x' dc_z' \tag{16}$$

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

$$R(c_x', c_y', c_z' : c_x, c_y, c_z) = \frac{2c_y'}{\pi(2 - \alpha_t)\alpha_t\alpha_n} T(c_x' : c_x)S(c_y' : c_y)T(c_z' : c_z), \tag{17}$$

$$T(x : y) = \exp\left[-\frac{[(1 - \alpha_t)y - x]^2}{\alpha_t(2 - \alpha_t)}\right], \tag{18}$$

$$S(x : y) = \widehat{I}_0\left[\frac{2(1 - \alpha_n)^{1/2}xy}{\alpha_n}\right]\exp\left[-\frac{[(1 - \alpha_n)^{1/2}y - x]^2}{\alpha_n}\right] \tag{19}$$

and, where, for computational convenience, we rewrite the modified Bessel function $I_0(z)$ as

$$\widehat{I}_0(z) = I_0(z)\mathrm{e}^{-z}. \tag{20}$$

In addition, since we are dealing with a half-space problem, we impose, in order to complete the definition of the temperature-jump problem, the Welander condition (Welander, 1954) on the temperature perturbation, at infinity, such that

$$\lim_{y\to\infty}\frac{\mathrm{d}}{\mathrm{d}y}T(y)=K, \tag{21}$$

where K is considered specified.

Once we have the problem defined by Eqs. (1), (15) or (16) and (21) we seek to compute some quantities, as, for example, the temperature and the density perturbations

$$T(y)=\frac{2}{3}\pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-c'^2}h(y,c_x,c_y,c_z)(\mathbf{c}^2-3/2)\mathrm{d}c_x\mathrm{d}c_y\mathrm{d}c_z \tag{22}$$

and

$$N(y)=\pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-c'^2}h(y,c_x,c_y,c_z)\mathrm{d}c_x\mathrm{d}c_y\mathrm{d}c_z. \tag{23}$$

3. A Reformulation

Looking back to Eqs. (22) and (23), we see that the quantities of interest are related to integrals of the distribution function h. Keeping that in mind and looking for simpler problems, more amenable to analytical procedures, we define

$$h_1(y,c_y)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi_1(c_x,c_z)h(y,c_x,c_y,c_z)\mathrm{d}c_x\mathrm{d}c_z \tag{24}$$

and

$$h_2(y,c_y)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi_2(c_x,c_z)h(y,c_x,c_y,c_z)\mathrm{d}c_x\mathrm{d}c_z \tag{25}$$

such that, if we multiply Eq. (1), firstly by (Barichello and Siewert, 2000)

$$\phi_1(c_x,c_z)=\frac{1}{\pi}e^{-({c_x}^2+{c_z}^2)} \tag{26}$$

and integrate over all c_x and c_z and next we repeat the procedure and multiply Eq. (1) by

$$\phi_2(c_x,c_z)=\frac{1}{\pi}({c_x}^2+{c_z}^2-1)e^{-({c_x}^2+{c_z}^2)} \tag{27}$$

and integrate over all c_x and c_z, we find we can write, for the BGK model ($\mathbf{K}$ defined in Eq. (9)), with $c_y=\xi$,

$$\xi\frac{\partial}{\partial y}\mathbf{H}(y,\xi)+\varepsilon\mathbf{H}(y,\xi)=\varepsilon\pi^{-1/2}\mathbf{Q}(\xi)\int_{-\infty}^{\infty}e^{-\xi'^2}\mathbf{Q}^T(\xi')\mathbf{H}(y,\xi')\mathrm{d}\xi', \tag{28}$$

for $y\in(0,\infty)$, $\xi\in(-\infty,\infty)$, where

$$\mathbf{H}(y,\xi)=\begin{bmatrix} h_1(y,\xi)\\ h_2(y,\xi)\end{bmatrix} \tag{29}$$

and

$$\mathbf{Q}(\xi)=\begin{bmatrix} (2/3)^{1/2}(\xi^2-1/2) & 1\\ (2/3)^{1/2} & 0\end{bmatrix}. \tag{30}$$

Following analogous procedure, to the one described above, with the boundary condition defined by Eq. (15) we obtain, for the Maxwell (diffuse-specular) boundary condition

$$\mathbf{H}(0,\xi)=(1-\alpha)\mathbf{H}(0,-\xi)+\mathbf{A}_*\int_{\mathbf{0}}^{\infty}\mathbf{e}^{-\xi'^2}\mathbf{H}(\mathbf{0},-\xi')\xi'\mathrm{d}\xi' \tag{31}$$

and, for the Cercignani-Lampis boundary condition defined by Eq. (16)

