Numerical Solution of Non-equilibrium Hypersonic Flows of Diatomic Gases Using the Generalized Boltzmann Equation

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Abstract: - The paper describes the methodology for computing hypersonic non-equilibrium shock wave flows of diatomic gases using the Generalized Boltzmann Equation (GBE) including both the vibrational - translational (VT) and rotational - translational (RT) relaxations. For the VT relaxation, GBE is always solved. For the RT relaxation, two approaches are employed. In the first approach, for the RT relaxation GBE is solved. This approach is computationally very intensive since it requires solving the complete GBE for both vibrational and rotational degrees of freedom. In the second approach, a two-level BGK type model of RT relaxation is employed. The second approach is much more efficient than the first (about 20 times faster). The paper describes the two-level RT relaxation model. The model is validated by computing the shock structure at high Mach numbers by comparing the results with the complete GBE solution. Computations are then performed for the shock structure accounting for both the vibrational and rotational excitations, using the second approach for the RT relaxations.

Key-Words: - Wang-Chang Uhlenbeck Equation, Hypersonic Flows, Rotational and Vibrational Relaxations

1 Introduction
For calculating the non-equilibrium flow of diatomic gases, currently DSMC method is the most widely used technique. In DSMC approach, one usually employs some empirical models [1], which very much resemble a BGK type relaxation model. In this paper, we describe a computational methodology for computing hypersonic non-equilibrium shock wave (SW) flows of diatomic gases such as Nitrogen and Oxygen using the Generalized Boltzmann Equation (GBE). In the GBE (similar to Wang-Chang Uhlenbeck equation (WC-UE) [2]), the internal and translational degrees of freedom are considered in the framework of quantum and classical mechanics respectively. The GBE [3] can be considered as a more general form of WC-UE and is also applicable when the energy levels are degenerated. The computational framework available for the classical Boltzmann equation is extended by including both the rotational and vibrational degrees of freedom in the GBE [4]. The whole problem that includes both the vibrational - translational (VT) and rotational - translational (RT) energy transfers is solved by applying a three-stage splitting procedure to the GBE. The three stages consist of free molecular transport, VT relaxation, and RT relaxation. For the VT relaxation, GBE is always solved. For the RT relaxation, two approaches are employed. In the first approach, for the RT relaxation GBE is solved. This approach is computationally very intensive since it requires solving the complete GBE for both vibrational and rotational degrees of freedom. In the second approach, a two-level BGK type model of RT relaxation that equilibrates rotational and translational energies is employed. The second approach is computationally less intensive than the first and therefore is much more efficient (about 20 times faster than the first approach). The paper describes the two-level RT relaxation model with a single relaxation time. The model is validated by computing the shock structure at high Mach numbers by comparing the results with the complete GBE solution for RT relaxations. Computations are then performed for the shock structure accounting for both the vibrational and rotational excitations; the second approach is employed for computing the RT relaxations.

2 Technical Approach
The shock wave structure in diatomic gases is studied using the GBE [5] that replaces the classical Wang Chang –Uhlenbeck Equation (WC-UE) for the case when energy levels are degenerated. In its mathematical form, the GBE is close to the WC-UE and differs from the later by a factor related to the
statistical weights of the levels. It should be noted that the GBE gives the equilibrium spectrum different from WC-UE. The GBE has the form:

\[
\frac{\partial f_i}{\partial t} + \xi \frac{\partial f_i}{\partial x} = R_i
\]  

(1)

The collision operator is given by:

\[
R_i = \sum_{jkl} \int \int \int (f_k f_l) \omega_{ij} - f_i f_j) P_{ij}^{kl} g b d b d \Phi d \xi
\]  

(2)

Here \( f_i \) is the distribution function for the energy level \( i \), \( P_{ij}^{kl} \) is the probability of the transfer from levels \( i, j \) to the levels \( k, l \), and the factor \( \omega_{ij} = (q_i q_j) / (q_i q_j) \); \( q_i \) being the energy level degeneration. For simple levels, the GBE changes to the WC-UE, therefore it can also be considered as a more general form of the later one. In [3], the GBE equation was obtained directly from WC-UE by grouping the \( q_i \) single levels that have the same energy and form a degenerated level. We consider molecular Nitrogen having the Lennard-Jones potential (6, 12) with the depth of the energy hole \( \varepsilon = 91K \), degeneration of rotational level \( q_i = 2i + 1 \), \( i = 0, 1, \ldots, \infty \), and the rotational energy of the level \( \varepsilon_i = \varepsilon_{ij}(i+1) \), \( \varepsilon_0 = 2.9K \). The molecular interaction during the collision consists of two phases. In the first phase, the molecules interact in an elastic manner according to the molecular potential. This stage determines the deviation angle of the relative velocity. In the second stage, the modulus of the relative velocity changes according to the energy conservation equation. For the transition probabilities \( P_{ij}^{kl} \) we apply the formulae given in [3] that are obtained by fitting the experimental data of molecular dynamics simulations of interactions of rigid rotors that model \( N_2 \) molecules.

