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Computation of Hypersonic Shock Wave Flows of Multi-Component Reactive Gas Mixtures Using the Generalized Boltzmann Equation

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TABLE OF CONTENTS

ABSTRACT.....	3
1. INTRODUCTION.....	5
2. TECHNICAL APPROACH.....	9
3. RESULTS	32
REFERENCES.....	38

ABSTRACT

In recent years, there has been a resurgence of interest in US Air Force in space access and therefore Air Force is interested in the hypersonic aerodynamics of its future space operations vehicles, long-range-strike vehicles and military-reusable launch vehicles. Hypersonic flows about space vehicles produce flow fields in thermodynamic non-equilibrium with local Knudsen numbers $K_n = \lambda / L$ (where λ is the mean free path of gas molecules and L is a characteristic length) which may lie in all the three regimes – continuum, transition and rarefied. Flows in continuum regime can be modeled accurately by the Navier-Stokes (NS) equations; however the flows in transition and rarefied regimes require a kinetic approach such as the Direct Simulation Monte Carlo (DSMC) method or the solution of the Boltzmann equation.

The objective of this research project has been to develop a computational methodology and a code for computing hypersonic non-equilibrium shock wave flows of multi-component reactive gas mixtures of diatomic gases using the Generalized Boltzmann Equation (same as the Wang-Chang Uhlenbeck equation which accounts for the degenerate energy levels) at Knudsen numbers in transitional and rarefied flow regimes. Several milestones have been achieved:

1. A 3D Generalized Boltzmann Equation (GBE) solver has been developed for a Cartesian mesh. The solver has been validated by computing the 1D shock structure in nitrogen for Rotational-Translational (R-T) relaxations and comparing the numerical results with the experimental data for Mach numbers up to 15. The solver has been exercised successfully for computing the 2D blunt body flows in nitrogen and 3D flow from a rectangular jet of nitrogen in vacuum for RT relaxations. The issues of stability of the algorithm and the possibility of reducing the number of rotational levels in the computations without compromising the accuracy of the solutions have been rigorously addressed.

2. A computational methodology has been developed to compute the hypersonic shock structure in diatomic gases including both the RT and Vibrational-Translational (V-T) relaxations. 1-D shock structure in nitrogen has been computed including both R-T and V-T relaxations and has been validated by comparing the results with the experimental data.

3. A computational methodology has been developed to compute the hypersonic shock structure in a non-reactive mixture of two diatomic gases. 1-D shock structure has been

computed in an inert mixture of nitrogen and oxygen for R-T relaxations. To accomplish this, the GBE is formulated and solved in "impulse space" instead of velocity space.

4. A new two-level kinetic model has been developed for computing the RT relaxations in a diatomic gas and has been validated by comparing the results with the solutions of complete GBE. The model is about twenty times more efficient than the GBE in computing the shock structure. It should be noted that the model is different than the BGK model; it accounts for both elastic and inelastic collisions.

1. INTRODUCTION

In recent years, there has been a resurgence of interest in US Air Force in space access and therefore Air Force is interested in the hypersonic aerodynamics of its future space operations vehicles, long-range-strike vehicles and military-reusable launch vehicles. Hypersonic flows about space vehicles produce flow fields in thermodynamic non-equilibrium with local Knudsen numbers $K_n = \lambda / L$ (where λ is the mean free path of gas molecules and L is a characteristic length) which may lie in all the three regimes— continuum, transition and rarefied. Therefore, there is an important need for a single unified Computational Fluid Dynamics (CFD) code that can treat all the three flow regimes in thermodynamic non-equilibrium accurately and efficiently. Flows in continuum regime can be modeled accurately by the Navier-Stokes (NS) equations; however the flows in transition and rarefied regimes require a kinetic approach such as the Direct Simulation Monte Carlo (DSMC) method or the solution of the Boltzmann equation.

One of the critical issues in accurate prediction of non-equilibrium flows is the ability to simulate the translational and internal energy mode relaxation of polyatomic (in particular diatomic) molecules present in these flows. Relaxation of diatomic molecules in non-equilibrium flows is very different from that of monoatomic molecules due to the internal degrees of freedom; therefore it is important to study the effect of the internal degrees of freedom upon the energy transfer between colliding diatomic molecules. It turns out that the simulation of internal energy mode relaxation is fundamentally different in the continuum (NS) and kinetic approaches. In the continuum approach, NS equations contain the source terms of reaction probabilities for quantifying the thermal and chemical non-equilibrium effects which are typically available from experiments for equilibrium conditions that have the translational temperature dependence. For flows with $Kn \sim 0.01$, this approach based on NS equations is very effective in computing hypersonic flows with small deviation from translational non-equilibrium [1]. However, at higher Kn for flows in transition and rarefied regimes, the kinetic methods based on the Boltzmann equation provide more detailed information on the degree of non-equilibrium.

During the past fifteen years, following Bird [2], DSMC methods have been developed for computing non-equilibrium flows of monoatomic and diatomic gases [3-5]. Typically, in most of the DSMC solvers, the diatomic molecules are modeled assuming quantized rigid rotors for rotational energy levels and anharmonic oscillators for vibrational energy levels. Elastic cross-

sections are based on Variable Hard Sphere (VHS) model and inelastic cross-sections (Rotational-Translational (R-T) and Vibrational-Translational (V-T)) are based on Borgnakke-Larsen model [6] assuming constant or temperature dependent collision numbers ZR . Dissociation cross-sections are based on the Weak Vibrational Bias model [7] or its variants. However, it has been shown that the non-equilibrium rarefied flows of diatomic gases, in which the gas molecules transfer energy among translational, rotational and vibrational degrees of freedom, cannot be accurately predicted by using the simple collision models in DSMC methods [8]. In recent years, considerable effort has also been devoted toward the development of approaches using simplified models of Boltzmann equation (e.g. BGK type models) that include the multi-translational temperatures, rotational relaxation, and dissociation kinetics [9,10], which have shown some promise. However, these approaches also have limitations, especially in prediction of strong shocks encountered in hypersonic non-equilibrium flows. Additionally, the transition and rarefied regimes are characterized by the formation of narrow boundary layers with sharp variation in flow parameters, the zones with considerable compression of a gas at the scale of the molecular mean free path, and the low density stagnation zones. Thus the most accurate description of the physics of these flows can be obtained by solving the Boltzmann equation for a diatomic gas, namely the Wang-Chang-Uhlenbeck Master Equation [11] or a generalized Boltzmann equation for a reactive mixture of gases.

In solving the Boltzmann equation by a finite-difference method, the principal difficulties arise in calculation of the multi-dimensional collision integral; the approximation to the collision integral must tend to the actual one as the mesh size in the velocity space tends to zero. In recent years, there has been significant progress toward the development of an efficient and accurate numerical method for the solution of Boltzmann equation for a monoatomic gas [12-15]. In this method, the Boltzmann equation is solved on fixed space and velocity grids by a finite-difference method. A projection method (that ensures that the velocities before and after collision belong to the same grid of discrete ordinates) is employed for the evaluation of the collision integral that ensures exact conservation laws for mass, momentum, and energy as well as zero value of the integral under thermodynamic equilibrium (when the distribution function is Maxwellian). The last property eliminates the numerical error of computing the principal part of the solution outside the Kundsen layers and shock waves and thus considerably increases the accuracy and

efficiency of the method. The differential part of the Boltzmann equation is approximated by an explicit second-order flux-conservative scheme. The combined system of difference equations (for the collision integral and the differential part) is solved by the splitting method which splits the solution process in two stages: the collision relaxation and free molecular flow. This method has been developed by Professor Chermisin of the Computing Center of the Russian Academy of Science [12-15]. It has been extensively applied by him and many other researchers [16] including the author of this report [17-21]. The key numerical features of this method are: (a) it is fully conservative, (b) it preserves the positiveness of the solution, (c) it does not disturb the thermodynamic equilibrium and therefore can be applied for computing flows approaching continuum regime, (d) it is essentially deterministic and therefore does not produce statistical noise, (e) it employs numerically efficient integration grids that make it very efficient, (f) it can employ a variable mesh that may exceed the local mean free path in the regions of low gradients, and (g) the method can be easily parallelized. It has several advantages over the DSMC method e.g. the DSMC method requires mesh spacing less the mean free path in the entire field, it employs not very realistic molecular potentials (like VHS) instead of the more accepted ones like the Lennard-Jones potential with established parameters for each gas (e.g. N₂ and O₂), and for inelastic collisions DSMC method employs models that are not physically justifiable. For example in the most commonly used Borgnakke-Larson model [6] in the DSMC method, the molecules are divided in two parts: the molecules in major part collide elastically and in the rest with internal –translational energy transfer that presumes a thermodynamic equilibrium. This model is therefore not very accurate.

The objective of this research project has been to develop a computational methodology and a code for computing hypersonic non-equilibrium shock wave flows of multi-component reactive gas mixtures of diatomic gases using the Generalized Boltzmann Equation (same as the Wang-Chang Uhlenbeck equation which accounts for the degenerate energy levels) at Knudsen numbers in transitional and rarefied flow regimes. It should be noted that in the GBE, the internal and translational degrees of freedom are considered in the framework of quantum and classical mechanics respectively. The general computational methodology for the solution of the GBE is similar to that for the classical BE for a monoatomic gas except that the evaluation of the collision integral becomes significantly more complex due to the quantization of rotational and

vibrational energy levels. The transition probabilities, elastic and inelastic cross-sections etc. of a gas molecule are needed for the solution of the collision integral. Lennard-Jones potential with two free parameters is used to obtain the elastic cross-section of the gas molecules, and the so called “combinatory relations” are used to obtain parameters of Lennard-Jones potential for an interaction of molecule A with molecule B knowing the parameters of A and B [11]. The probability of transition in inelastic collisions is determined using the approach by Beylich [22, 23]. These inputs allow for the calculation of the Boltzmann Collision Integral in GBE for a diatomic gas and a reactive mixture of gases.

Several milestones have been achieved:

1. A 3D Generalized Boltzmann Equation (GBE) solver has been developed for a Cartesian mesh. The solver has been validated by computing the 1D shock structure in nitrogen for Rotational-Translational (R-T) relaxations and comparing the numerical results with the experimental data for Mach numbers up to 15. The solver has been exercised successfully for computing the 2D blunt body flows in nitrogen and 3D flow from a rectangular jet of nitrogen in vacuum for RT relaxations. The issues of stability of the algorithm and the possibility of reducing the number of rotational levels in the computations without compromising the accuracy of the solutions have been rigorously addressed.

2. A computational methodology has been developed to compute the hypersonic shock structure in diatomic gases including both the RT and Vibrational-Translational (V-T) relaxations. 1-D shock structure in nitrogen has been computed including both R-T and V-T relaxations and has been validated by comparing the results with experimental data.

3. A computational methodology has been developed to compute the hypersonic shock structure in a non-reactive mixture of two diatomic gases. 1-D shock structure has been computed in an inert mixture of nitrogen and oxygen for R-T relaxations. To accomplish this, the GBE is formulated and solved in “impulse space” instead of velocity space.

4. A new two-level kinetic model has been developed for computing the RT relaxations in a diatomic gas and has been validated by comparing the results with the solutions of complete GBE. The model is about twenty times more efficient than the GBE in computing the shock structure. It should be noted that the model is different than the BGK model; it accounts for both elastic and inelastic collisions.