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

with

$$\mathbf{A}_* = \begin{bmatrix} 2\alpha & 0 \\ 0 & 0 \end{bmatrix}, \tag{33}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 0 & (1-\alpha_t)^2 \end{bmatrix} \tag{34}$$

and, for ξ, $\xi' \in (0,\infty)$,

$$f(\xi',\xi) = \frac{2\xi'}{\alpha_n}\exp\left[-\frac{[(1-\alpha_n)^{1/2}\xi-\xi']^2}{\alpha_n}\right]\widehat{I}_0\left[\frac{2(1-\alpha_n)^{1/2}\xi'\xi}{\alpha_n}\right]. \tag{35}$$

We then use the definitions of the components h_1 and h_2 to rewrite the quantities of interest, given by Eqs. (22) and (23) as

$$T(y) = \frac{2}{3}\pi^{-1/2}\int_{-\infty}^{\infty}\begin{bmatrix} \xi^2 - 1/2 \\ 1 \end{bmatrix}^T \mathbf{H}(y,\xi)e^{-\xi^2}\mathrm{d}\xi \tag{36}$$

and

$$N(y) = \pi^{-1/2}\begin{bmatrix} 1 \\ 0 \end{bmatrix}^T \int_{-\infty}^{\infty}\mathbf{H}(y,\xi)e^{-\xi^2}\mathrm{d}\xi. \tag{37}$$

Before proceeding the development of a solution for the **H** problem, we follow Siewert (Siewert, 2002) and note, as a special case regarding to the Cercignani-Lampis boundary conditions, that the cases $\alpha_n \to 0$ and $\alpha_n = 1$ lead, respectively, to specular and diffuse behavior, regarding to the boundary condition. However, it is not possible to obtain, from the Cercignani-Lampis boundary condition, as a particular case, the general diffuse-specular behavior.

4. A Discrete Ordinates Solution

To solve the vector problem **H** we develop a discrete ordinates solution, based on the ADO approach (Barichello and Siewert, 1999). Following previous work (Barichello and Siewert, 2000) and noting Eqs. (13), we define

$$\mathbf{G}(y,\xi) = \mathbf{Q}^{-1}(\xi)\mathbf{H}(y,\xi) \tag{38}$$

and

$$\mathbf{\Psi}(\xi) = \pi^{-1/2}\mathbf{Q}^T(\xi)\mathbf{Q}(\xi)e^{-\xi^2}, \tag{39}$$

where $\mathbf{Q}(\xi)$ is defined in Eq. (30), such that the problem given by Eq. (28) is rewritten, for $y \in (0,\infty)$ and $\xi \in (-\infty,\infty)$ as

$$\xi\frac{\partial}{\partial y}\mathbf{G}(y,\xi) + \mathbf{G}(y,\xi) = \int_{-\infty}^{\infty}\mathbf{\Psi}(\xi')\mathbf{G},(y,\xi')\mathrm{d}\xi' \tag{40}$$

the "so-called" G problem (Barichello and Siewert, 2000). Analogous transformation we apply to the boundary condition.

We write the discrete-ordinates version of Eq. (40)

$$\pm\xi_i\frac{d}{dy}\mathbf{G}(y,\pm\xi_i) + \mathbf{G}(y,\pm\xi_i) = \sum_{k=1}^{N}\omega_k\mathbf{\Psi}(\xi_k)[\mathbf{G}(y,\xi_k)+\mathbf{G}(y,-\xi_k)], \tag{41}$$

for $i = 1, 2, \ldots, N$. We note that, in writing Eqs. (41) we have used a "half-range" quadrature scheme with N nodes $\{\xi_k\}$ and weights $\{w_k\}$ defined in the interval $[0, \infty)$. Continuing to follow the usual procedure developed in earlier works, we seek for exponential solutions of Eqs. (41) and we find the general solution in a form

$$\mathbf{G}(y, \pm\xi_i) = \sum_{j=1}^{2N} [A_j \mathbf{\Phi}_{\pm}(\nu_j) e^{-y/\nu_j} + B_j \mathbf{\Phi}_{\mp}(\nu_j) e^{y/\nu_j}]. \quad (42a)$$

where $\mathbf{\Phi}_{\mp}(\nu_j)$ and ν_j are defined from the eigenvalue problem

$$(\mathbf{D} - 2\mathbf{W})\mathbf{U} = \lambda \mathbf{U} \quad (42b)$$

with $\lambda = (1/\nu^2)$ and

$$\mathbf{\Phi}_{\pm}(\nu_j) = \frac{1}{2\nu_j} \mathrm{diag}\Big\{(\nu_j \pm \xi_1)\mathbf{I}, (\nu_j \pm \xi_2)\mathbf{I}, \ldots, (\nu_j \pm \xi_N)\mathbf{I}\Big\} \mathbf{U}_j. \quad (42c)$$