\[
P_{ij}^{kl} = P_0 \omega_{ij}^k [\alpha_0 \exp(-\Delta_1 - \Delta_2 - \Delta_3 - \Delta_4) + \frac{1}{\alpha_0} \exp(-\Delta_1 - \Delta_4)]
\]

where

\[
\Delta_1 = |\Delta e_1 + \Delta e_2 | / e_{r0} , \quad \Delta_2 = 2 |\Delta e_2 - \Delta e_1 | / e_{rot} \\
\Delta_3 = 4 |\Delta e_1 | / (e_{r0} + e_{ri}) , \quad \Delta_4 = 4 |\Delta e_2 | / (e_{r0} + e_{rj})
\]

\[
\Delta e_1 = e_{ri} - e_{rk} , \quad \Delta e_2 = e_{rj} - e_{ri} , \quad \alpha_0 = 0.4 e_{rot} / e_{r0}
\]

The energy conservation law in a collision selects virtual collisions with non zero probability. From the equation

\[
m g^2 / 4 + e_{ri} + e_j = m g^2 / 4 + e_{rk} + e_{rj}
\]

it can be shown that \( P_{ij}^{kl} > 0 \), if \( q_i \geq 0 \), otherwise \( P_{ij}^{kl} = 0 \).

The elastic collision is a particular case of the collision. The probabilities obey the normalization condition: \( \sum_{i,j} P_{ij}^{kl} = 1 \). The kinetic equation (1) is solved by the splitting scheme. At a time step \( \tau < \tau_0 \), where \( \tau_0 \) is a mean inter-collision time, the equation (1) is replaced by the sequence of equations:

(a) \( \frac{\partial f_i}{\partial t} + \xi \frac{\partial f_i}{\partial x} = 0 \)

(b) \( \frac{\partial f_i}{\partial t} = R_i \)

The collision operator \( R_i \) is evaluated at the uniform grid \( S_0 \) in the velocity space by the conservative projection method proposed in [4].

3 Two-Level Kinetic Model for RT Relaxation in a Gas

The proposed model equation is aimed at simplifying the simulation of the rotational-translational (RT) energy exchange in a gas. Such simplification is highly needed for complex processes in which rotational excitation is accompanied by the vibration - translational (VT) energy transfer. The model consists of 2 levels: the ground level with the rotational energy \( \varepsilon_1 = 0 \) and the excited level with some energy \( \varepsilon_2 > T_{\text{max}} \), where \( T_{\text{max}} \) is the maximum temperature in the problem under consideration. We call the proposed model as “2LRT” model. The distribution function is also composed of two parts, \( f_1 \) and \( f_2 \) with corresponding populations of the levels \( n_1 \) and \( n_2 \).

The gas density is \( n = n_1 + n_2 \) and the rotational energy is \( E_{rot} = \varepsilon_2 n_2 \). Let the density of the gas at some point be \( n \), the kinetic energy \( E_{\text{kin}} \), and the rotational energy \( E_{\text{rot}} \). One can then determine the
populations of the levels by the simple formulas \( n_2 = \frac{E_{rot}}{e_2} \) and \( n_1 = n - n_2 \). Maximal value of \( E_{rot} \) is given by \( E_{rot} = nT_{max} \), therefore \( n_2 < nT_{max} / e_2 \), and one obtains \( 0 < n_2 < n \) and \( n_1 > 0 \). Having \( E_{kin} \), one can determine the equilibrium temperature, \( T_{eq} = \frac{2(E_{kin} + E_{rot})}{5n} \) and the equilibrium rotational populations \( n_{2eq} < nT_{eq} / e_2 \), \( n_{eq} = n - n_{2eq} \). These parameters determine the equilibrium distribution functions \( f_{1eq} \) and \( f_{2eq} \). For construction of the model equation we begin with the Wang Chang–Uhlenbeck equation (WC-UE) for the considered 2 levels system \((i, j, k) = 1, 2\).

\[
\frac{\partial f_{ij}}{\partial t} = \sum_{k,l} \int p_{ik,j}^{kl}(f_{ik,j} - f_i f_j) g_{i,j} bdbdqd\xi_j \tag{3}
\]