2. TECHNICAL APPROACH

As mentioned before in Section 1, gas flows in continuum-transition regime, where the Knudsen number K_n is $O(1)$ [$0.1 < K_n < 10$], are characterized by the formation of narrow, highly non-equilibrium zones (Knudsen layers) of thickness of the order of molecular free path λ ; the flow structure is then determined by the fast kinetic processes. Moreover, in case of unsteady flows, an initial Knudsen time interval is of the order $\tau_0 = \lambda/v$, where v is the molecular velocity. Thus, the Knudsen layer can be computed accurately only by directly solving the Boltzmann equation. Alternative approaches which approximate the Boltzmann equation to account for departure from equilibrium, namely the higher-order continuum equations such as the Burnett equations [24, 25], Grad's moment equations [26] or Eu's equations [27] as well the particle methods such as DSMC [2-4], have been shown to have limitations.

2.1 Solution Method for the Classical Boltzmann Equation

In this section, we briefly describe the finite-difference method that is currently employed for solving the classical Boltzmann equation (BE) of classical mechanics for a monatomic gas in translational non-equilibrium. In solving the Boltzmann equation by a finite-difference method, the principal difficulties arise in calculation of the multi-dimensional collision integral; the approximation to the collision integral must tend to the actual one as the mesh size in the velocity space tends to zero. In recent years, there has been significant progress toward the development of an efficient and accurate numerical method for the solution of Boltzmann equation for a monoatomic gas [12-15]. In this method, the Boltzmann equation is solved on fixed space and velocity grids by a finite-difference method. A projection method (that ensures that the velocities before and after collision belong to the same grid of discrete ordinates) is employed for the evaluation of the collision integral that ensures exact conservation laws for mass, momentum, and energy as well as zero value of the integral under thermodynamic equilibrium (when the distribution function is Maxwellian). The last property eliminates the numerical error of computing the principal part of the solution outside the Knudsen layers and shock waves and thus considerably increases the accuracy and efficiency of the method. The differential part of the Boltzmann equation is approximated by an explicit second-order flux-conservative scheme. The combined system of difference equations (for the collision integral and

differential part) is solved by the splitting method which splits the solution process in two stages: the collision relaxation and free molecular flow. The method described below is second-order accurate and is quite efficient; it is due to Cheremisin and his colleagues [12-15].

Consider a gas of molecules without internal degrees of freedom and seek a solution to the 2-D Boltzmann equation:

$$\frac{\partial f}{\partial t} + \xi_x \cdot \frac{\partial f}{\partial x} + \xi_y \cdot \frac{\partial f}{\partial y} = I(f, f) \equiv -L(f, f) + G(f, f) \quad (1)$$

In equation (1), collisions in $L(f, f) \equiv v(f)f$ and $G(f, f)$ have the form

$$L(f, f) = \int_{-\infty}^{\infty} \int_0^{2\pi b_m} \int f \cdot f_1 \cdot g \cdot b \cdot db \cdot d\varepsilon \cdot d\xi_1 \text{ and } G(f, f) = \int_{-\infty}^{\infty} \int_0^{2\pi b_m} \int f' \cdot f'_1 \cdot g \cdot b \cdot db \cdot d\varepsilon \cdot d\xi_1. \quad (2)$$

A standard notation is used in equation (2): b and ε are the impact parameters of a molecular collision; f, f_1, f' and f'_1 are functions of velocity vectors ξ, ξ_1, ξ' and ξ'_1 respectively. The first two vectors are the pre-collision velocities; the last two are the post-collision ones; $g = |\xi - \xi_1|$; b_m is the upper limit of the impact parameter; and the vector ξ has the components ξ_x, ξ_y and ξ_z . The space of velocity ξ is restricted to a domain Ω where an N-point uniform grid is defined, with grid points ξ_β and a mesh size vector $h = (h_1, h_2, h_3)$. Equation (1) is approximated by a set of N equations for f_β as:

$$\frac{\partial f_\beta}{\partial t} + \xi_{\beta,x} \frac{\partial f_\beta}{\partial x} + \xi_{\beta,y} \frac{\partial f_\beta}{\partial y} = I_\beta. \quad (3)$$

The method used for calculating the collision integrals described in [12, 13] ensures that a computation performed to any numerical accuracy is consistent with the conservation laws. If

Ψ_β denotes the collision invariant vector, $\Psi_\beta = (1, \xi_\beta, \xi_\beta^2)$, then

$$\sum_{\beta} \Psi_\beta I_\beta = 0 \quad (4)$$

and at any grid point ξ_β

$$I_\beta(f_{M,\beta}, f_{M,\alpha}) = 0. \quad (5)$$

Here, $f_{M,\beta}$ is the equilibrium Maxwellian distribution function for gas molecules at a grid point ξ_β . The last condition substantially improves the accuracy of calculation of the integral I_β in those subdomains where the state of the gas is close to the thermodynamic equilibrium [14].

System of equations (3) is solved by the method of splitting with respect to physical processes [15, 16]. On an interval $[t^j, t^{j+1}]$, we consecutively solve the collisionless transport equations

$$\frac{\partial f_\beta^*}{\partial t} + \xi_{\beta,x} \cdot \frac{\partial f_\beta^*}{\partial x} + \xi_{\beta,y} \cdot \frac{\partial f_\beta^*}{\partial y} = 0, \quad f_\beta^{*,j} = f_\beta^j \quad (6)$$

and the collisional relaxation equations

$$\partial f_\beta / \partial t = I_\beta, \quad f_\beta^j = f_\beta^{*,j+1}, \quad (7)$$

written for each grid point (the grid-point index is dropped).

By splitting with respect to spatial variables, system of equations (6) is approximated by a second-order accurate (in h_x and h_y) explicit scheme [28]. The set of nonlinear equation (6) is solved by an integral form [15]. For time step $\tau = \tau^{j+1} - \tau^j$:

$$f_\beta^{i+1} = f_\beta^i + \int_{\tau^i}^{\tau^{i+1}} I_\beta d\tau \quad (8)$$

To resolve fast kinetic process, the condition $\tau < \tau_0$ where τ_0 is the mean time between collisions, should be satisfied. Cheremisin and his colleagues have written a Boltzmann solver using the above method. This solver has been extensively validated by computing flows with Knudsen numbers ranging from 0.01 to 10 by the author of this report and Professor Cheremisin for computing hypersonic flows with translational non-equilibrium [17]. This solver was extended for solving the Generalized Boltzmann Equation (GBE) for diatomic gases; the methodology is described in Section 2.2.

2.1.1 The Stability Condition for the Algorithm Described Above in Section 2.1

The main algorithm of the conservative projection method described above in Section 2.1 has two parts. First, there is the splitting of the advection equation and second the integration of relaxation equation. For the advection equation, when an explicit 1st order method is applied, the

CFL condition defined by the maximum molecular velocity should be satisfied, i.e. $\xi_{\max} \tau_{CFL} / h \leq 1$. For a higher-order explicit method, instead of unity on the right hand side of above condition, a number less than 1 (for example 0.5) appears.

For the solution at the relaxation stage, there are no exactly defined stability parameters. However an important role is played by the parameter ε_r that limits the proportion of rejected contributions. It should be sufficiently small. Usually, it should be of the order of E-4 or E-5. For strict computation, it should be equal to 0, but then the CPU time becomes very large. In practice, the optimal choice of ε_r depends on a problem. The wrong choice may influence the results of the solution, and even lead to the divergence of the solution. When ε_r is chosen and the number of integration (Korobov's) nodes is given, the maximal value of the time step τ_r at the relaxation step can be determined. For the stability of the computations, the time step of the algorithm should be chosen as $\tau = \min(\tau_{CFL}, \tau_r)$.

The Boltzmann equation covers gas flows in all regimes: from free molecular, which is extremely viscous from the view point of continuum fluid dynamics, to the Euler gas dynamics with zero viscosity. The algorithm contains a number of parameters whose values depend on a particular problem. These parameters are: the discretization steps in coordinate and velocity variables, the time step, and the limits in the velocity space. If these parameters are not chosen correctly, the solution may be wrong or diverge, because it doesn't correspond to the physical reality. For example, if the gas is very far from the thermodynamic equilibrium, and one takes the coordinate step $h > \lambda$ (local mean free path) or the time step is not sufficiently less the mean molecular inter-collision time, the algorithm will produce wrong results and may diverge. The use of the same parameters for a near continuum flow however may be O.K. The situation is analogous to the application of the Euler gas dynamics equations to a viscous low Reynolds flow. Therefore the parameters of the algorithm that define the approximation of a particular problem should be properly chosen. The same conclusions are true for the algorithm employed for the solution of GBE or the Wang-Chang Uhlenbeek equation described in Section 2.2

2.2 Solution Method for the Generalized Boltzmann Equation for a Diatomic Gas (Wang-Chang-Uhlenbeck Equation)

Nonequilibrium processes in a gas with internal degrees of freedom of molecules can be studied by using the generalized Boltzmann equation or the Wang-Chang-Uhlenbeck equation, where the internal and translational degrees of freedom are considered in the framework of quantum and classical mechanics respectively. For small deviations from local thermodynamic equilibrium, an asymptotic method developed for this equation yields hydrodynamic equations including the effect of the internal degrees of freedom on the viscosity and thermal conduction of the gas [11]. The GBE or Wang-Chang-Uhlenbeck equation (WC-UE) for a diatomic gas in thermodynamic non-equilibrium can be written in the form:

$$\frac{\partial f_i}{\partial t} + \xi_i \frac{\partial f_i}{\partial x} = \sum_{j,k,l} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (f_k f_l - f_i f_j) g \sigma_{ij}^{kl} d\Omega d\xi_j \quad (9)$$

In Equation (9), $d\Omega = \sin \theta d\theta d\varphi$, $f_i \equiv f(i, \xi, x, t)$ is the distribution function, where i is the set of quantum numbers determining the internal state of the molecule; ξ_i is the velocity of the molecule in the i th state; $g = |\xi_i - \xi_j|$; indices i, j and k, l correspond to the molecular states before and after the collision respectively; and σ_{ij}^{kl} is the cross section for the collision responsible for this change of the internal states. There is no summation with respect to the repeated index i .

The cross sections for direct and inverse collisions are related as

$$g \sigma_{ij}^{kl}(g, \theta, \varphi) d\xi_i d\xi_j = g^* \sigma_{ij}^{kl}(g^*, \theta, \varphi) d\xi_k d\xi_l \quad (10)$$

The magnitude $g^* = |\xi_k - \xi_l|$ of the velocity after the collision and velocities ξ_k and ξ_l are determined from the laws of conservation.

$$g^* = g \sqrt{1 - \frac{4\Delta e}{mg^2}}, \xi_k = \xi_0 - 0.5g^*, \text{ and } \xi_l = \xi_0 + 0.5g^*. \quad (11)$$

In equation (11), m is the molecular mass; $\Delta e = e_i + e_k - e_j - e_l$, where e_i is the energy of the i th internal state and $\xi_0 = 0.5(\xi_i + \xi_j)$. The condition $mg^2 \geq 4\Delta e$ determines the

admissibility of the transition $(i, j) \rightarrow (k, l)$. We set $\sigma_{ij}^{kl} = 0$ for forbidden transitions. The probability of the transition $(i, j) \rightarrow (k, l)$ is defined as

$$p_{ij}^{kl} = \frac{\sigma_{ij}^{kl}}{\sigma_{ij}}, \text{ where } \sigma_{ij}^{kl} = \sum_{k,l} \sigma_{ij}^{kl} \quad (12)$$

and satisfies the condition $0 \leq p_{ij}^{kl} \leq 1$ and the normalization condition

$$\sum_{k,l} p_{ij}^{kl} = 1. \quad (13)$$

We assume that σ_{ij} is independent of the internal molecular state and is equal to the elastic scattering cross section $\sigma_{ij} = \sigma_0(g, \theta)$. The introduction of quantities σ_0 and p_{ij}^{kl} obviously transforms equation (9).

2.2.1 Numerical Solution Procedure for GBE

The problem of numerically solving the Wang-Chang-Uhlenbeck (WC-U) equation [29] reduces to the construction of a method of calculating its right-hand side, the generalized collision operator, which can be represented as $I_i = -L_i + G_i$, where

$$L_i = \sigma_0 \sum_{j,k,l} \int_V \int_{\Omega} f_i f_j p_{ij}^{kl} g d\Omega d\xi_j \quad (14)$$

and

$$G_i = \sigma_0 \sum_{j,k,l} \int_V \int_{\Omega} f_k f_l p_{ij}^{kl} g d\Omega d\xi_j. \quad (15)$$

As in the case of the classical Boltzmann equation (1), an effective numerical method must ensure that the collision operator must be (i) conservative and (ii) be equal to zero on the equilibrium distribution function.

Operators L_i and G_i are calculated on the $j_m \times S_0$ lattice, where S_0 is the uniform lattice in volume V of velocity space and j_m is the number of quantum levels.

Similar to the case of a one-atom gas, we consider the functional

$$Q(\Phi, f_i) = \sigma_0 \sum_{i,j,k,l} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{\Omega} \Phi f_i f_j p_{ij}^{kl} d\Omega d\xi_i d\xi_j \quad (16)$$

Taking functions $\Phi(\xi)$ in the form

$$\Phi' = 0.5[\partial_{ni}\partial(\xi^* - \xi_i) + \partial_{nj}\partial(\xi^* - \xi_j)] \text{ and} \quad (17)$$

$$\Phi^* = 0.5[\partial_{nk}\partial(\xi^* - \xi_k) + \partial_{nl}\partial(\xi^* - \xi_l)], \quad (18)$$

where ∂_{nq} is the Kronecker delta and $\partial(\xi^* - \xi)$ is the three-dimensional delta function, we obtain

$$L_n(\xi^*) = Q(\Phi', f_i) \text{ and} \quad (19)$$

$$G_n(\xi^*) = Q(\Phi^*, f_i). \quad (20)$$

Functions (19) and (20) are calculated on the uniform cubic lattice consisting of N_v sites $S_v = \{i, j, k, l, \xi_i, \xi_j, \theta, \varphi\}_v$ such that $(\xi_i)_v, (\xi_j)_v \in S_0$. Let $(\xi_i)_v \equiv \xi_{\alpha_v}$ and $(\xi_j)_v \equiv \xi_{\beta_v}$. The values $(\xi_k)_v$ and $(\xi_l)_v$ for each site of this lattice are calculated by equation (11). The arrangement of vectors ξ_i, ξ_j, ξ_k , and ξ_l for the v th site of cubic lattice S_0 is schematically shown in Fig. 1, where the three-dimensional velocity lattice is given as a plane lattice and subscript v is omitted. The value $L'_{n,\gamma} = L'_n(\xi_\gamma)$ calculated in site $\xi^* = \xi_\gamma \in S_0$ by equation (19) is determined by the part of the cubic sum for $i_v = n, \alpha_v = \gamma$ and $j_v = n, \beta_v = \gamma$ as

$$L'_{n,\gamma} = B \sum_v (\partial_{ni_v} \partial_{\gamma\alpha_v} + \partial_{nj_v} \partial_{\gamma\beta_v}) \Delta_v, \quad (21)$$

$$\text{where } B = \frac{2\pi\sigma_0 j_m^2 V}{N_v}, \quad \Delta_v = f_{i,\alpha_v} f_{j,\beta_v} (p_{ij}^{kl})_v g_v \sin \theta_v, \quad \Delta_v = f_{i,\alpha_v} f_{j,\beta_v} (p_{ij}^{kl})_v g_v \sin \theta_v, \quad \text{and}$$

$f_{i,\alpha} \equiv f(i, \xi_\alpha, x, t)$. In what follows, the subscript v will be omitted where possible. Since velocities ξ_k and ξ_l are not in the sites of lattice S_0 , $G'_{n,\gamma}$ is calculated with the replacement of equation (18) by projector Φ^{**} into pairs of sites $\xi_\lambda, \xi_{\lambda+s}$ and $\xi_\mu, \xi_{\mu-s}$, which are nearest to ξ_k and ξ_l and are shown in Fig. 13:

$$\Phi^{**}(\xi_\gamma) = (1-r)[\partial_{n\lambda}\partial(\xi_\gamma - \xi_\lambda) + \partial_{n\mu}\partial(\xi_\gamma - \xi_\mu)] + r[\partial_{n,\lambda+s}\partial(\xi_\gamma - \xi_{\lambda+s}) + \partial_{n,\mu-s}\partial(\xi_\gamma - \xi_{\mu-s})], \quad (22)$$

where $s = (s_1, s_2, s_3)$ is the vector whose components take values 0, -1, and 1 and that determines the site that is nearest to ξ_k and shown in Fig. 1. As a result,

$$G'_{n,\gamma} = B \sum_v \{[(1-r)(\partial_{nk}\partial_{\gamma\lambda} + \partial_{nl}\partial_{\gamma\mu}) + r(\partial_{nk}\partial_{\gamma,\lambda+s} + \partial_{nl}\partial_{\gamma,\mu-s})]\Delta\}_v. \quad (23)$$

The coefficient r_v is determined from the laws of conservation for each site of the cubic formula, i.e., for each contribution Δ_v to operators $L'_{n,\gamma}$ and $G'_{n,\gamma}$. The conservation of mass follows from the form of Φ^{**} , and the conservation of momentum follows from the symmetric arrangement of lattice sites $\xi_\lambda, \xi_{\lambda+s}$ and $\xi_\mu, \xi_{\mu-s}$ with respect to vectors ξ_k and ξ_l . In terms of the notation

$$E_0 = \frac{m\xi_k^2}{2} + \frac{m\xi_l^2}{2}, E_1 = \frac{m\xi_\lambda^2}{2} + \frac{m\xi_\mu^2}{2}, \text{ and } E_2 = \frac{m\xi_{\lambda+s}^2}{2} + \frac{m\xi_{\mu-s}^2}{2}, \quad (24)$$

the law of energy conservation, when contribution Δ_v is split, has the form $E_0 = (1-r)E_1 + rE_2$.

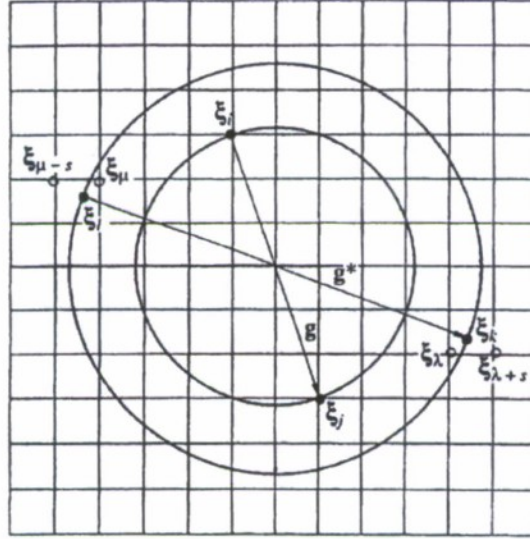


Figure 1: Schematic of an Inelastic Collision

Therefore $r = \frac{E_0 - E_1}{E_2 - E_1}$, which satisfies the condition $0 \leq r \leq 1$ because either $E_1 \leq E_0 \leq E_2$ or $E_2 \leq E_0 \leq E_1$. It is important that r_v is independent of Δ_v . For this reason, additional lattice sites $\xi_{\lambda_v}, \xi_{\mu_v}, \xi_{\lambda_v+s_v}$, and $\xi_{\mu_v-s_v}$ and coefficient r_v can be preliminarily determined for each site of cubic lattice S_v , and then extended lattice S_v^* can be used repeatedly, e.g., in various sites of physical space. Each contribution Δ_v can be treated as the result of a "collision" transferring molecules from sites i, j to sites λ, μ and $\lambda+s, \mu-s$. In order to ensure that condition (ii) above is satisfied, we consider a pair of inverse collisions to sites i, j from sites λ, μ and $\lambda+s, \mu-s$,

$\mu-s$ with weights $(1-r^*)$ and r^* , respectively. The probability p_{ij}^{kl} is determined from equation (10), and coefficient r^* from the condition

$$E_1\Delta^{(1)}(1-r^*) + E_1\Delta^{(2)} = E_0[\Delta^{(1)}(1-r^*) + \Delta^{(2)}r^*], \quad (25)$$

where

$$\Delta^{(1)} = f_{k,\lambda} f_{l,\mu} p_{ij}^{kl} g \sin(\theta) \text{ and} \quad (26)$$

$$\Delta^{(2)} = f_{k,\lambda+s} f_{l,\mu-s} p_{ij}^{kl} g \sin(\theta). \quad (27)$$

$$\text{As a result, } r^* = \frac{\Delta^{(1)}r}{\Delta^{(1)}r + \Delta^{(2)}(1-r)}. \quad (28)$$

An analysis similar to the above gives the contribution of inverse collisions in the form

$$L_{n,\gamma}^* = B \sum_v \{ (1-r^*)(\partial_{nk}\partial_{\gamma\lambda} + \partial_{nl}\partial_{\gamma\mu})\Delta^{(1)} + r(\partial_{nk}\partial_{\gamma,\lambda+s} + \partial_{nl}\partial_{\gamma,\mu-s})\Delta^{(2)} \}_v, \text{ and} \quad (29)$$

$$G_{n,\gamma}^* = B \sum_v \{ (\partial_{ni}\partial_{\gamma\alpha} + \partial_{ni}\partial_{\gamma\beta})[(1-r^*)\Delta^{(1)} + r^*\Delta^{(2)}] \}_v. \quad (30)$$

Finally, the collision operators are determined as

$$L_{n,\gamma} = \frac{1}{2}(L_{n,\lambda}' + L_{n,\lambda}^*), \quad G_{n,\gamma} = \frac{1}{2}(G_{n,\lambda}' + G_{n,\lambda}^*). \quad (31)$$

For any arbitrarily lattice of integration sites S_v , condition (ii) is satisfied to within an accuracy no worse than $O(h)$, where h is the step of lattice S_0 . For degenerate levels of internal energy, equation (9) must be modified so as to reduce the number of substantial levels.

Let j_m levels be separated into J_m groups of degenerate levels, $J=0,1,\dots,J_M$, with degeneration degree q_j . We determine the distribution function as $F_j = \sum_q f_q = q_j f_{q_j}$, where $q \in J$. Substituting $\sigma_{ij}^{kl} = \sigma_0 p_{ij}^{kl}$ into equation (9), summing this equation over the groups of levels i, j, k , and l forming degenerate levels I, J, K and L , and returning to the old notation, we arrive at the equation

$$\frac{\partial f_i}{\partial t} + \xi_i \frac{\partial f_i}{\partial x} = \sigma \sum_{j,k,l} \int_{-\infty}^{\infty} \int_{\Omega} (q_i q_j f_k f_l - q_k q_l f_i f_j) g p_{ij}^{kl} d\Omega d\xi_j \quad (32)$$

for which equations (21), (23), (29) and (30) are valid with the change $\Delta \rightarrow q_k q_l \Delta$, $\Delta^{(1)} \rightarrow q_k q_l \Delta^{(1)}$, and $\Delta^{(2)} \rightarrow q_k q_l \Delta^{(2)}$.

2.2.2 Modeling of Transition Probabilities, Elastic & Inelastic Cross-Sections

The computation of collision integral in equation (9) requires the knowledge of the collision cross-section σ_{ij}^{kl} responsible for the change of internal states of the molecules. This cross-section can be calculated from equation (12) if the probability of transition $(i, j) \rightarrow (k, l)$, p_{ij}^{kl} and the elastic scattering cross-section σ_{ij} are known for a given gas or a mixture of gases.

For DSMC simulations of real gases, Koura [7] has given models of elastic cross-section, rotationally and vibrationally inelastic cross-sections, and dissociation and recombination cross-sections. These cross-sections can be used for shock wave simulations in Nitrogen, Oxygen, and in a mixture of Oxygen and Nitrogen. In the simulations, one may use these models (or similar models used in DSMC simulations [4]) as well as other models, which have proven to be more accurate. It has been recently shown by Beylich [30] that Lennard-Jones (LJ) model gives better prediction for the structure of normal shock waves in Helium and Argon than Hard-Sphere (HS) model because the scattering behavior of LJ is very different from the HS model. In our calculations, we employ the LJ model [11] for calculating the elastic cross-section of diatomic gases e.g. Nitrogen, Oxygen, and a mixture of Nitrogen and Oxygen. For calculating the rotationally inelastic cross-sections, we employ the transition probability model due to Beylich [22, 23] based on an interlaced system of rigid rotors which has shown excellent results for shock wave structure in Nitrogen. The model gives the transition probabilities as follows:

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

where $\Delta_1 = |\Delta e_1 + \Delta e_2| / e_{ir0}$, $\Delta_2 = 2 |\Delta e_2 - \Delta e_1| / e_{tot}$,

$$\Delta_3 = 4 |\Delta e_1| / (e_{ir0} + e_{ri}), \Delta_4 = 4 |\Delta e_2| / (e_{ir0} + e_{rj}), \quad (33)$$

and $\omega_{ij}^{kl} = q_k q_l / (q_i q_j)$, $e_{ir0} = mg^2 / 4$, $e_{tot} = e_{ir0} + e_{ri} + e_{rj}$.

In equation (33), q_i is the degeneracy, and e_i is the rotational energy of the i -th level. This model can be easily extended to Oxygen. For calculating the vibrationally inelastic cross-sections, we employ the transition probability model described in Reference [7].

2.2.3 Computation of Shock Structure in a Diatomic Gas

These computations were performed for validation of the Generalized Boltzmann Solver. In particular, both the computations with other methods such as DSMC and BGK-type models [9] as well as experimental data [31, 32] are available for shock structure in Nitrogen for both weak and strong shocks. The calculation of the shock structure using equation (9) requires the calculation of relaxation of vibrational levels and rotational levels. The energy of j th vibrational level is given by $e_j^v = \hbar\omega\left(j + \frac{1}{2}\right)$ and the equilibrium distribution for the vibrational temperature T_v is given by

$$n_j^v = nZ_v^{-1} \exp\left[-\frac{\hbar\omega(j + \frac{1}{2})}{T_v}\right], \quad (34)$$

where Z_v is the vibrational partition function. For Nitrogen, $\frac{\hbar\omega}{k} = 3340K$ and for Oxygen it is $2230 K$, where k is the Boltzmann's constant. The energy level with the rotational quantum number j has the degeneracy of degree $q_j = 2j + 1$ and energy $e_j^r = -\frac{\hbar^2 j(j+1)}{2I_r}$, where I_r is the moment of inertia of the molecule. The equilibrium distribution of the gas density n over levels for temperature T_r is given by the expression

$$n_j^r = nZ_r^{-1} (2j + 1) \exp\left[-\frac{\hbar^2 j(j+1)}{2I_r T_r}\right]. \quad (35)$$

The rotational constant for Nitrogen $\frac{\hbar^2}{2I_r k} = 2.9K$ and for Oxygen it is $2.1 K$. The values of

$\frac{\hbar\omega}{k}$ and $\frac{\hbar^2}{2I_r k}$ for a nitrogen and oxygen molecule have been obtained from [33]. From the

values of vibrational and rotational constant for nitrogen and oxygen, it is obvious that the vibration levels are excited at high temperatures, but the rotational levels are excited at any temperature. Therefore in most of the cases, only a few vibration levels can be considered. At room temperature for Nitrogen, about 20 rotational levels are sufficient for calculations, and at least 25 levels are needed for Oxygen. When the temperature rises, the needed number of levels

increases. For shock wave in Nitrogen at Mach 2 to 11, about 30 to 60 levels may be needed. Although the computational difficulty in number of arithmetic operations increases more than J^2 times, fortunately, for a large number of levels one can consider the spectrum as continuous and use the reduced number of efficient levels. Such is the approach applied in statistical physics where the statistical sum is replaced by an integral. When a reduced number of levels are used, one can consider the rotational levels in GBE or WC-UE in the framework of classical mechanics. In fact, Beylich [22, 23] has successfully employed this approach; he computed the probability of R-T transfer for continuous spectrum, and then made it discrete using the notion of a rotational quantum. One could do the same, but with an arbitrary "quantum".

The SW structure is formed as a final stage of the evolution of a discontinuity in the initial distribution function. The problem is considered for the interval $-L_1 \leq x \leq L_2$ 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

$$f_i^{1,2}(\xi, x) = n^{1,2} [m/(2\pi T^{1,2})]^{3/2} \exp\left[-\frac{m(\xi - u^{1,2})^2}{2T^{1,2}}\right] \frac{2i+1}{Q_r} \exp\left(-\frac{e_{ri}}{T^{1,2}}\right), \quad (36)$$

where Q_r 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. The characteristic dimensional parameters needed in the computation are the gas density n , the initial translational temperature T_0 , and the mean-free-path time τ at this temperature. The initial distribution function at $t=0$ can be taken as Maxwellian with translational velocities. Lattices S_0 and S_v with about 5000 and 0.5×10^6 sites respectively are sufficient. Time integration is performed according to the scheme in [12, 14] using an appropriate time step, e.g. $\Delta t = 0.005\tau$ based on the calculations performed in [17]. In Section 3, the results of computations for SW structure in nitrogen at high Mach numbers are presented for R-T relaxations, for both R-T and V-T relaxations, and for an inert mixture of two diatomic gases.

2.2.4 The Choice of Efficient Rotational Levels

For real gases, except for some light ones like Hydrogen, the rotational energy quantum ε_{rot} is very small compared to the thermal energy (at the usual conditions when the gas temperature is not close to the absolute 0 K). For example, for Nitrogen one has $\varepsilon_{rot} / k = 2.9K$, and for Oxygen $\varepsilon_{rot} / k = 2.1K$. Let the characteristic gas temperature be T_0 . We then define the non- dimensional parameter $\chi = \varepsilon_{rot} / kT_0$. When $\chi \ll 1$ the spectrum contains a large number of levels and is dense. It can be considered as a “near continuous” spectrum. Because it may be difficult in some cases to compute the real spectrum with all the levels, an approximate approach can be employed without loss of accuracy. *It is not a strict approximation, but rather a reasonable model of the spectrum.* One considers the spectrum as continuous and applies some step of the discretization ε_{rot}^* preserving the degeneration rules. From physical consideration, one should preserve the condition $\chi^* = \varepsilon_{rot}^* / kT_{min} \ll 1$, or at least $\chi^* < 1$. This condition signifies that the energy threshold for the excitation of the rotations everywhere in the flow remains sufficiently small, as it is for the real spectrum. One may therefore suppose that better approximation is obtained with small χ^* , but larger value of χ^* leads to a fewer number of the efficient levels and may save the computational effort. According to our test computations of the SW problem for a wide range of Mach numbers from $M= 2$ to 25, the choice $\chi^* \leq 0.25$ gives quite satisfactory results. Additionally, it can be noted from equation (33) that for Nitrogen the probabilities of transitions from the levels i, j to the levels k, l don't explicitly contain the value of the rotational quantum. This gives an additional support for the proposed reduction in the rotational levels.

2.3 Solution of Classical / Generalized Boltzmann Equation for a Mixture of Monoatomic / Diatomic Gases

For solving the classical Boltzmann equation for a mixture of monoatomic gases or the Generalized Boltzmann equation for a mixture of diatomic gases, these equations are formulated in impulse space. These formulations are described below. *It should be noted that these formulations and solution methodology are completely new and have been developed for the first time by us for 3D Generalized Boltzmann equation.* Some previous work for an inert binary

mixture of monoatomic gases for the solution of 1D classical Boltzmann equation with cylindrical symmetry in velocity space has been reported by Raines [34].

2.3.1 Mixture of Monoatomic Gases

The system of Boltzmann kinetic equations for a mixture of monoatomic gases containing K components is usually written in the form

$$\frac{\partial f_i}{\partial t} + \xi_i \frac{\partial f_i}{\partial \mathbf{x}} = I_i, \quad i = 1, \dots, K \quad (37)$$

The collision integrals have the form

$$I_i = \sum_j \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f'_i f'_j - f_i f_j) g b d b d \varphi d \xi_j, \quad i = 1, \dots, K, j = 1, \dots, K \quad (38)$$

Here b_m is the maximum interaction distance and the following abbreviations have been used:

$f_i \equiv f_i(\xi_i, \mathbf{x}, t)$, $f_j \equiv f_j(\xi_j, \mathbf{x}, t)$, $f'_i \equiv f_i(\xi'_i, \mathbf{x}, t)$, $f'_j \equiv f_j(\xi'_j, \mathbf{x}, t)$, where $g = |\xi_i - \xi_j|$, b and φ being the impact parameters of the binary collision. The six components of the post collision velocities vectors ξ'_i and ξ'_j are defined by the three scalar conservation laws for the impulse, the energy conservation law, and by the two impact parameters. For construction of the conservative method of evaluation of the collision integrals for a gas mixture one needs to transform the equations from velocity variables to the impulse variables defined as $\mathbf{p}_i = m_i \xi_i$, m_i being the molecular mass. Thus,

$$(\xi_i, \mathbf{x}, t) \rightarrow (\mathbf{p}_i, \mathbf{x}, t), \quad f_i(\xi_i, \mathbf{x}, t) \rightarrow f_i^*(\mathbf{p}_i, \mathbf{x}, t). \quad (39)$$

From the condition of normalization on the particle density n_i of a specie

$$\int f_i d\xi = \int f_i^* d\mathbf{p} = n_i, \quad \text{one obtains}$$

$$f_i^* = m_i^{-3} f_i \quad (40)$$

In new impulse variables, the system of Boltzmann equations takes the form

$$\frac{\partial f_i^*}{\partial t} + \frac{\mathbf{p}_i}{m_i} \frac{\partial f_i^*}{\partial \mathbf{x}} = I_i^*, \quad i = 1, \dots, K \quad (41)$$

The collision integrals take the form

$$I_i^* = \sum_j \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_i^* f_j^* - f_i^* f_j^*) g^* b d b d \varphi d \mathbf{p}_j, \quad g^* = |\mathbf{p}_j / m_j - \mathbf{p}_i / m_i| \quad (42)$$

Note that in the subsequent equations, asterisks in equations (41) and (42) will be omitted. The integrals will be computed on a limited Cartesian impulse space Ω .

The system (41) is solved on a uniform 3-dimensional grid $\mathbf{p}_\gamma$ with N_0 points in impulse space Ω . For brevity, the values of the collision integrals and distribution functions in the grid nodes are marked as $I_{i,\gamma}$ and $f_{\alpha,\gamma}$. The system (41) of K equations is transformed in the system of $N_0 K$ equations

$$\frac{\partial f_{i,\gamma}}{\partial t} + \frac{\mathbf{p}_{i,\gamma}}{m_i} \frac{\partial f_{i,\gamma}}{\partial \mathbf{x}} = I_{i,\gamma}, \quad i = 1, \dots, K, \quad \gamma = 1, \dots, N_0 \quad (43)$$

For evaluation of the integrals (42), one builds the 8-dimensional uniform integration grid $\Xi = \xi_{i_v}, \xi_{j_v}, b_v, \varphi_v$ in impulse spaces $\Omega \times \Omega \times 2\pi \times b_m$ with N_v nodes in such a way that impulse nodes $\mathbf{p}_{\alpha,v}$ and $\mathbf{p}_{\beta,v}$ belong to the grid $\mathbf{p}_\gamma$. The integration grid nodes for which the post-collision impulses $\mathbf{p}'_{i,v}$ or $\mathbf{p}'_{j,v}$ fall outside Ω are excluded.

Consider a mixture component κ at the grid node γ . Introduce a combination of Dirac δ -functions and Kroneker symbols $\delta_{n,l}$, with $\delta_{n,l} = 1$, if $n = l$, and $\delta_{n,l} = 0$, if $n \neq l$.

$$\phi_{n,\gamma} = \delta_{n,i} \delta(\mathbf{p}_i - \mathbf{p}_{i,\gamma}) + \delta_{n,j} \delta(\mathbf{p}_j - \mathbf{p}_{j,\gamma}) - \delta_{n,i} \delta(\mathbf{p}'_i - \mathbf{p}_{i,\gamma}) + \delta_{n,j} \delta(\mathbf{p}'_j - \mathbf{p}_{j,\gamma}) \quad (44)$$

The collision operator for the n -th component at the node γ can be written in the form

$$I_{n,\gamma} = \frac{1}{4} \sum_i \sum_j \int_{\Omega} \int_0^{2\pi} \int_0^{b_m} \phi_{n,\gamma} (f'_i f'_j - f_i f_j) g \, b db d\varphi d\mathbf{p}_i d\mathbf{p}_j \quad (45)$$

The integral is evaluated as a sum at the grid Ξ .

The conservative projection method for evaluation of (45) consists of replacing the two last δ -functions in (44) by decompositions with a splitting coefficient $r_v \leq 1$ that has to be defined from the energy conservation law. For each contribution to the integral sum, omitting the sub-index v , one makes the decomposition

$$\begin{aligned} \delta(\mathbf{p}'_i - \mathbf{p}_{i,\gamma}) &= (1-r) \delta(\mathbf{p}_{i,\lambda} - \mathbf{p}_{i,\gamma}) + r \delta(\mathbf{p}_{i,\lambda+s} - \mathbf{p}_{i,\gamma}) \\ \delta(\mathbf{p}'_j - \mathbf{p}_{j,\gamma}) &= (1-r) \delta(\mathbf{p}_{j,\mu} - \mathbf{p}_{j,\gamma}) + r \delta(\mathbf{p}_{j,\mu-s} - \mathbf{p}_{j,\gamma}) \end{aligned} \quad (46)$$

In (46) the grid nodes $\mathbf{p}_{i,\lambda}$ and $\mathbf{p}_{j,\mu}$ are the nearest ones to the post collision vectors $\mathbf{p}'_i$ and $\mathbf{p}'_j$ correspondingly, when $\mathbf{p}_{i,\lambda+s}$, $\mathbf{p}_{j,\mu-s}$ are some complimentary nearly located grid nodes. Hence, the contributions to the collision integral in two near grid points are replaced by the weighted contributions in two pairs of the closest nodes.

The necessary condition to make this decomposition conservative is the fulfillment of the impulse conservation law. The transformation of the kinetic equation to the impulse space and the application of the uniform grid in Ω provide this condition.

Let $\mathbf{p}_i$ and $\mathbf{p}_j$ be the impulses before collision, and $\mathbf{p}'_i$, $\mathbf{p}'_j$ are the post collision impulses. We select the initial impulses at the grid nodes, therefore they can be presented as $\mathbf{p}_i = \mathbf{k}_1 h$ and $\mathbf{p}_j = \mathbf{k}_2 h$, where $\mathbf{k}_1$ and $\mathbf{k}_2$ are integer vectors and h is the mesh of the impulse space.

The impulse conservation law gives

$$\mathbf{p}_i + \mathbf{p}_j = \mathbf{p}'_i + \mathbf{p}'_j \quad (47)$$

Let the grid node nearest to $\mathbf{p}'_i$ be $\mathbf{p}_\lambda = \mathbf{k}_3 h$ and that nearest to $\mathbf{p}'_j$ be $\mathbf{p}_\mu$. Let $\mathbf{p}_\lambda = \mathbf{p}'_i - \Delta h$.

From (47) one gets $\mathbf{p}'_j = (\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3)h - \Delta h$, therefore $\mathbf{p}_\mu = \mathbf{p}'_j + \Delta h$ and one gets

$$\mathbf{p}_i + \mathbf{p}_j = \mathbf{p}_\lambda + \mathbf{p}_\mu \quad (48)$$

In a similar way, if the nodes $\mathbf{p}_{\lambda+s}$ and $\mathbf{p}_{\mu-s}$ are properly chosen, one can prove the equality

$$\mathbf{p}_i + \mathbf{p}_j = \mathbf{p}_{\lambda+s} + \mathbf{p}_{\mu-s} \quad (49)$$

From (48) and (49) it results that the decomposition (46) preserves the impulse conservation law.

The decomposition coefficient r can be defined from the energy conservation law.

Let the ν -th energy contribution to the nodes $\mathbf{p}_i$ and $\mathbf{p}_j$ be

$$-E_0 = \Delta_\nu \cdot \left(\frac{p_i^2}{2m_i} + \frac{p_j^2}{2m_j} \right), \quad (50)$$

where $\Delta_\nu = \frac{2\pi V^2}{4N_\nu N_0} f_i f_j g_\nu b_\nu$, V being the volume of the Ω space. Then the contribution to the nodes $\mathbf{p}_\lambda$, $\mathbf{p}_\mu$ is

$$E_1 = \Delta_v \cdot \left(\frac{p_\lambda^2}{2m_i} + \frac{p_\mu^2}{2m_j} \right), \quad (51)$$

and the contribution to the nodes $\mathbf{p}_{\lambda+s}$, $\mathbf{p}_{\mu-s}$ is

$$E_2 = \Delta_v \cdot \left(\frac{p_{\lambda+s}^2}{2m_i} + \frac{p_{\mu-s}^2}{2m_j} \right) \quad (52)$$

One should select the nodes $\mathbf{p}_{\lambda+s}$, $\mathbf{p}_{\mu-s}$ in such a way that the value E_0 lies between E_1 and E_2 .

The coefficient r_v can be defined from the energy conservation law $E_0 = (1-r_v)E_1 + r_v E_2$ that gives

$$r_v = \frac{E_0 - E_1}{E_2 - E_1}, \quad 0 \leq r_v \leq 1. \quad (53)$$

We have demonstrated that the transformation of the variables in the system of the Boltzmann kinetic equations from velocity space to the impulse space makes it possible to build the conservative projection method for the evaluation of the collision integrals.

2.3.2 Mixture of Diatomic Gases

The extension of the method described in section 3.3.1 to a mixture of diatomic gases described by a system of Wang Chang-Uhlenbeck equations (WC-UE) or generalized Boltzmann equations (GBE) can be done in an analogous manner. The GBE for a single component gas can be written in the velocity space as

$$\frac{\partial f_\alpha}{\partial t} + \xi_\alpha \frac{\partial f_\alpha}{\partial \mathbf{x}} = \sum_{\beta \chi \delta} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_\chi f_\delta \omega_{\alpha\beta}^{\chi\delta} - f_\alpha f_\beta) P_{\alpha\beta}^{\chi\delta} g_{\alpha\beta} b db d\varphi d\xi_\beta \quad (54)$$

Here indices $\alpha, \beta, \chi, \delta$ mark the energy levels, $\omega_{\alpha\beta}^{\chi\delta} = (q_\chi q_\delta) / (q_\alpha q_\beta)$, q_α is the degeneration of the energy level α , $P_{\alpha\beta}^{\chi\delta}$ is the probability of transition from levels α, β to the levels χ, δ , $g_{\alpha\beta} = |\xi_\alpha - \xi_\beta|$. For rotational levels one has $q_\alpha = 2\alpha + 1$ in most cases. For vibrational levels, the degeneration is absent and $q_\alpha = 1$. We assume that the degenerations are the same for all components of the mixture.

The generalization of (54) to the mixture of gases is quite evident:

$$\frac{\partial f_{i,\alpha}}{\partial t} + \xi_{i,\alpha} \frac{\partial f_{i,\alpha}}{\partial \mathbf{x}} = \sum_j \sum_{\beta \chi \delta} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_{i,\chi} f_{j,\delta} \omega_{\alpha\beta}^{\chi\delta} - f_{i,\alpha} f_{j,\beta}) P_{i,\alpha\beta}^{j,\chi\delta} g_{\alpha\beta} b db d\varphi d\xi_{j,\beta} \quad (55)$$

To build the conservative method of evaluation of the collision operator on the right hand side of (55), the equation is transformed to the impulse space in a similar way as in the case of the mixture of mono atomic gases. One gets

$$\frac{\partial f_{i,\alpha}}{\partial t} + \frac{\mathbf{p}_{i,\alpha}}{m_i} \frac{\partial f_{i,\alpha}}{\partial \mathbf{x}} = \sum_j \sum_{\beta \chi \delta} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_{i,\chi} f_{j,\delta} \omega_{\alpha\beta}^{\chi\delta} - f_{i,\alpha} f_{j,\beta}) P_{i,\alpha\beta}^{j,\chi\delta} g_{\alpha\beta} b db d\boldsymbol{\varphi} d\mathbf{p}_{j,\beta} \quad (56)$$

The important feature of inelastic collisions is that the impulse conservation law holds in the same form as given in equation (47) for the elastic collisions. As a consequence, the similar decomposition of the additions in the collision operator can be made with the single difference that the formulae (50-52) contain the energy ΔE transferred between the translational and internal degrees of freedom. One can exclude this value from consideration by choosing E_0 as the kinetic energy after the collision

$$E_0 = \Delta_v \cdot \left(\frac{p_{i,\chi}^2}{2m_i} + \frac{p_{j,\delta}^2}{2m_j} \right) \quad (57)$$

The formula (53) for the splitting coefficient r_v remains the same.

2.3.3 Special Case: Solution Methodology for a Binary Mixture of Diatomic Gases

In this section, we describe the solution method for a binary mixture of two diatomic gases as a special case of general methodology described in section 2.3.2. This methodology has been successfully coded to compute the hypersonic shock structure in an inert mixture of two gases as shown in Figure 11. It should be noted that it is applicable to a reactive mixture as well. We denote the distribution functions for the mixture components as $f_i^\alpha(\mathbf{p}, \mathbf{x}, t)$, where upper index α marks the specie, and index i marks the internal energy level. The generalized Boltzmann kinetic equations for the two components of the mixture can be written as:

$$\frac{\partial f_i^1}{\partial t} + \frac{\mathbf{p}}{m_1} \frac{\partial f_i^1}{\partial \mathbf{x}} = R_i^{(1,1)} + R_i^{(1,2)} \quad (58)$$

$$\frac{\partial f_i^2}{\partial t} + \frac{\mathbf{p}}{m_2} \frac{\partial f_i^2}{\partial \mathbf{x}} = R_i^{(2,2)} + R_i^{(2,1)}$$

where the collision operators are given by:

$$\begin{aligned}
R_i^{(1,1)} &= \sum_{jkl} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_k^1 f_l^1 \omega_{ij}^{kl} - f_i^1 f_j^1) P^{(1,1)kl}_{ij} g_{ij} b db d\phi d\mathbf{p}_{1,j} \\
R_i^{(2,2)} &= \sum_{jkl} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_k^2 f_l^2 \omega_{ij}^{kl} - f_i^2 f_j^2) P^{(2,2)kl}_{ij} g_{ij} b db d\phi d\mathbf{p}_{2,j} \\
R_i^{(1,2)} &= \sum_{jkl} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_k^1 f_l^2 \omega_{ij}^{kl} - f_i^1 f_j^2) P^{(1,2)kl}_{ij} g_{ij} b db d\phi d\mathbf{p}_{2,j} \\
R_i^{(2,1)} &= \sum_{jkl} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{b_m} (f_k^2 f_l^1 \omega_{ij}^{kl} - f_i^2 f_j^1) P^{(2,1)kl}_{ij} g_{ij} b db d\phi d\mathbf{p}_{1,j}
\end{aligned}$$

These equations have been written in the impulse space $\mathbf{p} = (p_x, p_y, p_z)$ in order to apply the conservative projection method described in section 2.3.2. The molecular masses should be normalized by some characteristic mass, for example $m_0 = 2m_1 m_2 / (m_1 + m_2)$, or simply $m_0 = m_1$. For masses close in values, the choice between two methods of normalizations is not important. We consider two main cases:

Case1: The characteristic length of the flow is not large enough for the vibration levels to be excited.

In this case the vibration levels are frozen and one may consider only the energy transfer between translational and rotational levels (RT transfer). The collision operators $R_i^{(1,1)}, R_i^{(2,2)}, R_i^{(1,2)}, R_i^{(2,1)}$ include only purely elastic collisions and those with RT energy transfer. For most gases, including Nitrogen and Oxygen, because of small value of the rotational energy quantum all the collisions are not elastic. The characteristic time of the RT process is 4 to 5 times larger than that for the elastic relaxation toward the local thermodynamic equilibrium. The main problem consists in evaluation of collision operators $R_i^{(1,1)}, R_i^{(2,2)}, R_i^{(1,2)}, R_i^{(2,1)}$. When this is done, the solution of the system (58) can be obtained by the application of the usual splitting procedure described in section 3.1 at a time step τ :

Step (a)

$$\frac{\partial f_i^{1*}}{\partial t} + \frac{\mathbf{p}}{m_1} \frac{\partial f_i^{1*}}{\partial \mathbf{x}} = 0 \quad (59a)$$

$$\frac{\partial f_i^{2*}}{\partial t} + \frac{\mathbf{p}}{m_2} \frac{\partial f_i^{2*}}{\partial \mathbf{x}} = 0$$

Step (b)

$$\frac{\partial f_i^1}{\partial t} = R_i^{(1,1)} + R_i^{(1,2)} \quad (59b)$$

$$\frac{\partial f_i^2}{\partial t} = R_i^{(2,2)} + R_i^{(2,1)}$$

At the second step the collision operators are evaluated with the functions marked by (*). It is natural to apply at this step a sub-splitting in the form

$$\frac{\partial f_i^{1**}}{\partial t} = R_i^{(1,1)} \quad (60a)$$

$$\frac{\partial f_i^1}{\partial t} = R_i^{(1,2)} \quad , \quad (60b)$$

and a similar procedure for the second equation of (59b). Here in (60a) the collision operator is computed by the distribution function f_i^{1*} and in (60b) by the distribution function f_i^{1**} .

A simple symmetric modification wherein the equation (60a) is solved at $\tau/2$, then (60b) is solved at τ , and finally (60a) is solved at $\tau/2$ can be applied for to increase the accuracy.

Case2: The characteristic length of the flow is so large that the vibration levels are also excited.

In this case one should take into account the huge difference in characteristic relaxation times for RT and VT processes. Let $\tau_{vib} = \varepsilon \tau_{rot}$, and Q_{vib} denote the VT collision operator. Then the inelastic parts of the corresponding collision operators can be estimated as $Q_{vib} = \varepsilon R_{rot}$, $\varepsilon \ll 1$, where the indices on the components and the energy levels have been omitted. The kinetic equations then take the form (vibration level is marked by the index α)

$$\frac{\partial f_{i,\alpha}^1}{\partial t} + \frac{\mathbf{p}}{m_1} \frac{\partial f_{i,\alpha}^1}{\partial \mathbf{x}} = R_{i,\alpha}^{(1,1)} + R_{i,\alpha}^{(1,2)} + Q_{i,\alpha}^{(1,1)} + Q_{i,\alpha}^{(1,2)} \quad (61a)$$

$$\frac{\partial f_{i,\alpha}^2}{\partial t} + \frac{\mathbf{p}}{m_1} \frac{\partial f_{i,\alpha}^2}{\partial \mathbf{x}} = R_{i,\alpha}^{(2,2)} + R_{i,\alpha}^{(2,1)} + Q_{i,\alpha}^{(2,2)} + Q_{i,\alpha}^{(2,1)} \quad (61b)$$

In principle, all the collision operators can be evaluated as the GBE operators, but this task is enormously difficult because the total number of levels now is equal to $i_{\max} \cdot \alpha_{\max}$, where the index indicates the numbers of the rotational and vibration levels. To make the problem solvable for a mixture one may apply the two-level model approach for the RT collision operators described below (without loss of accuracy), while the operators of VT exchange being evaluated in the complete GBE form. In this case the total number of the energy levels will be only two times the number of vibration levels thereby significantly reducing the computational effort.

2. 4 Two Levels Kinetic Model for R-T Relaxation in a Diatomic 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 $\varepsilon_2 > T_{\max}$, where $T_{\max}$ 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 being 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_{kin} , and the rotational energy E_{rot} . One can then determine the populations of the levels by the simple formulas $n_2 = E_{rot} / \varepsilon_2$ and $n_1 = n - n_2$. Maximal value of E_{rot} is given by $E_{rot} = n T_{\max}$, therefore $n_2 < n T_{\max} / \varepsilon_2$, and one obtains $0 < n_2 < n$ and $n_1 > 0$. Having E_{kin} , one can determine the equilibrium temperature $T_{eq} = 2(E_{kin} + E_{rot}) / 5n$, and the equilibrium rotational populations $n_{2,eq} < n T_{eq} / \varepsilon_2$, $n_{1,eq} = n - n_{2,eq}$. These parameters determine the equilibrium distribution functions $f_{1,M}$ and $f_{2,M}$.

For construction of the model equation we begin with the Wang Chang–Uhlenbeck equation (WC-UE) for the considered 2 levels system ($\{i, j, k\} = 1, 2$).

$$\partial f_i / \partial t = \sum_{j,k,l} \int p_{i,j}^{k,l} (f_k f_l - f_i f_j) g_{i,j} b db d\varphi d\xi_j \quad (62)$$

In equation (62), 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 [35], 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:

$$Q_{i,el} = \sum_j \int (f_i' f_j' - f_i f_j) g_{i,j} b db d\varphi d\xi_j \quad (63)$$

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

$$Q_{r,i} = -\nu_r (f_i - f_{i,M}^*) \quad (64)$$

It was found by a number of numerical experiments that the choice for $f_{i,M}^*$ in equation (64) 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

$$f_{i,M}^* = n_{i,eq} \left(\frac{m}{2\pi k} \right)^{3/2} (T_{xx}^* T_{yy}^* T_{zz}^*)^{-1/2} \exp(-mc_x^2 / 2kT_{xx}^* - mc_y^2 / 2kT_{yy}^* - mc_z^2 / 2kT_{zz}^*), \quad (65)$$

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

$$T_{aa}^* = T_{aa} (T_{eq} / T_{kin}) \quad (66)$$

The use of the function given in equation (65), 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 ν of the BGK model equation

$$\nu_r = a_1 \nu \quad (67)$$

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 R-T relaxation model contains two operators, the inelastic operator given by equation (64) with the frequency given by the equation (67), and the elastic operator $Q_{i,el}^* = (1 - a_2 \nu_r) Q_{i,el}$. The coefficients a_1 and a_2 can be determined from comparisons of the solutions of the proposed model with solutions of the WC-U equation. This model has been successfully applied to compute the hypersonic shock structure in Nitrogen with RT energy transfer as shown in Figures 12 and 13. There is good agreement between the results of two levels RT model and those obtained with solution of complete GBE.

3. RESULTS

Several milestones have been achieved which are described below. The details are given in References [18-21]. In what follows, some key computational results are presented.

1. A 3D Generalized Boltzmann Equation (GBE) solver has been developed for a Cartesian mesh. The solver has been validated by computing the 1D shock structure in nitrogen for Rotational-Translational (R-T) relaxations and comparing the numerical results with the experimental data for Mach numbers up to 15. Figure 2 shows the comparison of computed solution with the experimental data of Alsemeyer [31] for shock structure in nitrogen at Mach 10; excellent agreement is obtained [19]. Figures 3, 4 and 5 show the details of the computed solutions for shock structure at $M=15$ [19]. Figure 3 shows the variation in flow properties over the shock thickness, Figure 4 shows the rotational spectrum i.e. the variation in population density of various rotational energy levels at different locations in the shock wave, and Figure 5 shows the variation in rotational spectral populations in the shock region and upstream and downstream of the shock. Figures 4 and 5 are very instructive in providing the information as to which rotational energy levels contribute most to the shock structure. The solver has been exercised successfully for computing the 2D blunt body flows in nitrogen up to Mach 7 and for Knudsen numbers ranging from 0.01 to 10 [20]. Figure 6 shows the flow field contours for density and rotational temperature at $Kn = 0.1$ when the flow is in transitional regime. Figures 7 and 8 show the flow properties along the stagnation line. These results are in good agreement with the DSMC calculations performed by Dr. Bondar in Professor Ivanov's group in Novosibirsk, Russia using the "SMILE" code. The solver has also been exercised successfully for computing 3D flow from a rectangular jet of nitrogen exiting in vacuum for RT relaxations. Figures 9(a) – 9(c) show density, temperature and rotational temperature contours respectively in $z = 0$ plane, and Figure 9(d) shows the variation in density, temperature and rotational temperature along the centerline of the 3D rectangular jet of nitrogen exiting in vacuum. The issues of stability of the algorithm and the possibility of reducing the number of rotational levels in the computations without compromising the accuracy of the solutions have also been rigorously addressed.

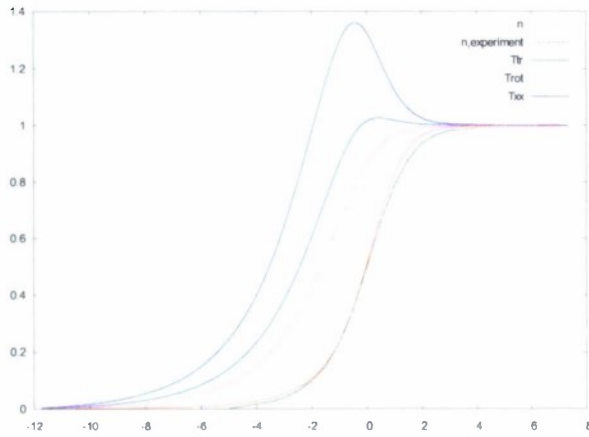


Figure 2: Shock Wave Structure in Nitrogen for $M=10$; n = computed density, $n_{\text{experimental}}$ = experimental density, T = total temp, T_{xx} = translational temp, T_{rot} = rotational temp (normalized)

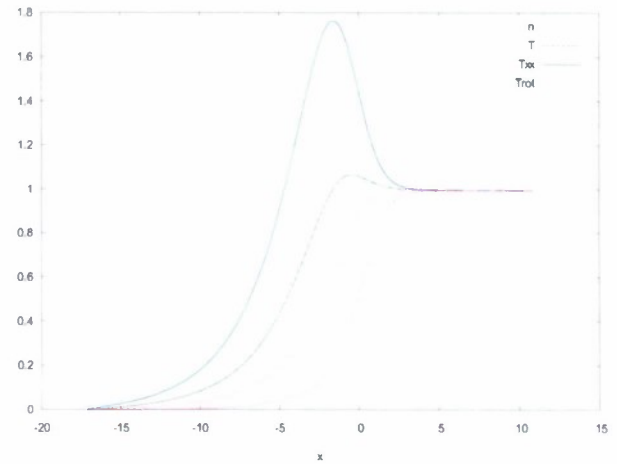


Figure 3: Shock Wave Structure in Nitrogen for $M=15$, n = computed density, T = total temp, T_{xx} = Translational temp, T_{rot} = rotational temp (normalized)

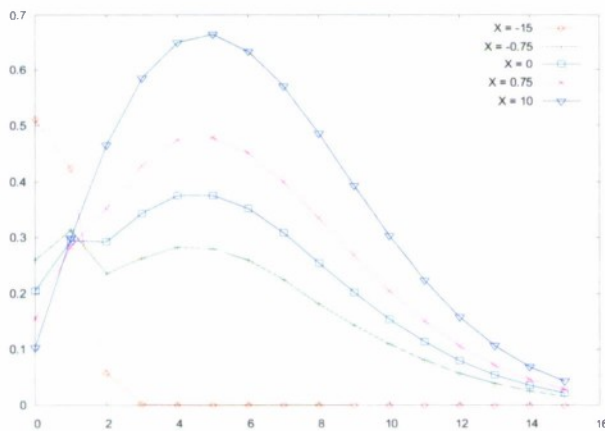


Figure 4: Rotational Spectrum in SW in Nitrogen at $M=15$

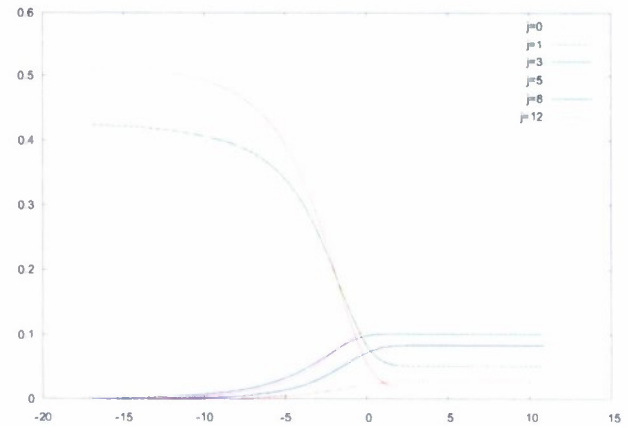
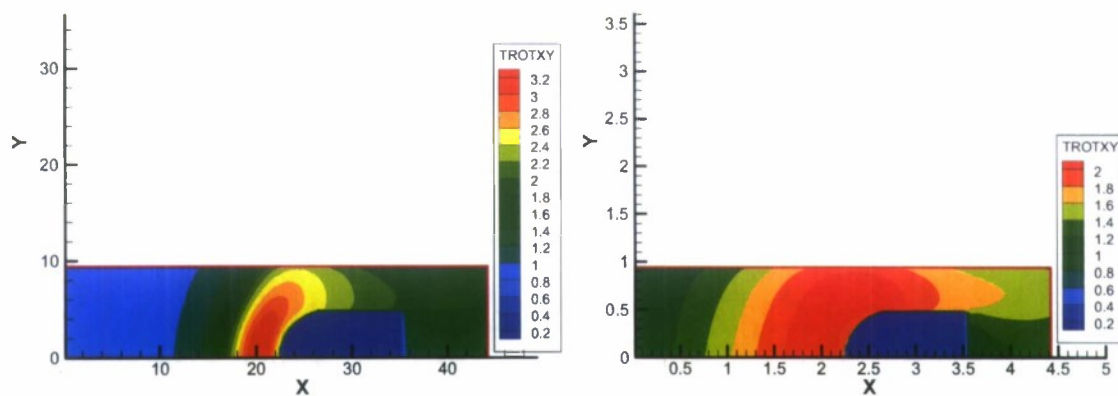


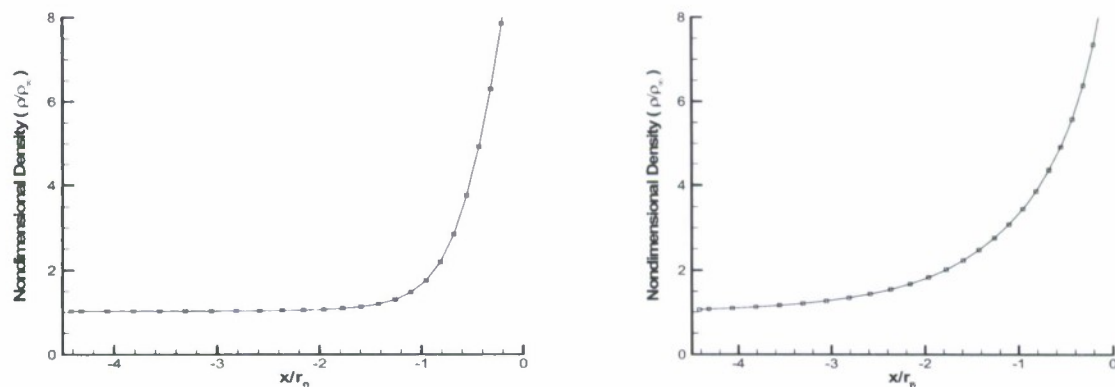
Figure 5: Variation of Spectral Population in SW in Nitrogen at $M=15$



$Kn = 0.1$

$Kn = 1.0$

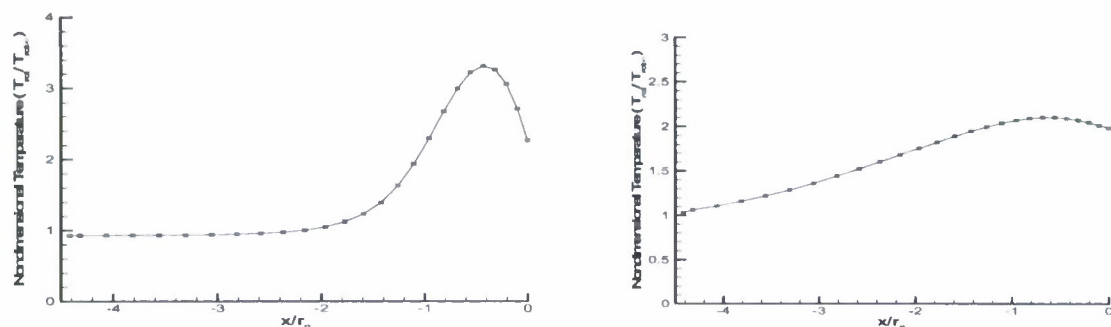
Figure 6: Rotational Temperature Contours for Flow Past a Blunt Body; $M = 7$



$Kn = 0.1$

$Kn = 1.0$

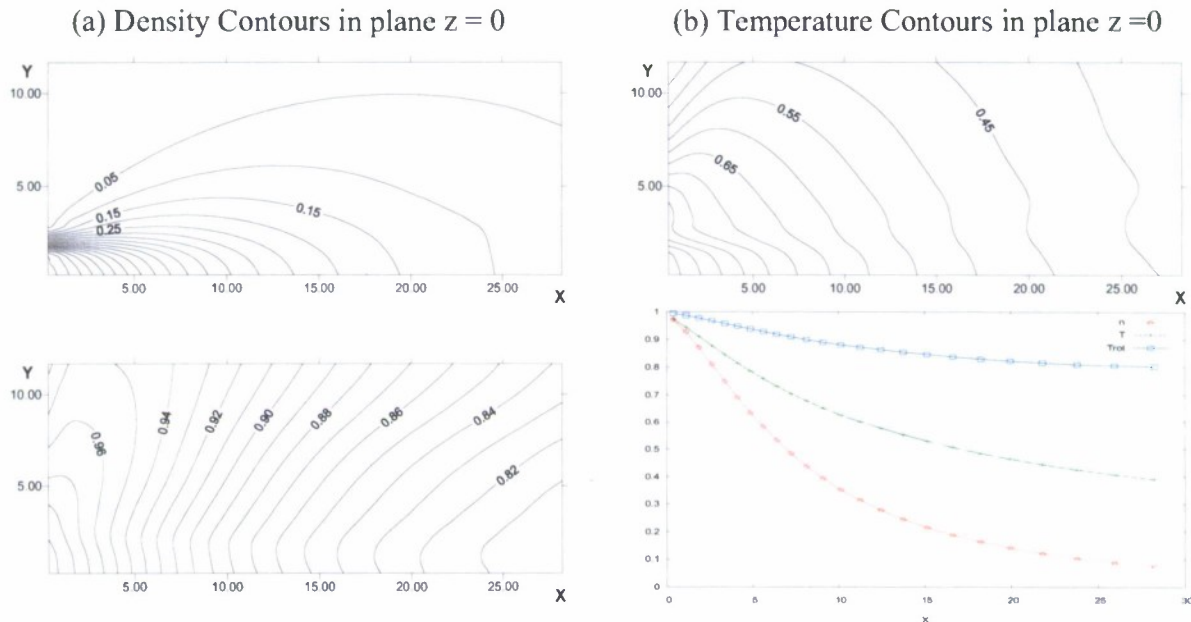
Figure 7: Density along the Stagnation Line for Flow Past a Blunt Body, $M = 7$



$Kn = 0.1$

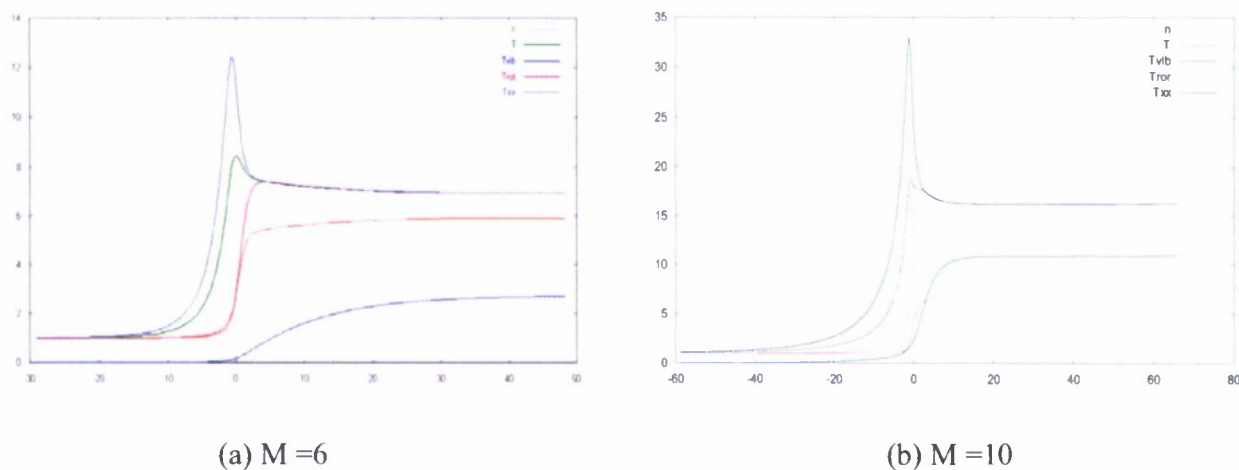
$Kn = 0.1$

Figure 8: Rotational Temperature along the Stagnation Line for Flow Past a Blunt Body, $M = 7$



(e) Rotational Temperature Contours in $z = 0$ (d) Variation in Properties along the Jet Centerline
Figure 9: 3D Supersonic Flow of a Rectangular N_2 Jet in Vacuum, $M=2$, $T_0 = 200K$, $dy = 2\lambda$, $dz = 8\lambda$

2. A computational methodology has been developed to compute the hypersonic shock structure in diatomic gases including both the RT and Vibrational-Translational (V-T) relaxations [18]. 1-D shock structure in nitrogen has been computed including both R-T and V-T relaxations and has been validated by comparing the results with experimental data. The V-T methodology is currently being extended to 3D in the 3D Boltzmann solver described in the item 1 above. Figure 10 shows the variation in flow properties across the shock at $M=6$ and $M=10$.



(a) $M = 6$ (b) $M = 10$
Figure 10: SW in Nitrogen including both R-T and V-T Relaxations

3. A computational methodology has been developed to compute the hypersonic shock structure in a non-reactive mixture of two diatomic gases. 1-D shock structure has been computed in an inert mixture of two gases with R-T relaxations. To accomplish this, the GBE is formulated and solved in “impulse space” instead of velocity space. Figure 11 shows the shock structure in a binary mixture of two gases of mass ratio $m_2/m_1 = 2$, and the ratio of molecular diameters $d_2/d_1=1.5$. It should be noted that it is easier to compute the shock structure in an inert mixture of oxygen and nitrogen because the mass ratio is 1.143 and molecular diameter ratio is 1.0. The code can be easily applied to a mixture containing an arbitrary number of species.

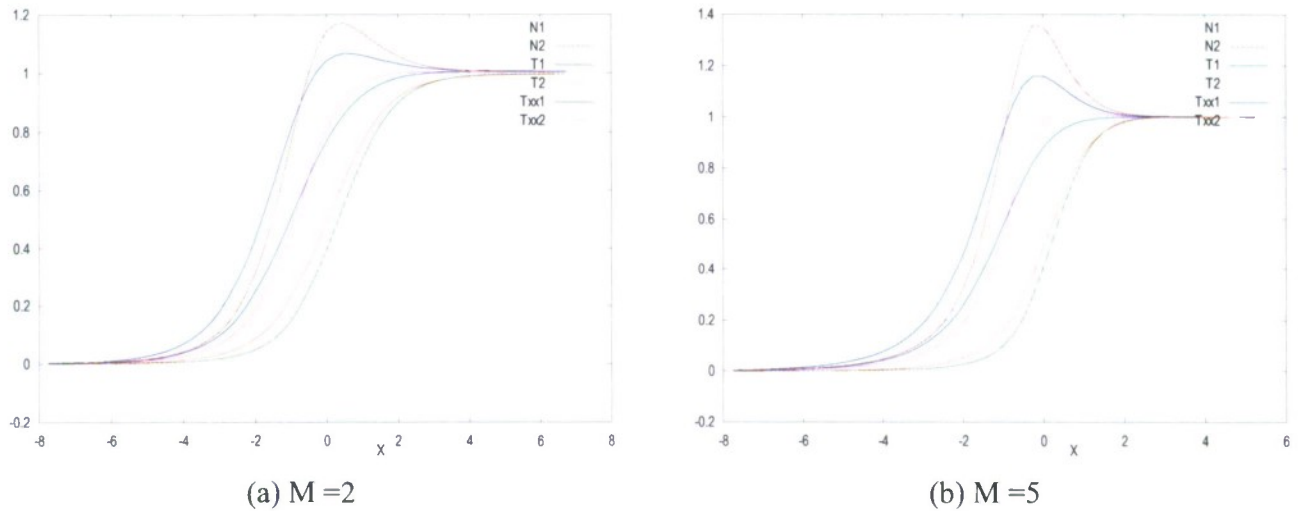


Figure 11: SW in an Inert Mixture of Two Diatomic Gases

4. A new two-level kinetic model has been developed for computing the RT relaxations in a diatomic gas and has been validated by comparing the results with the solutions of complete GBE [18]. The model is about twenty times more efficient than the GBE in computing the shock structure. It should be noted that the model is different than the BGK model; it accounts for both elastic and inelastic collisions. Figures 12 and 13 show the comparisons of flow properties using the two-level kinetic level and the complete GBE for hypersonic shock structure in nitrogen with R-T relaxations at $M = 2.4$ and 10. The agreement between the two solutions is excellent at lower Mach number of 2.4 and is reasonable at $M = 10$. It should be noted that a similar model is currently under development for V-T relaxations. These models can provide extremely efficient

solutions for gas flows of diatomic gases with both R-T and V-T relaxations with acceptable accuracy.

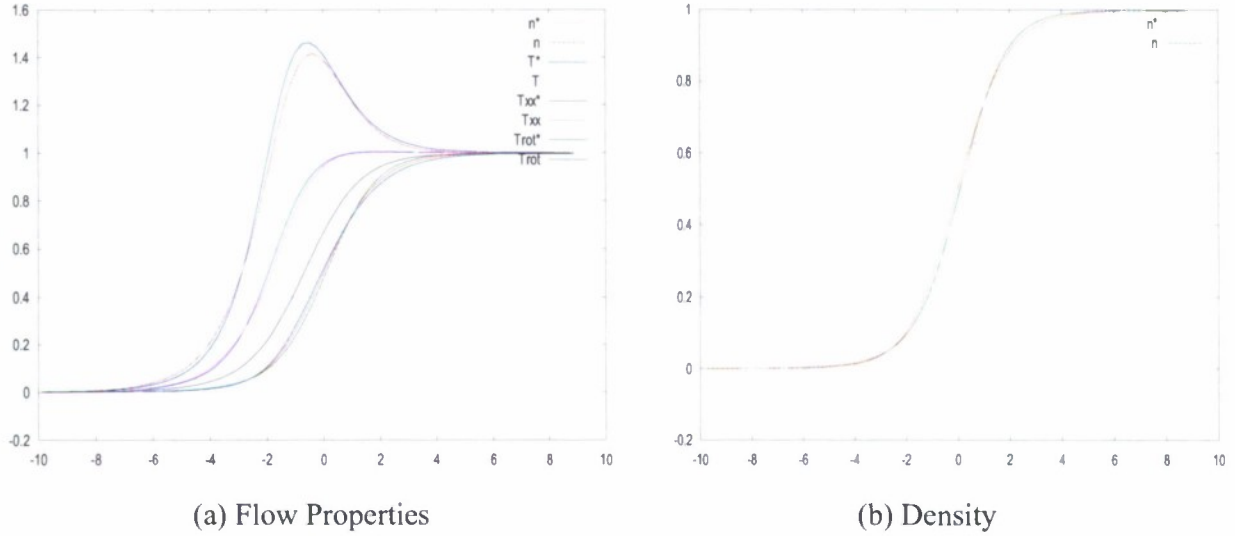


Figure 12: Comparison of SW in Nitrogen with R-T Relaxations with Complete GBE and Two-Level R-T Model (shown by *), $M=2.4$

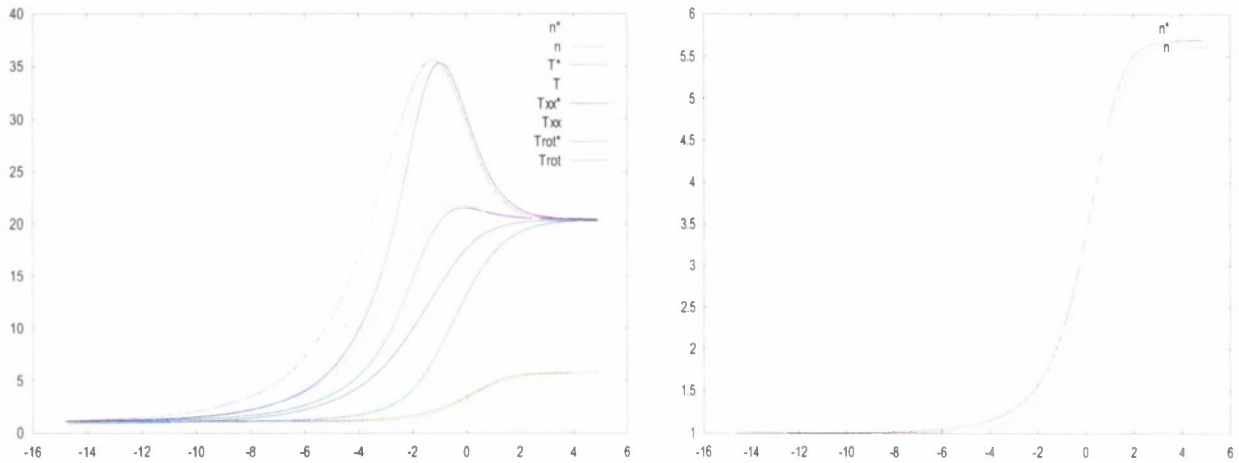


Figure 13: Comparison of SW in Nitrogen with R-T Relaxations with Complete GBE and Two-Level R-T Model (shown by *), $M=10$.

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