Here, the block matrix

$$\mathbf{D} = \mathrm{diag}\Big\{(1/\xi_1)^2\mathbf{I}, (1/\xi_2)^2\mathbf{I}, ..., (1/\xi_N)^2\mathbf{I}\Big\}, \quad (42d)$$

where $\mathbf{I}$ is the 2×2 identity matrix and $\mathbf{W}$ is a $2N \times 2N$ matrix, where each $2 \times 2N$ submatrix is given by

$$\mathbf{R}_i = (1/\xi_i)^2 \Big[\omega_1 \mathbf{\Psi}(\xi_1) \quad \omega_2 \mathbf{\Psi}(\xi_2) \quad \ldots \quad \omega_N \mathbf{\Psi}(\xi_N)\Big], \quad (42e)$$

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

Since it is a conservative problem, we have to add a number of exact solutions, once some of the separation constants ν_j are unbounded. For this specific case we consider

$$\mathbf{F_1}(\xi) = (2/3)^{(1/2)} \begin{bmatrix} \xi_i^2 - 1/2 \\ 1 \end{bmatrix} \quad \text{and} \quad \mathbf{F}_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad (43a,b)$$

and going back to $\mathbf{H}(y, \xi)$ we write

$$\mathbf{H}(y, \pm\xi_i) = \Big[A_1 + B_1(y - \xi)\Big]\mathbf{F}_1(\xi) + \Big[A_2 + B_2(y - \xi)\Big]\mathbf{F}_2 + \mathbf{Q}(\xi_i) \sum_{j=3}^{2N} A_j \mathbf{\Phi}_{\pm}(\nu_j) e^{-y/\nu_j} \quad (44)$$

where, based on the expected behavior of the solution at infinity, we consider $B_j = 0$ for $j = 3, \cdots, 2N$. To have the solution completely established, we still have to determinate the other arbitrary constants. In this sense, from the Welander condition, given by Eq. (21), we obtain that $B_1 = K(3/2)^{1/2}$. On the other hand, since $\mathbf{F}_2$ satisfies the homogeneous version of the boundary conditions we follow previous works and use the normalization condition (Kriese et al., 1974; Onishi, 1997)

$$\lim_{y \to \infty} \big[N(y) + T(y)\big] = 0. \quad (45)$$

which give us that $A_2 = -(2/3)^{1/2} A_1$ and $B_2 = -(2/3)^{1/2} B_1$. In this way, we write our final solution as

$$\mathbf{H}(y, \pm\xi_i) = (2/3)^{1/2} A_1 \begin{bmatrix} \xi_i^2 - 3/2 \\ 1 \end{bmatrix} + (y \mp \xi_i) K \begin{bmatrix} \xi_i^2 - 3/2 \\ 1 \end{bmatrix} + \mathbf{Q}(\pm\xi_i) \sum_{j=3}^{2N} \Big[A_j \mathbf{\Phi}_{\pm}(\nu_j) e^{-y/\nu_j}\Big] \quad (46)$$

where the remaining $2N - 1$ unknowns are obtained (least squares) by using the $2N$ boundary conditions given by either Eq. (31) or (32).

Thus, the final expressions, considering $K = 1$, for the temperature perturbation is

$$T(y) = y + (2/3)^{1/2} A_1 + 2/3 \sum_{j=3}^{2N} A_j \; e^{-y/\nu_j} \Big[(2/3)^{1/2} M_1(\nu_j) + M_2(\nu_j)\Big], \quad (47)$$

with

$$M_1(\nu_j) = \pi^{-1/2} \sum_{k=1}^{N} \omega_k e^{-\xi_k{}^2} (\xi_k^4 - \xi_k^2 + 5/4)[\Phi(\nu_j, \xi) + \Phi(\nu_j, -\xi)], \quad (48)$$

where $\Phi(\nu_j, \pm\xi)$ are the components of the vectors defined in Eq. (42c) and

$$M_2(\nu_j) = \pi^{-1/2} \sum_{k=1}^{N} \omega_k e^{-\xi_k{}^2} (\xi_k^2 - 1/2)[\Phi(\nu_j, \xi) + \Phi(\nu_j, -\xi)]. \tag{49}$$

We also express the density perturbation as

$$N(y) = -y - (2/3)^{1/2} A_1 + \sum_{j=3}^{2N} A_j \; e^{-y/\nu_j} \left[(2/3)^{1/2} M_3(\nu_j) + M_4(\nu_j) \right], \tag{50}$$

with

$$M_3(\nu_j) = \pi^{-1/2} \sum_{k=1}^{N} \omega_k e^{-\xi_k{}^2} (\xi_k^2 - 1/2)[\Phi(\nu_j, \xi) + \Phi(\nu_j, -\xi)] \tag{51}$$

and

$$M_4(\nu_j) = \pi^{-1/2} \sum_{k=1}^{N} \omega_k e^{-\xi_k{}^2} [\Phi(\nu_j, \xi) + \Phi(\nu_j, -\xi)]. \tag{52}$$

The temperature-jump coefficient is written in terms of the asymptotic behavior

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

where

$$T_{asy}(y) = y + (2/3)^{1/2} A_1 \tag{54}$$

and

$$\zeta = \left(\frac{2}{3}\right)^{1/2} A_1. \tag{55}$$

5. Computational Aspects and Concluding Comments

The computational procedures, in order to implement the discrete-ordinates solution, has been widely described in a series of papers on these RGD problems based on the ADO approach (Barichello et al., 2001; Barichello and Siewert, 2000; Barichello et al., 2002) . We briefly repeat here, however, some basic steps. To evaluate Eqs. (47), (50) and (55), the first thing we have to do is to define a quadrature scheme. One of the very good aspects in regard to the ADO approach is the use of arbitrary quadrature schemes, which allow us to deal with class of problems using the same basic methodology. In general (Barichello et al., 2001; Barichello et al., 2002) the interval of interest is mapped to the interval $[0, 1]$ and then the Gauss-Legendre scheme is linearly mapped to this interval. As a second step the eigenvalue problem, given by Eq. (42b) is solved (using known libraries as LAPACK) and finally the linear system to define the arbitrary constants in the solution is solved. The discrete-ordinates solution based on this (ADO) approach has been shown to be easy to implement, fast, accurate and adequate to deal with a wide class of problems in RGD, in particular, the temperature-jump problem.

In regard to the results presented in Tables 1 to 4, and Figs. 1 and 2, we note, in agreement with previous papers, that the temperature-jump coefficient varies very slightly depending on the model to be used. In opposition, the accommodation coefficient is an important parameter to be taken into account in this analysis.

For an appropriate choice of the mean-free-path, both constant collision frequency models used here, the BGK and the S model, lead to the same jump coefficient and provide good approximations when compared with the LBE results. A slightly difference in regard to the temperature and density perturbations (Knackfuss and Barichello, 2004) is noted. However, in using the ADO approach to develop a solution for the derived **H** vector problem, based on the S model, more intensive analytical tools have to be used (Knackfuss and Barichello, 2004).

As extension of this work, the temperature-jump problem has been evaluated for mixtures of binary gases, including the analysis of the Cercignani-Lampis boundary conditions.

Table 1: The Temperature-Jump Coefficient, $\alpha = 0.5$, Diffuse-specular boundary conditions.

Model	ζ
BGK	3.629125[a,b]
Williams	3.435960[b]
Rigid-sphere	3.476180[b]
S ($\varepsilon = 1$)	5.44369[c]
S ($\varepsilon = 3/2$)	3.62912[c]
LBE	3.5485[d]

Ref[a]=(this work; LBB & CES,2000) Ref[b]=(MC, 2003)
Ref[c]=(RFK & LBB, 2004) Ref[d]=(CES, 2003a)

Table 2: The Temperature-Jump Coefficient, $\alpha_t = 0.5$, $\alpha_n = 0.5$ Cercignani-Lampis boundary conditions.

Model	ζ
BGK	2.78041[a]
S ($\varepsilon = 1$)	4.17061[b]
S ($\varepsilon = 3/2$)	2.78041[b]
S	4.170[c]
LBE	2.7282[d]

Ref[a]=(this work) Ref[b]=(RFK & LBB, 2004)
Ref[c]=(FS, 2003) Ref[d]=(CES, 2003b)

Table 3: BGK model, The Temperature- Jump Coefficient ζ, Cercignani-Lampis boundary conditions

α_t	$\alpha_n = 0.25$	$\alpha_n = 0.5$	$\alpha_n = 0.75$	$\alpha_n = 1$
0.25	5.7895	3.8418	2.7241	2.0055
0.5	3.8859	2.7804	2.0584	1.5566
0.75	3.2223	2.3660	1.7797	1.3598
1	3.0447	2.2509	1.7003	1.3027

Table 4: The temperature $T(y)$ and density $N(y)$ perturbations, BGK Model, Cercignani-Lampis boundary conditions, $\alpha_t = 0.5$, $N = 40$

y	$T(y)$ $\alpha_n = 0.5$	$N(y)$ $\alpha_n = 0.5$	$T(y)$ $\alpha_n = 1$	$N(y)$ $\alpha_n = 1$
0.0	2.10157	–2.56938	1.18961	–1.08900
0.1	2.34143	–2.71400	1.37629	–1.30803
0.2	2.51598	–2.83371	1.51921	–1.46634
0.3	2.67076	–2.94749	1.64968	–1.60728
0.4	2.81423	–3.05829	1.77328	–1.73864
0.5	2.95014	–3.16724	1.89241	–1.86377
0.6	3.08054	–3.27491	2.00837	–1.98451
0.7	3.20674	–3.38167	2.12194	–2.10196
0.8	3.32960	–3.48770	2.23367	–2.21686
0.9	3.44976	–3.59315	2.34391	–2.32975
1.0	3.56767	–3.69812	2.45293	–2.44099
2.0	4.67538	–4.73195	3.50592	–3.50413
3.0	5.72288	–5.75046	4.52874	–4.52919
4.0	6.74708	–6.76147	5.54032	–5.54115
5.0	7.76037	–7.76823	6.54671	–6.54745
6.0	8.76804	–8.77248	7.55042	–7.55099
7.0	9.77261	–9.77519	8.55266	–8.55307
8.0	10.7754	–10.7769	9.55404	–9.55433
9.0	11.7772	–11.7781	10.5549	–10.5551
10.0	12.7783	–12.7788	11.5555	–11.5556
20.0	22.7804	–22.7804	21.5565	–21.5566

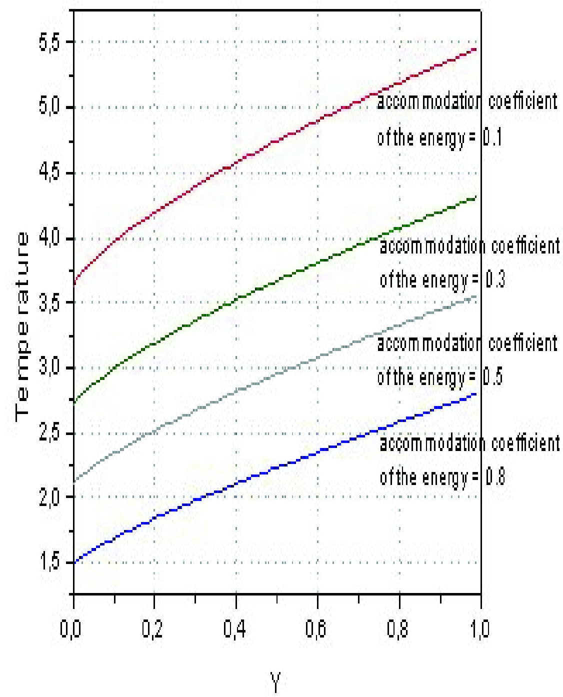

Figure 1: Temperature, $N = 40$ and $\alpha_t = 0.5$

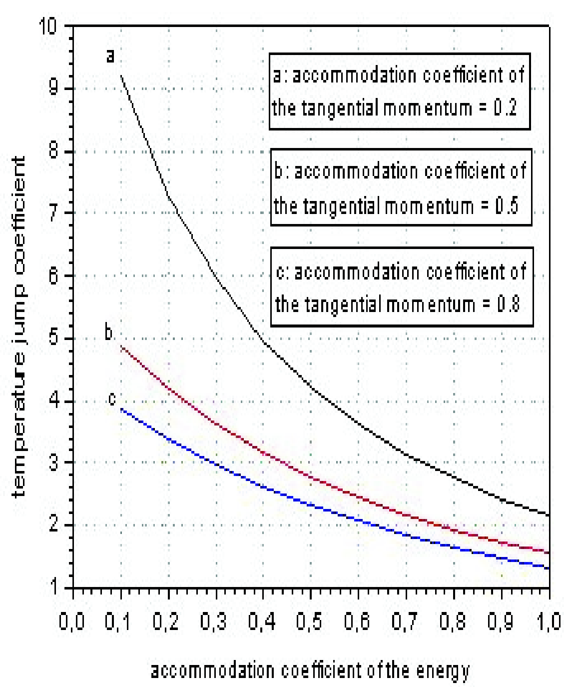

Figure 2: Temperature jump coefficient, $N = 40$

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7. References

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