In equation (3), we replace the collision operator by an elastic collision operator \( Q_{el} \) and the non-elastic operator \( Q_r \). This replacement can not be strictly justified, as it is assumed in [5], because for RT exchange the purely elastic collisions present an exception, and about all the collisions are accompanied with the transfer of relatively small part of kinetic energy to/from the rotational energy. On the other hand, because of small inelasticity of interactions the main collision relaxation process is close to the case of elastic collisions, except that one should take into account the inelastic transfer of the energy. The elastic operator is the same as the Boltzmann collision integral for a two-component gas mixture:

\[
Q_{el} = \sum_j \int (f_{i}^* f_{j} - f_i f_j) g_{i,j} bdbdqd\xi_j \tag{4}
\]

The non-elastic operator is taken in a relaxation form:

\[
Q_r = -\nu_r (f_i - f_{i,M}^*) \tag{5}
\]

It was found by a number of numerical experiments that the choice for \( f_{i,M}^* \) in equation (5) as the Maxwellian distribution functions \( f_{i,M} \) is possible, but is not the best. The function \( f_{i,M}^* \) represents the elliptic distribution defined by the diagonal elements of the temperature tensor.

\[
f_{i,M}^* = n a_2 (\frac{m}{2\pi kT_{eq}})^{3/2} \exp(-m \xi_i^2 / 2kT_{eq}) \tag{6}
\]

where \( c_x = \xi_x - u, c_y = \xi_y - v, c_z = \xi_z - w \), and \( u, v, w \) are the components of the bulk velocity vector. The components \( T_{aa}^* \) of the temperature tensor are defined by self-similar transformation of the initial components as

\[
T_{aa}^* = T_{aa} (T_{eq} / T_{kin}) \tag{7}
\]

The use of the function given in equation (6), instead of the Maxwellian, means that the inelastic operator \( Q_r \) preserves to some extent the shape of the distribution function in the velocity space. The RT relaxation frequency can be defined as a part of the relaxation frequency \( \nu \) of the BGK model equation

\[
\nu_r = a_1 \nu . \tag{8}
\]

The non-elastic operator contributes to the evolution of the velocity distribution function toward the equilibrium state. To take into account its influence one should diminish the elastic collision operator by a factor \((1 - a_2 \nu_r)\), \( 0 < a_2 < 1 \). Finally, the proposed RT relaxation model contains two operators, the inelastic operator given by equation (5) with the frequency given by the equation (8), and the elastic operator \( Q_{el} = (1 - a_2 \nu_r)Q_{el} \). The coefficients \( a_1 \) and \( a_2 \) can be determined from comparisons of the solutions of the proposed model with solutions of the WC-UE equation. Note that some additional fitting parameters can also be applied in the model to obtain good agreement.

### 4 Results on Computation of Shock Wave (SW) Structure

The results on the computation of shock structure are presented in three parts: (a) the computations are presented for shock structure in Nitrogen including the rotational degrees of freedom up to Mach 15 by solving the complete GBE with a number of energy levels, (b) the computations are presented for SW in Nitrogen including the rotational degrees of freedom using the two-level kinetic model and are compared with the solution obtained in part (a), and (c) the computations are presented for SW
in Nitrogen with both rotational and vibrational degrees of freedom by solving the complete GBE for VT relaxations and employing the two-level kinetic model for RT relaxations.

(a) The SW structure is formed as a final stage of the evolution of discontinuity in the initial distribution function. The problem is considered for the interval \(-L \leq x \leq L\) with the discontinuity at \(x = 0\). The initial distribution function on both sides of the discontinuity is described by the velocities and spectral levels. It has the form

\[
\begin{align*}
    \rho_i^{(2)}(\xi,x) &= n_i^{(2)} \left[ \frac{m(2\pi T_i^{(2)})^{3/2}}{2T_i^{(2)}} \right] \exp \left( \frac{m(\xi-u_i^{(2)})^2}{2T_i^{(2)}} \right) \exp \left( \frac{e_i}{T_i^{(2)}} \right)
\end{align*}
\]

where \(Q_i\) denotes the statistical sum. Parameters \((n, T, u)^{1,2}\) are defined by the Rankine-Hugoniot relations with \(\gamma = 7/5\). At the boundary, the initial distribution function is kept constant.

