Numerical Solution Of One-Dimensional Problems In Binary Gas Mixture On The Basis Of The Boltzmann Equation

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Abstract. One-dimensional problems for a binary gas mixture are studied on the basis of numerical solution of the complete kinetic Boltzmann equation. The collision integral is evaluated by conservative discrete ordinate method.

DESCRIPTION OF THE METHOD AND THE BASIC EQUATIONS

Basic equations

In this paper we consider the problems for binary gas mixtures: shock wave structure and heat transfer between two parallel plates with diffusive reflection on the wall. Both of them are important and classical problems in rarefied gas dynamics and have been investigated experimentally [1, 2] and theoretically [3, 4, 5, 6, 7, 8, 9, 10, 11] by different methods.

For evaluation of the collision integral we apply a generalization of the conservative discrete ordinate method (the kernel method for a single gas was developed by Tcheremissine [12]) for binary gas mixtures and for the case of cylindrical symmetry [13]. This discrete ordinate method ensures 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. For the evaluation of collision integrals we use the algorithm which includes the “inverse collisions”.

The system of Boltzmann equations in the momentum space for two gas components consisting of hard sphere molecules with the masses $m_i$ and the diameters $d_i$ may be written as

$$\frac{\partial f_i}{\partial t} + \vec{p}_m \frac{\partial f_i}{\partial \vec{x}} = I_i = -L_i + G_i, \quad i = 1, 2$$

where $f_i$ is the distribution function which depends on the vector of momentum $\vec{p}_m$, the vector of configuration space $\vec{x}$ and the time $t$. Here the “loss” term $L_i$ and the “gain” term $G_i$ are defined as

$$L_i = \sum_{j=1}^{2} \int \int \int_{-\infty}^{+\infty} f_i f_j \frac{1}{2} \left( \frac{d_i + d_j}{2} \right)^2 q_{ji} \sin \theta d\theta d\phi d\vec{p}_s$$

$$G_i = \sum_{j=1}^{2} \int \int \int_{-\infty}^{+\infty} f_i f_j \frac{1}{2} \left( \frac{d_i + d_j}{2} \right)^2 q_{ji} \sin \theta d\theta d\phi d\vec{p}_s.$$  

In kinetic momentum space we have the following equalities for the vectors of momentum $\vec{p}, \vec{p}_s$ before the collision and $\vec{p}', \vec{p}_s'$ after the collision

$$\vec{p}' = \vec{p} + \frac{2m_i m_j}{(m_i + m_j)} \left( \vec{g}_{ji} \cdot \vec{n} \right) \vec{n}$$

$$\vec{p}_s' = \vec{p}_s - \frac{2m_i m_j}{(m_i + m_j)} \left( \vec{g}_{ji} \cdot \vec{n} \right) \vec{n}$$
Evaluating the integrals (6), (7), we exclude those values of variables \( \Phi \) taking for each node of the momentum grid will have two coordinates \( \vec{p}_0 \) and \( \vec{p}_1 \) in the configuration space \( \vec{x} \) and the time \( t \).

We introduce in the limited domain of the physical space a fixed grid \( \vec{x} \) and impose limits on the momentum variables in (1)–(3) by introducing a domain \( \Omega \) of the volume \( V \). In \( \Omega \) we construct a discrete grid containing \( N_0 \) equidistant points \( \vec{p}_\beta \) with the step \( h \).

The Boltzmann equation in a discrete form becomes

\[
\frac{\partial f_{i\beta}}{\partial t} + \frac{\vec{p}_\beta}{m_i} \frac{\partial f_{i\beta}}{\partial \vec{x}} = I_{i\beta} = -L_{i\beta} + G_{i\beta}. \tag{5}
\]

Equation (1) is solved by the splitting procedure. On each interval \( \Delta t \) we split the process into the two stages: free-molecular flow and collisional relaxation. For the first stage we have the divergence finite-difference scheme of the molecular flow and collisional relaxation. For the first stage we have the divergence finite-difference scheme of the configuration space is realized in a conservative way. For the second stage we apply the Euler’s method which provides the satisfaction of conservation laws in each \( x \) node. The steady problems were solved by the stabilization method based on the splitting procedure.

### Conservative discrete ordinate method

Let us consider the integral operator

\[
Q_i(\Phi) = \frac{1}{2} \int_{0}^{2\pi} \int_{\rho_0}^{\infty} \int_{\phi_0}^{\pi} \Phi f_i f_j \frac{1}{2} \left( \frac{d_j + d_i}{2} \right)^2 q_{ji} \sin \theta d\theta d\phi d\vec{p}_j d\vec{p}_i
\]

Taking for \( \Phi \) a three dimensional \( \delta \)-function, we reduce the integrals to the following form

\[
L_i(\vec{p}^*) = \frac{1}{2} Q_i(\delta(\vec{p}^* - \vec{p}_j) + \delta(\vec{p}^* - \vec{p}_i)) \tag{6}
\]

\[
G_i(\vec{p}^*) = \frac{1}{2} Q_i(\delta(\vec{p}^* - \vec{p}_j) + \delta(\vec{p}^* - \vec{p}_i)) \tag{7}
\]

Evaluating the integrals (6), (7), we exclude those values of variables \( \theta, \phi \) which remove the vectors \( \vec{p}_j, \vec{p}_i \) out of the domain \( \Omega \times \Omega \). For this purpose we multiply the integrand by the characteristic function \( \chi(\vec{p}_j, \vec{p}_i) \) where \( \chi = 1 \) if \( (\vec{p}_j, \vec{p}_i) \in \Omega \times \Omega \) and \( \chi = 0 \) if \( (\vec{p}_j, \vec{p}_i) \notin \Omega \times \Omega \).

While transforming the integral operator to cylindrical coordinates one should take into account the relations \( \vec{p} = \vec{p}(p, \rho, \gamma) \), \( d\vec{p} = \rho dp d\rho d\gamma \). The integral operator becomes

\[
Q_i(\Phi) = \frac{1}{2} \int_{0}^{2\pi} \int_{0}^{\pi} \Phi f_i f_j \frac{1}{2} \left( \frac{d_j + d_i}{2} \right)^2 q_{ji} \chi \sin \theta d\theta d\phi d\vec{p}_j d\vec{p}_i
\]

In cylindrical coordinates each node of the momentum grid will have two coordinates \( \vec{p}_\beta(p_\beta, \rho_\beta) \) with the step \((h, h)\). It is important to note that the method needs the same grid with a constant mesh in momentum space for all components of the mixture. At the same time the steps in each momentum coordinate could be different. We construct the cubature formula for the evaluation of the integral \( I_{i\beta} \) satisfying the conservation laws

\[
\sum_\beta \psi_\beta^i I_{i\beta} = 0, \quad \psi_\beta^i = \{1, \vec{p}_\beta, \vec{p}_\beta^2\}
\]
and also the condition

\[ I_{ij}(f_{iMB} \cdot f_{jMa}) = 0 \]

at each nod \( \vec{p}_{B} \) of the momentum grid. Here \( f_{iMB} \) is the Maxwellian distribution function at the nod \( \vec{p}_{B} \).

Introduce the uniform integration grid \( p_{\alpha}, p_{\beta}, p_{\rho} \) with \( N \) nodes in such a way that \( p_{\alpha}, p_{\beta}, p_{\rho} \) belong to the momentum grid while the angles are distributed uniformly in the corresponding intervals. The multiple integral is calculated as the 8-fold sum over all the nodes while the distribution functions do not depend on \( \gamma, \gamma_{v} \). One obtains the following result

\[ \tilde{L}_{i}(\vec{p}) = A \sum_{v=1}^{N} \sum_{j=1}^{2} J_{ij}^{\nu} \left( \delta(\vec{p} - \vec{p}_{\alpha}) + \delta(\vec{p} - \vec{p}_{\beta}) \right) \]

where

\[ J_{ij}^{\nu} = f_{i\alpha} f_{j\beta} \frac{1}{2} \left( \frac{d_{\alpha} + d_{\beta}}{2} \right) a_{ij\nu} \sin \theta_{\nu} \beta_{\alpha} \beta_{\beta} \]

and \( A = V^{2} \pi^{2}/N \).

The integral \( \tilde{L}_{i\beta} \) is calculated straightforwardly

\[ \tilde{L}_{i\beta} = B \sum_{v=1}^{N} \sum_{j=1}^{2} \left( J_{ij}^{\nu} + J_{ij}^{\nu' \nu} \right) \]

Here \( B = V^{2} \pi^{2}/(N_{v}/N_{\nu}) \), the primes and double primes mark the values \( J_{ij}^{\nu} \) with \( \alpha_{\nu} = \beta \) and \( \beta_{\nu} = \beta \), respectively.

It is not possible to use the same way for obtaining the values of \( G_{i\beta} \) because the singularities in the formula (9) do not coincide with the nodes of the momentum grid. The correct way of evaluating the values of \( G_{i\beta} \) is to decompose each term in the parentheses in (9) into \( \delta \)-functions which have singularities at discrete ordinate nodes. Here \( p_{\alpha_{\nu}} \) and \( \tilde{p}_{\beta_{\nu}} \) are the nodes nearest to \( \vec{p}_{\alpha_{\nu}} \) and \( \vec{p}_{\beta_{\nu}} \), respectively. We introduce the notation

\[ \tilde{\Delta}_{\alpha_{\nu}} = p_{\alpha_{\nu}} - \tilde{p}_{\alpha_{\nu}}, \tilde{\Delta}_{\beta_{\nu}} = \tilde{p}_{\beta_{\nu}} - \tilde{p}_{\beta_{\nu}} \]

From (4) we have

\[ \tilde{\Delta}_{\nu} = -\tilde{\Delta}_{\nu} \]

We denote \( \tilde{\Delta} = \tilde{\Delta}_{\nu}/h = (\Delta_{1}, \Delta_{2}), \tilde{\Delta} = \tilde{\Delta}_{\nu}/h = (\tilde{\Delta}_{1}, \tilde{\Delta}_{2}) \) where \( |\Delta_{k}| \leq 1/2 \) and \( |\tilde{\Delta}_{k}| \leq 1/2 \) for \( k = 1, 2 \). Let us introduce the vectors of displacements along the grid \( \vec{s}(\delta_{1}, \delta_{2}) \) and \( \vec{s}(\tilde{\delta}_{1}, \tilde{\delta}_{2}) \) where \( \delta_{k} = 0 \) or \( \delta_{k} = \text{sign}(\Delta_{k}) \), \( \tilde{\delta}_{k} = 0 \) or \( \tilde{\delta}_{k} = \text{sign}(\tilde{\Delta}_{k}) \) for \( k = 1, 2 \). Then the 2 sets of the 4 nodes surrounding the points \( p_{\alpha_{\nu}} \) and \( \tilde{p}_{\beta_{\nu}} \) can be presented as \( p_{\alpha_{\nu} + \vec{s}} \) and \( \tilde{p}_{\beta_{\nu} + \vec{\tilde{s}}} \). These nodes form two cells being their vertices. From (11) we have \( \vec{s} = -\vec{\tilde{s}} \). However, in cylindrical coordinates on the momentum grid we have only one equality for the first coordinates

\[ \tilde{\Delta}_{1} = -\Delta_{1} \implies \tilde{\delta}_{1} = -\delta_{1}. \]

We replace the expressions in parentheses in (9) by

\[ \delta(\tilde{p} - \tilde{p}_{\alpha_{\nu}}) + \delta(\tilde{p} - \tilde{p}_{\beta_{\nu}}) \]

\[ = \sum_{x} r_{x} \left( \delta(\tilde{p} - \tilde{p}_{\alpha_{\nu} + \vec{s}}) + \delta(\tilde{p} - \tilde{p}_{\beta_{\nu} + \vec{\tilde{s}}}) \right) \]

The coefficients \( r_{x} \) can be found from the conditions of conservation of density, kinetic momentum and energy in the decomposition (12) for a pair of above mentioned cells including their vertices. For economy of computations it would be preferable to have a decomposition with a minimum of terms. Such a solution exists and contains due to (11) only two non-zero coefficients: the first one \( (1 - r_{x}) \) corresponds to \( \vec{s} = 0, \vec{\tilde{s}} = 0 \) and the second one \( r_{x} \) corresponds to some \( \vec{s} = \vec{s} \neq 0, \vec{\tilde{s}} = \vec{\tilde{s}} \neq 0 \) and depends on a combination of parameters in the energy equation. Thus, the expansion
the concentration of the light component is large. One can see it more clearly when the shock wave is not weak and the light component reach their downstream uniform values earlier than for the heavy component. The temperature of masses $0$. The problem of the shock wave in a binary gas mixture was studied for the Mach numbers $1 \leq \alpha \leq 5$. The numerical density and flow velocity (momentum) for masses $0$ presented at this paper were obtained by modified algorithm. To the nodes $p_1$ and $p_2$ do not belong to the grid. According to the formula (10) this collision gives the contributions $\tilde{G}_{ij}^\nu$ to the integral $L_{ij}$ at the nodes $p_1$ and $p_2$. It would give the same contributions to the integral $G_{ij}$ at the points $p_1$ and $p_2$ only if they coincide with the nodes of the momentum grid. Since this condition is not satisfied, these contributions are distributed in the ratio $0 \leq (1 - r_\nu)/r_\nu \leq 1$ between the nodes $p_3$, $p_4$ nearest to $p_1$ and $p_2$ and another pair of nodes $p_5$, $p_6$ chosen from the vertices of the cells containing the points $p_1$, $p_2$. The nodes $p_3$, $p_4$, and $p_5$, $p_6$ do not belong to the grid only if they coincide with the nodes of the momentum grid. Since this condition is not satisfied, these contributions are distributed in the ratio $0 \leq (1 - r_\nu)/r_\nu \leq 1$ between the nodes $p_3$, $p_4$ nearest to $p_1$ and $p_2$ and another pair of nodes $p_5$, $p_6$ chosen from the vertices of the cells containing the points $p_1$, $p_2$. The nodes $p_3$, $p_4$, and $p_5$, $p_6$ do not belong to the grid only if they coincide with the nodes of the momentum grid. 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nodes and $\Delta t = 0.01$ (on the figures). For $Mach = 3$, $m_2/m_1 = 0.5$, $d_2/d_1 = 1$ and various concentrations we take the following values of the parameters: 11 858 nodes of the momentum grid (154 points for $p$ and 77 points for $\rho$) with the step $h = 0.1$, 90 nodes of the $x$-grid with the step $h_x = 0.2$, 198 000 integration nodes and $\Delta t = 0.01$ (on the figures). The period of stabilization of the solution is equal to $20\tau - 27\tau$. With this method we can obtain the results on rough grids (1 800 nodes of the momentum grid with the step $h = 0.26$, 90 nodes of the $x$-grid with the step $h_x = 0.2$, 66 000 integration nodes, $\Delta t = 0.01$) which coincide well with more detailed results. The computing time for one iteration step is 4.2 sec, for the whole problem — 2.7 hours.

Our results were compared with the results obtained in [5]. Figure 4 shows the profiles of macroscopic variables for the mixture. Here we observe a good agreement. In [5] the computing time for one iteration step in a parallel computation using ten CPU’s on Fujitsu VPP800 computer is 142 sec. for $M = 2$ and 99 sec. for $M = 3$. The computer memory for $M = 2$ is 1.7 GB, for $M = 3$ is 1.4 GB. In this work the computations were made on a personal computer with the processor Pentium 3 with the frequency 550 Mhz and the memory 128 Mb. The computing time for one iteration step for $M = 2$ is 36 sec., for the whole problem is 23 hours, computer memory is 8.5 Mb. The same data for $M = 3$ are 19.3 sec, 13 hours and 8.5 Mb respectively. One can see a good agreement between numerical results obtained in the present study and experiments [1] (Fig. 5, 6, 7).

The problem of the heat transfer between two parallel plates is studied for $m_2/m_1 = 0.5$, $d_2/d_1 = 1$, $T_{II}/T_I = 2$, $n_2av/n_1av = 1$ ($n_{iav}$ is the average molecular numerical density of $i$-component in the domain between two parallel plates, $0 < X < D$) and $Kn = 0.1$, $1$, $10$ (Fig. 8, Fig. 9).

This method for a mixture solves problems with acceptable preciseness, small time of calculations, small computer memory and with a good agreement with theoretical and experimental data of other authors.
FIGURE 3. Profiles of molecular number densities, flow velocities, and temperatures for \( M_- = 2, m_2/m_1 = 0.1, d_2/d_1 = 1, \) and \( \chi_{2-} = 0.5. \) See the caption on the Fig. 1.

FIGURE 4. Comparison with the results of Kosuge et. al. [5]: profiles of molecular number density, flow velocity and temperature for the mixture: \( M_- = 3, m_2/m_1 = 0.5, d_2/d_1 = 1, \) and \( \chi_{2-} = 0.9. \) The results obtained by the method of Kosuge et. al. are shown by the rhombuses (n), triangles (U), and squares (T). The results of the present method are shown by +, ×, and * respectively.

FIGURE 5. Profiles of parallel and radial temperatures for argon for \( M_- = 1.58, m_2/m_1 = 0.1, d_2/d_1 = 0.593, \) and \( \chi_{2-} = 0.9. \) The results obtained by Harnett and Muntz are shown by squares \( (T_\parallel) \), and rhombuses \( (T_\perp) \). The results of the present method are shown by × and + respectively.
FIGURE 6. Profiles of parallel and radial temperatures for helium with the same parameters and notation as in Fig. 5.

FIGURE 7. Profiles of total temperature for argon and helium for \( M_- = 1.58, m_2/m_1 = 0.1, d_2/d_1 = 0.593, \) and \( \chi_2- = 0.9 \). The results obtained by Harnett and Muntz are shown by squares \((T_{\text{argon}})\), and rhombuses \((T_{\text{helium}})\). The results of the present method are shown by + and \( \times \) respectively.

FIGURE 8. Profiles of number densities \( n_1 \) and \( n_2 \) for \( Kn = 0.1, 1, \) and 10; \( m_2/m_1 = 0.5, d_2/d_1 = 1, T_{II}/T_I = 2, n_{2av}/n_{1av} = 1 \). \( n_{iav} \) is the averaged molecular number density of the \( i \)-component in the domain \( 0 < X < D \). Here for \( Kn = 0.1: n_1 — \text{rhombuses}, n_2 — \times \); for \( Kn = 1: n_1 — \text{squares}, n_2 — \times \); for \( Kn = 10: n_1 — \text{triangles}, n_2 — + \).
FIGURE 9. Profiles of the total temperature for the mixture. Here for $Kn = 0.1$ — rhombuses, for $Kn = 1$ — +, for $Kn = 10$ — squares.

REFERENCES