Heat transfer in a gas mixture

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The problem of heat transfer and temperature distribution between two parallel plates with different temperatures is one of the classical problems in rarefied gas dynamics. The large number of theoretical and experimental works has been devoted to this problem both for a single gas and for a mixture. In this paper we study the problem of heat transfer and temperature distribution for a binary gas mixture on the basis of the complete kinetic Boltzmann equation with the following assumptions: the molecules are hard spheres and the interaction between two gas molecules is a completely elastic collision; the molecules of each component are reflected according to the diffusion reflection condition on the walls. The Boltzmann equation was solved by the stabilization method based on the splitting procedure - free molecular flow and collisional relaxation. For the first stage we use the divergence finite-difference scheme of the 2nd order. For the second stage we use the Euler's method, which provides the satisfaction of conservation laws at $\vec{x}$ node. For calculation of collision integrals we use the extension of the numerical kernel method [1], originally developed for a single gas, to the binary gas mixture and the case of cylindrical symmetry [2]. Here for the evaluation of collision integrals we use the modification of the algorithm, which includes "inverse collisions". The inclusion of the "inverse collisions" makes the method more economical and more precise for the calculation of weakly non-equilibrium flows. This projection method ensures the strict conservation of mass, momentum and energy. The conservativeness of the method is achieved by special projecting of integrand values, calculated at non-node points, to the nodes of the momentum grid closest to them.

The problem of heat transfer is solved for different values of *Kn*, various ratios of masses, number densities and diameters of the components. The heat flow of a mixture is investigated for different parameters and temperature jumps on the cold and hot walls are studied.

PROBLEM

Consider a rarefied mixture of two gases, say corresponding to i =1, 2, in the domain $0 < X = X_1 < D$ between two parallel plane walls at rest, where X_i is rectangular coordinate system in the space. Let the wall at X_1 =0 be kept at temperature T_1 and the other one at $X_1 = D$ at temperature T_2. Investigate the steady behavior of the mixture on the basis of kinetic theory under the assumptions: a) the molecules of each component are hard spheres and the interaction between two molecules is a perfectly elastic collision; b) the molecules of each component are reflected with the full diffusive condition on the walls.

BASIC EQUATION

The system of the Boltzmann equations in the momentum space for two gas components without internal degrees of freedom consisting of hard sphere molecules with the masses m_i and diameters d_i may be written in the form

$$\frac{\partial f_\mathrm{i}}{\partial t} + \frac{\vec{p}}{m_\mathrm{i}} \frac{\partial f_\mathrm{i}}{\partial \vec{x}} = -L_\mathrm{i} + G_\mathrm{i}, \qquad \mathrm{i} = 1, 2,$$

where f_i is the distribution function, which depends on the vector of momentum $\vec{\mathrm{p}}$, vector of configuration space $\vec{x}$ and time t. Here the "loss" term L_i and the 'gain' term G_i are defined as

$$L_\mathrm{i} = \sum_{\mathrm{j}=1}^{2} \int_{-\infty}^{+\infty} \int_0^{2\pi} \int_0^{\pi} f_\mathrm{i} f_\mathrm{j} \frac{1}{2} \left(\frac{d_\mathrm{i} + d_\mathrm{j}}{2} \right)^2 q_\mathrm{ji} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\varphi \, \mathrm{d}\vec{\mathrm{p}}_* ,$$

$$G_\mathrm{i} = \sum_{\mathrm{j}=1}^{2} \int_{-\infty}^{+\infty} \int_0^{2\pi} \int_0^{\pi} f_\mathrm{i}' f_\mathrm{j}' \frac{1}{2} \left(\frac{d_\mathrm{i} + d_\mathrm{j}}{2} \right)^2 q_\mathrm{ji} \sin\theta d\theta d\varphi d\vec{p}_* ,$$

$$q_\mathrm{ji} = \left| \left(\vec{g}_\mathrm{ji} \vec{n} \right) \right| .$$

In the kinetic momentum space we have the following equalities for vectors of the pre-collisional momenta $\vec{p}, \vec{p}_*$ and post-collisional momenta $\vec{p}', \vec{p}_*'$

$$\vec{p}' = \vec{p} + \frac{2m_i m_j}{(m_i + m_j)}(\vec{g}_{ji}\vec{n})\vec{n} \ , \quad \vec{p}_*' = \vec{p}_* - \frac{2m_i m_j}{(m_i + m_j)}(\vec{g}_{ji}\vec{n})\vec{n},$$

$$\vec{g}_{ji} = \frac{\vec{p}_*}{m_j} - \frac{\vec{p}}{m_i}, \qquad \vec{n} = \vec{n}(\cos\theta, \sin\theta\cos\varphi, \sin\theta\sin\varphi).$$

Here $\vec{n}$ is a unit vector directed along the interection line of molecules, $\vec{g}_{ji}$ is their relative velocity, θ, φ are collision angles.

The boundary conditions on the walls

$$f_i(\vec{p}, X) = n_{iw}\left(\frac{1}{2\pi k m_i T_w}\right)\exp\left(-\frac{\vec{p}^2}{2km_i T_w}\right), \quad \vec{p}^{\,2} = p^2 + \rho^2,$$

$$\text{X=0}, T_w = T_1, \ n_{iw} = -\sqrt{\frac{2\pi m_i}{kT_w}}\int\limits_{p<0} f_i \, p d\vec{p}\,, \quad \text{X=D}, \ T_w = T_2, \ n_{iw} = \sqrt{\frac{2\pi m_i}{kT_w}}\int\limits_{p>0} f_i \, p d\vec{p}.$$

The densities are found from the conditions of equality of the flows to the walls and from the walls.

If we rewrite the equation and the boundary condition in a dimensionless form, we find that the problem is characterized by the following five parameters $m_2/m_1, d_2/d_1, \ T_2/T_1, \ n_{av}^2/n_{av}^1$ and Kn. Here $n_{av}^i (i = 1, 2)$ is the average molecular number density of the ith component in the domain $0 < X_1 < D$, and $Kn = l_0/D$ is the Knudsen number, where $l_0 = [\sqrt{2}\pi(d_1)^2 n_{av}]^{-1}$ is the mean free path of molecules of the first component when it is in the equilibrium state at rest with the number density $n_{av} = n_{ev}^1 + n_{ev}^2$.

RESULTS OF ANALYSIS

The computations were carried out for $T_2/T_1 = 2$, (m_2/m_1 , d_2/d_1) = (0.25, 0.5) and (0.5, 1), n_{av}^2/n_{av}^1 =0.1, 1, 10, Kn = 0.1,1,10 and the single computation for $m_2/m_1 = 0.1, \ d_2/d_1 = 1$, n_{av}^2/n_{av}^1 =0.01 and Kn = 0.01. In the physical space we divided the interval $0 < X_1 < D$ into 100 uniform segments for Kn = 1, 10 and 100 non-uniform segments (of the minimum size $10^{-3}D$ at $X_1 = 0$, $X_1 = D$ and of the maximum size 0.0320 D in the middle) for Kn = 0.1. In the momentum space we use the uniform grid for parameters of the distribution functions.

We show profiles of the molecular number densities n^α of the ith component (i = 1, 2), profiles of the temperature *T* of the total mixture for Kn = 0.1, 1 and 10 and the velocity distribution functions f_1 and f_2 at two points near the walls for all the cases given above.

The interesting phenomenon is the jumps of the temperatures (both of the total one and of each component) on the cold and hot walls that depend on the rarefying parameter. These jumps are determined by temperatures T_1 and T_2 of the walls, temperatures of the gas near the cold and hot walls, $T(0)$, $T(1)$, and the temperature $T_\infty = \sqrt{T_1 T_2}$, which corresponds to the free-molecular regime. Thus, we use the formula

$$\alpha = -\frac{T(0) - T_1}{T_1 - T_\infty}, \ \beta = \frac{T(1) - T_2}{T_2 - T_\infty}.$$

We compare our results with the results of [3] concerning the maximum variation of the heat flow of the total mixture: $q_i = (q_1, 0, 0)$, $2q_1 = \int p\,|\vec{p}\,|^2 \left(\frac{F_1}{m_1^2} + \frac{F_2}{m_2^2}\right) d\vec{p}$. Note that in the present problem the flow velocity of each component vanishes identically and the heat flow q_1 is independent of X_1 because of the mass and energy conservation. The maximum variation of q_1 over $0 \le X_1 \le D$ relative to q_{1av}: $\Delta = \max |\, q_1 - q_{1av} \,| / q_{1av}$, which gives a good measure of accuracy of the computation, is shown in percentage. We have a good agreement of our results with the results of [3].

The computing time for one iteration step is 1.8 s, while for the whole problem it is 3 hours for *Kn* = 1.10 and 22 hours for *Kn* = 0.1.

The method for a mixture solves the problem with acceptable preciseness, small time of calculations and small computer memory. The computations have been made on PC with the processor AMD, the frequency 2200 mHz and the memory 1024 mb.

REFERENCES

[1] F.G. Tcheremiissine, Comput. Math. Appl., **35**, 215-221 (1998)
[2] A.A. Raines, Eur. J. Mech. B Fluids, **21**, 599-610 (2002)
[3] S. Kosuge, K. Aoki, S. Takata, Eur. J. Mech. B Fluids, **20**, 87-126 (2001)

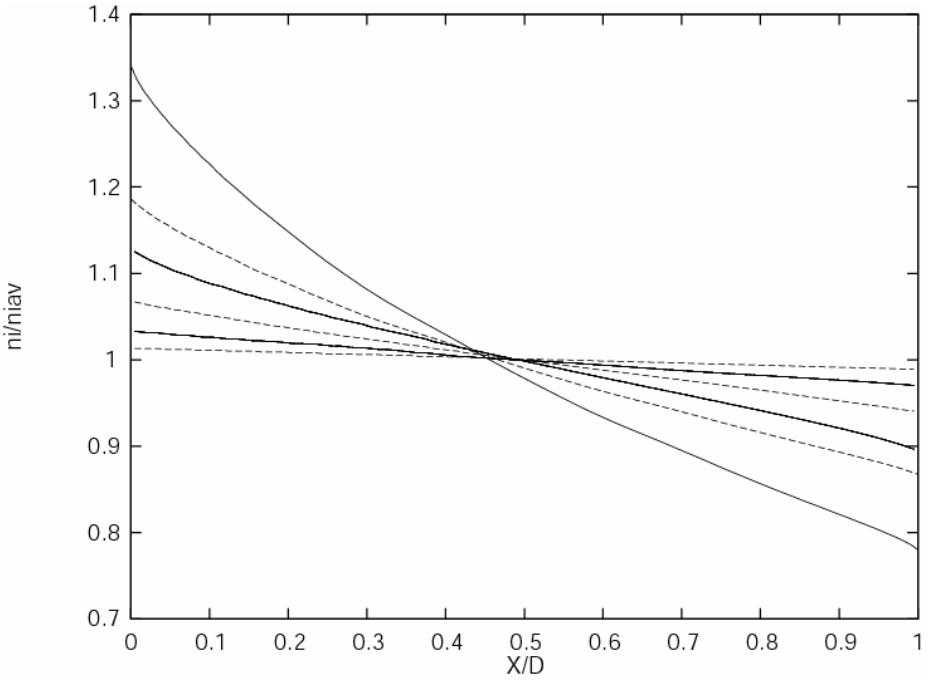

FIGURE 1. Profiles of number densities of the components n_1, n_2 for $n_2/n_1 = 0.1, m_2/m_1 = 0.25, d_2/d_1 = 0.5$. Here $n_i / n^i{}_{av}$ (i=1,2) along the y-axis. The density of the first component n_1 is upper then the density n_2 for the second component. In the direction from the left to the right before intersection:
the upper pair of the curves is for *Kn* = 0.1,
the next pair of the curves is for *Kn* = 1,
the last pair of the curves is for *Kn* = 10.
After the intersection the curves are in the reverse order.

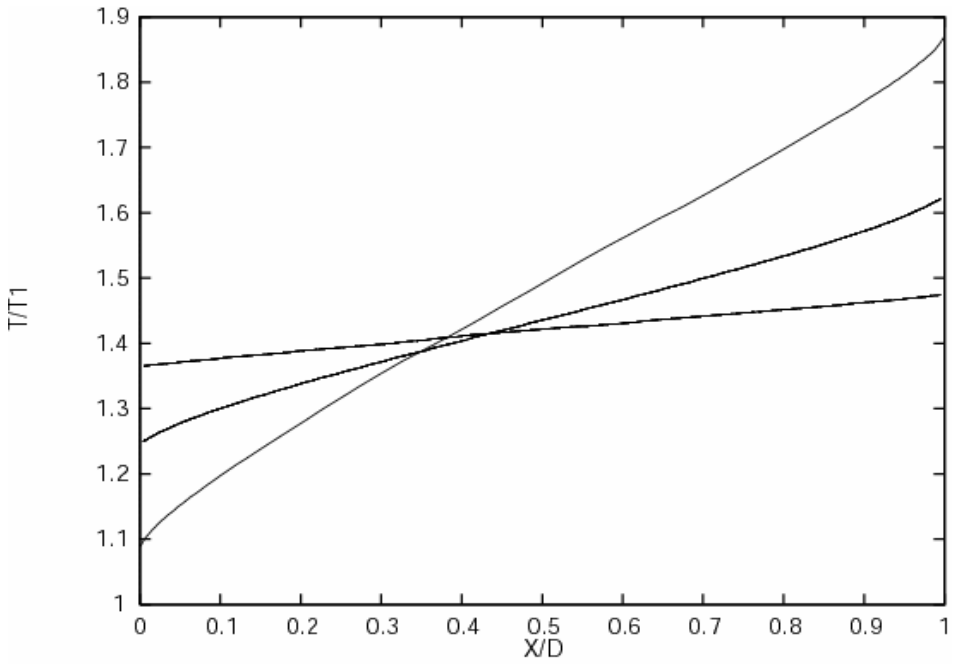

FIGURE 2. Temperature profiles of the total temperature T for $n_2 / n_1 = 0.1, m_2 / m_1 = 0.25, d_2 / d_1 = 0.5$.
In the direction from the left to the right before the intersection:
the upper curve is *Kn* = 10,
the next curve is *Kn* = 1,
the last curve is *Kn* = 0.1.
After the intersection the curves are in the reverse order.

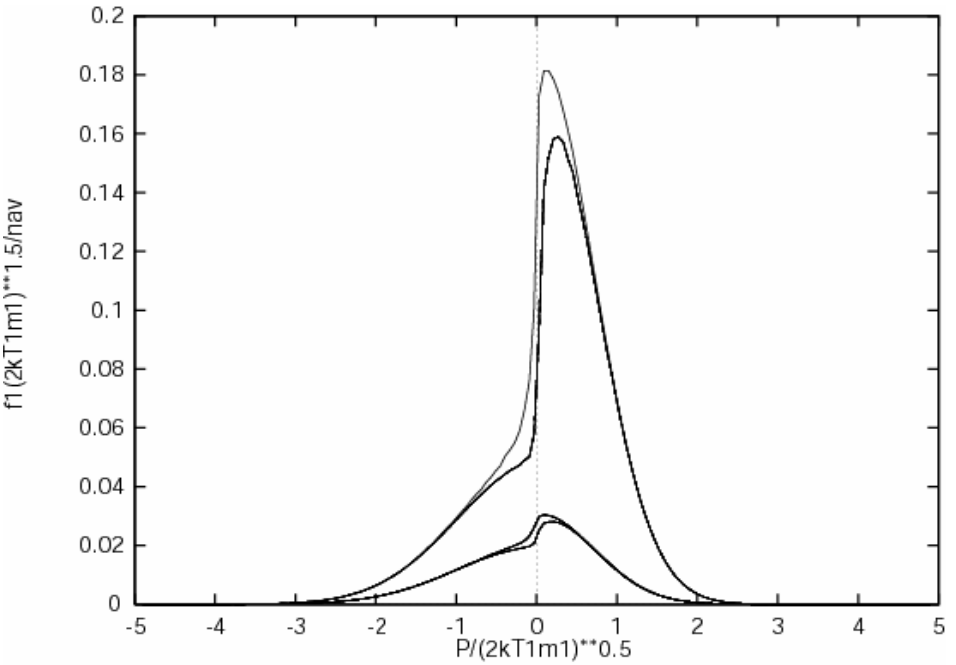

FIGURE 3. The profiles of distribution function of the first component in two points near the walls for $n_2 / n_1 = 0.1$, $m_2 / m_1 = 0.25$, $d_2 / d_1 = 0.5$, *Kn* = 10. In the direction from the top to the bottom:
the first curve is for $X / D = 0.095$, $\rho / \sqrt{2kt_1 m_1} = 0.15$; the second curve is for $X / D = 0.905$, $\rho / \sqrt{2kt_1 m_1} = 0.15$; the third curve is for $X / D = 0.095$, $\rho / \sqrt{2kt_1 m_1} = 1.35$;
the fourth curve is for $X / D = 0.905$, $\rho / \sqrt{2kt_1 m_1} = 1.35$.

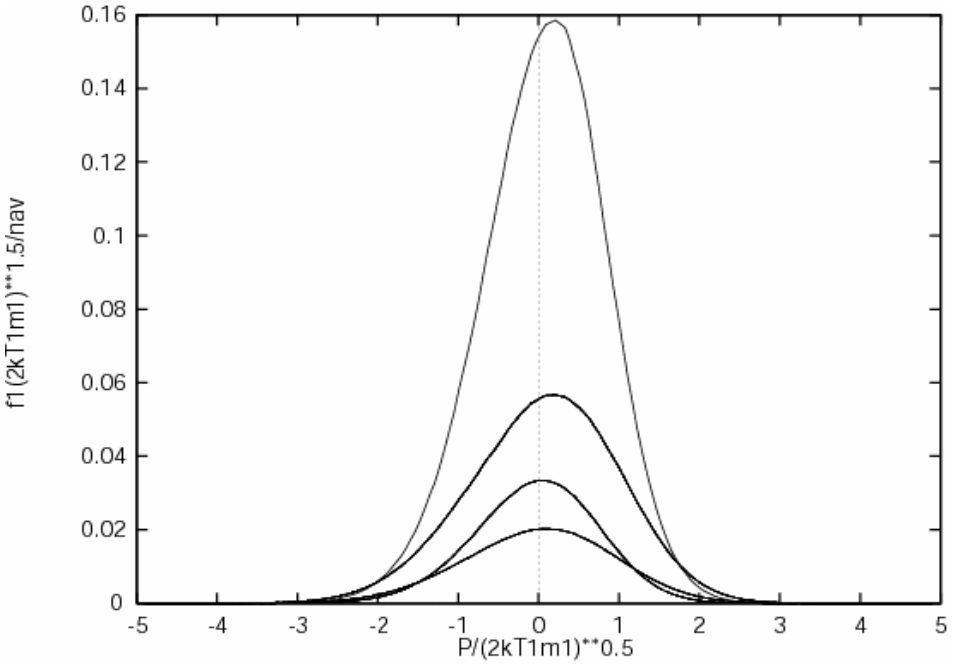

FIGURE 4. The profiles of distribution function of the first component in two points near the walls for $n_2 / n_1 = 0.1$, $m_2 / m_1 = 0.25$, $d_2 / d_1 = 0.5$, *Kn* = 0.1. In the direction from the top to the bottom:
the first curve is for $X / D = 0.091$, $\rho / \sqrt{2kt_1 m_1} = 0.15$; the second curve is for $X / D = 0.91$, $\rho / \sqrt{2kt_1 m_1} = 0.15$; the third curve is for $X / D = 0.091$, $\rho / \sqrt{2kt_1 m_1} = 1.35$;
the fourth curve is for $X / D = 0.91$, $\rho / \sqrt{2kt_1 m_1} = 1.35$.

n2/n1	Kn	m2/m1=0.5	d2/d1= 1	m2/m1=0.25	d2/d1=0.5
		$q_1 / \left(p_0 (2kT_1)^{1/2} \right)$	Δ%	$q_1 / \left(p_0 (2kT_1)^{1/2} \right)$	Δ%
0.1	1	-0.514 (-0.509)	0.11 (0.19)	-0.552 (-0.547)	0.12 (0.19)
0.1	10	-0.658 (-0.656)	0.023 (0.049)	-0.695 (-0.693)	0.019 (0.047)
1	1	-0.594 (-0.589)	0.14 (0.15)	-0.819 (-0.814)	0.064 (0.13)
1	10	-0.765 (-0.763)	0.023 (0.047)	-0.967 (-0.966)	0.013 (0.03)
10	1	-0.683 (-0.677)	0.055 (0.10)	-1.129 (-1.124)	0.041 (0.025)
10	10	-0.873 (-0.871)	0.035 (0.038)	-1.246 (-1.244)	0.0043 (0.014)
0.1	0.1	-0.188 (-0.184)	0.48 (0.45)	-0.211 (-0.207)	0.37 (0.72)
1	0.1	-0.213 (-0.209)	0.52 (0.34)	-0.375 (-0.370)	0.41 (0.67)
1 *	0.1	-0.213 (-0.209)	0.18 (0.34)		
10	0.1	-0.250 (-0.245)	0.48 (0.34)	-0.667 (-0.659)	0.29 (0.19)
10 *	0.1	-0.250 (-0.245)	0.21 (0.34)		

TABLE 1. Heat flow $q_1 = (q_1, 0, 0)$ of the total mixture for $T_2 / T_1 = 2$.
Here $p_0 = kn_{\text{av}} T_1$ is the reference pressure. In the parentheses the results from [3] are shown.
In [3] $dx_{\text{w}} = 10^{-6}$ near the walls. In this work $dx_{\text{w}} = 10^{-3}$. For the cases with asterisks we have a uniform grid with $dx = 10^{-3}$.