For moderate Mach numbers, the SW structure in Nitrogen can be computed with real value of the spectral energy gap \(\varepsilon_0\), but for the hypersonic case the needed number of levels becomes too high (up to 50-70 levels) and therefore the computations become very time consuming. To facilitate this problem it is possible to increase this energy gap and thereby reduce the number of levels. By conducting numerical experiments at Mach number \(M = 4\), we determined that this increase in spectral energy gap does not influence the results of calculations in any significant way. Figure 1 shows an example of hypersonic SW structure in Nitrogen at Mach 15, computed with 16 levels instead of nearly 70 “natural” levels. These types of calculations compare well with the experiments of Alsmeyer [6] for density “n” for reported Mach numbers up to 10. Figure 2 shows the comparison for density distribution at Mach 10 between the computation and experimental data; excellent agreement is obtained.

(b) In part (a), the shock structure in Nitrogen was computed for RT relaxation using the complete collision integral in GBE with a number of energy levels. In this part, we show the SW calculations using a two-level kinetic model for RT relaxations. We choose the fixed coefficients \(a_1\) and \(a_2\) in such a way that the solution of the 2LRT model is close to the solution of the GBE for large number of Mach numbers.

\[
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\[
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The comparisons between the two set of solutions have been made at \(M = 2.4\) and \(M = 10\), and also for several intermediate Mach numbers. The solutions of the GBE equation shown in part (a) were obtained for Lennard-Jones molecular interaction potential and real rotational spectrum. For 2LRT model, we have applied the (12) inverse power repulsive potential which gives \(n < n (T_{kin})^{0.33}\). After a number of tests, the following best fitting parameters were determined as \(a_1 = 0.36, a_2 = 0.9\). The comparison of solutions of the 2LRT model with the solution of GBE for \(M = 2.4\) are given in Figures 3 and 4, and for \(M = 10\) in Figures 5 and 6. The solutions of GBE
were computed by the method described in [6]. The graphs for flow variables using 2LRT model are marked by stars.

![Normalized Flow Variables at M = 2.4.](image)

![Normalized Density at M = 2.4.](image)

(c) In this part we consider the gas with both rotational and vibrational degrees of freedom. The interaction potential is again in the form of the Lennard-Jones potential with parameters of Nitrogen taken at room temperature of 300K. The vibrational spectrum corresponds to Nitrogen with energy gap of 3340K. For rotational spectrum the energy quantum was increased against the actual (which is equal to 2.9K) for reducing the number of the levels as described before in the Introduction and part (a). The probabilities of R-T transfers are taken from the data of mathematical simulation by Beylich [3]. The probabilities of V-T transfers are generally accepted to be much smaller than those of the R-T transfers and are in the range of 0.005 – 0.001 of the elastic collision probability. As mentioned above in the technical approach, VT transfers are computed using GBE and the RT transfer are computed using the two-level kinetic model to simplify the computations. Computations are performed at Mach 6 and 10. In computation of the shock structure, we calculate the vibration energy as $E_{vib} = \sum_{j=0}^{j_{max}} j^2 \epsilon_{vib} n_j$. Assuming that the vibrations possess two degrees of freedom, one can associate the vibration energy with the classic
vibrational temperature $T_{\text{vib,cl}} = E_{\text{vib}} / k$. This temperature measures the amount of energy stored in the vibrations. From the viewpoint of quantum mechanics, the vibrations form the Bose gas in which the temperature in the thermodynamic equilibrium is related to the vibrational energy by the formula $E_{\text{vib}} = \frac{\epsilon_{\text{vib}}}{\exp(\epsilon_{\text{vib}} / kT_{\text{vib,q}}) - 1}$ [7]. In the classical limit, one obtains $T_{\text{vib,q}} \rightarrow T_{\text{vib,cl}}$. In Figures 7 and 8, we present both vibration temperatures along with the density, kinetic translational, longitudinal translational and rotational temperatures. It should be noted that the quantum vibrational temperature reaches the thermodynamic equilibrium value, but the classic vibrational temperature is below this limit. At $M = 6$, the vibrational spectrum consists of 4 levels which are sufficient to cover the entire energy range. At $M = 10$, the number of needed levels is eight. In Figures 7 and 8, the part of the x axes is shown. The computations were made for $x/\lambda = (-120, 250)$.

5 Conclusions
A numerical methodology has been developed for computing hypersonic non-equilibrium shock wave flows of diatomic gases using the Generalized Boltzmann Equation (GBE) including both the vibrational - translational (VT) and rotational - translational (RT) relaxations. In order to speed up the calculations for RT relaxations, a two-level BGK type model has also been developed which has been validated by comparing its results with that of complete GBE. The method can be easily extended to compute 2-D and 3-D non-equilibrium hypersonic flows of diatomic gases.

Fig. 7: SW Structure in Nitrogen at $M = 6$.

Fig. 8: SW Structure in Nitrogen at $M =10$.

References: