

A Macroscopic Gas Model with Translational and Rotational Nonequilibrium

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Abstract—A mathematical model of viscous compressible gas flows is constructed, which makes allowance for nonequilibrium of the system with respect to translational and rotational degrees of freedom. In the equilibrium case, the constructed equations are reduced to a previously derived quasi-gasdynamic system for a polyatomic gas. Numerical results obtained for shock-wave flows and for a relaxation problem are discussed and compared with those based on the kinetic approach.

1. INTRODUCTION

An original mathematical model of viscous compressible gas flows, called the quasi-gasdynamic (QGD) equations, was proposed in [1, 2]. These equations were shown to be well suited for computing several gas-dynamics problems, in particular, for simulation of moderately rarefied gas flows [3]. This study extends the QGD equations to gases with translational–rotational thermal nonequilibrium, which is characteristic of rarefied flows of diatomic or polyatomic gases [4–6].

A molecule is treated as a rigid body having only translational and rotational degrees of freedom. This description is valid if the gas temperature is neither too high (the vibrational degrees of freedom are not excited) nor too low (the rotational degrees of freedom can be treated in the classical approximation).

2. MOLECULAR MODEL AND DISTRIBUTION FUNCTIONS

2.1. Expressions for the energy of molecules. All molecules are assumed to be identical rigid rotators. The total energy of a molecule is then equal to its kinetic energy and can be written as

$$E_m = \frac{m_0}{2} \xi^2 + E_r,$$

where E_r is the rotational energy; m_0 is the mass of the molecule; and $\xi = \mathbf{u} + \mathbf{c}$ is the velocity of its center of mass, which can be represented as the sum of macroscopic velocity \mathbf{u} and thermal velocity \mathbf{c} .

In the case of a polyatomic molecule, the rotational energy is

$$E_r^{(3)} = \frac{1}{2}(I_1^0 \omega_1^2 + I_2^0 \omega_2^2 + I_3^0 \omega_3^2), \quad (2.1)$$

where I_1^0 , I_2^0 , and I_3^0 are the principal moments of inertia of the molecule and ω_1 , ω_2 , and ω_3 are the angular velocities relative to the principal axes denoted by the indices 1–3 (see [7, p. 128]). The molecule has six degrees of freedom, of which three are translational and three are rotational (the number of internal degrees of freedom is $\zeta = 3$). In what follows, this system is referred to as the 3R gas.

In the case of linear (e.g., diatomic) molecules, which have two rotational degrees of freedom ($\zeta = 2$), the rotational energy is written as

$$E_r^{(2)} = \frac{I^0}{2}(\omega_1^2 + \omega_2^2), \quad (2.2)$$

where I^0 is the principal moment of inertia with respect to the axis perpendicular to the symmetry axis of the molecule. This model is referred to as the 2R gas.

2.2. Distribution functions and equations of state. The state of a gas of rigid rotators can be described by a single-particle distribution function $f(t, \mathbf{R}, \xi, \omega)$, which depends on time t , coordinate \mathbf{R} , center-of-mass velocity ξ , and angular velocity ω . This function is normalized by the relation

$$d\rho = f d\xi d\omega,$$

where ρ is the mass density of the gas.

We consider the locally equilibrium two-temperature Maxwell–Boltzmann distribution function [6, p. 109]

$$f_{0r} = f_0 f_r, \quad (2.3)$$

which is the product of the Maxwell distribution over the translational degrees of freedom

$$f_0 = \rho \left(2\pi \frac{\mathcal{R}}{\mathcal{M}} T_t \right)^{-3/2} \exp\left(-\frac{\mathbf{c}^2}{2(\mathcal{R}/\mathcal{M})T_t} \right)$$

and the Hinshelwood distribution function over the rotational degrees of freedom [4, p. 104]

$$f_r = \mathcal{A} \exp\left(-\frac{E_r}{kT_r} \right),$$

where \mathcal{A} is the normalization constant. For a gas with two rotational degrees of freedom (2R), the distribution has the form

$$f_r^{2R} = \left(2\pi \frac{\mathcal{R}}{I} T_r \right)^{-1} \exp\left(-\frac{\omega_1^2 + \omega_2^2}{2(\mathcal{R}/I)T_r} \right).$$

For a gas with three rotational degrees of freedom (3R gas), it has the form

$$f_r^{3R} = (2\pi \mathcal{R} T_r)^{-1} (I_1 I_2 I_3)^{1/2} \exp\left(-\frac{\omega_1^2}{2(\mathcal{R}/I_1)T_r} - \frac{\omega_2^2}{2(\mathcal{R}/I_2)T_r} - \frac{\omega_3^2}{2(\mathcal{R}/I_3)T_r} \right).$$

Here, \mathcal{R} is the universal gas constant, \mathcal{M} is the molar mass of the gas, $I = I^0 N_A$, $I_\alpha = I_\alpha^0 N_A$ ($\alpha = 1, 2, 3$), N_A is Avogadro's number, $k = \mathcal{R}/N_A$ is the Boltzmann constant, T_t is the translational temperature (equal for all translational degrees of freedom of a molecule), and T_r is the rotational temperature (equal for all rotational degrees of freedom of a molecule).

The normalization constant \mathcal{A} is determined by the condition

$$\int f_r d\boldsymbol{\omega} = 1.$$

This representation of the distribution function is valid if the gas temperature is neither too high (no vibrational degrees of freedom are excited) nor too low (i.e., the rotational degrees of freedom can be treated in the classical approximation) [8].

The distribution functions f and f_{0r} are interrelated and determine macroscopic characteristics of the gas:

$$\int f d\xi d\boldsymbol{\omega} = \int f_{0r} d\xi d\boldsymbol{\omega} = \rho, \quad (2.4)$$

$$\int \xi f d\xi d\boldsymbol{\omega} = \int \xi f_{0r} d\xi d\boldsymbol{\omega} = \rho \mathbf{u}. \quad (2.5)$$

Hereafter, the limits of integration are infinite. Note that

$$\int \mathbf{c} f d\xi d\boldsymbol{\omega} = \int \mathbf{c} f_{0r} d\xi d\boldsymbol{\omega} = 0.$$

The translational temperature is determined by the kinetic energy of thermal translational motion:

$$\frac{3}{2} \rho \frac{\mathcal{R}}{\mathcal{M}} T_t = \frac{1}{2} \int \mathbf{c}^2 f d\xi d\boldsymbol{\omega} = \frac{1}{2} \int \mathbf{c}^2 f_{0r} d\xi d\boldsymbol{\omega}.$$

The pressure associated with the translational temperature of a particle is defined as

$$p_t = \frac{1}{3} \int \mathbf{c}^2 f d\xi d\boldsymbol{\omega} = \frac{1}{3} \int \mathbf{c}^2 f_{0r} d\xi d\boldsymbol{\omega} = \rho \frac{\mathcal{R}}{\mathcal{M}} T_t.$$

The rotational energy ε_ω of a particle (see [8]) is defined for the 2R gas as

$$\varepsilon_\omega^{2R} = \frac{I}{2\mathcal{M}} (\omega_1^2 + \omega_2^2), \quad (2.6)$$

and for the 3R gas as

$$\varepsilon_{\omega}^{3R} = \frac{1}{2\mathcal{M}}(I_1\omega_1^2 + I_2\omega_2^2 + I_3\omega_3^2). \quad (2.7)$$

In the new variables, the distribution functions of the rotational energy are written as

$$f_r^{2R} = \frac{I}{2\pi\mathcal{R}T_r} \exp\left(-\frac{\varepsilon_{\omega}^{2R}}{(\mathcal{R}/\mathcal{M})T_r}\right)$$

and

$$f_r^{3R} = \frac{\sqrt{I_1 I_2 I_3}}{2\pi\mathcal{R}T_r} \exp\left(-\frac{\varepsilon_{\omega}^{3R}}{(\mathcal{R}/\mathcal{M})T_r}\right).$$

The temperature T_r and pressure p_r associated with the rotational energy of particles are defined as

$$\rho \frac{\mathcal{R}}{\mathcal{M}} T_r = p_r = \int \varepsilon_{\omega}^{2R} f d\xi d\omega = \int \varepsilon_{\omega}^{2R} f_{0r} d\xi d\omega \quad (2.8)$$

for the 2R gas and

$$\rho \frac{\mathcal{R}}{\mathcal{M}} T_r = p_r = \frac{2}{3} \int \varepsilon_{\omega}^{3R} f d\xi d\omega = \frac{2}{3} \int \varepsilon_{\omega}^{3R} f_{0r} d\xi d\omega \quad (2.9)$$

for the 3R gas.

The relations above imply that the kinetic energy per unit mass of the gas, which includes the translational and rotational energies, can be written as

$$E = \int \left(\frac{\xi^2}{2} + \varepsilon_{\omega} \right) f d\xi d\omega = \int \left(\frac{\xi^2}{2} + \varepsilon_{\omega} \right) f_{0r} d\xi d\omega = E_t + E_r, \quad (2.10)$$

where

$$\begin{aligned} E_t &= \frac{1}{2} \int \xi^2 f d\xi d\omega = \frac{1}{2} \int \xi^2 f_{0r} d\xi d\omega = \frac{\rho \mathbf{u}^2}{2} + \frac{3}{2} p_t, \\ E_r^{2R} &= \int \varepsilon_{\omega}^{2R} f d\xi d\omega = \int \varepsilon_{\omega}^{2R} f_{0r} d\xi d\omega = \rho \frac{\mathcal{R}}{\mathcal{M}} T_r = p_r, \\ E_r^{3R} &= \int \varepsilon_{\omega}^{3R} f d\xi d\omega = \int \varepsilon_{\omega}^{3R} f_{0r} d\xi d\omega = \frac{3}{2} \rho \frac{\mathcal{R}}{\mathcal{M}} T_r = \frac{3}{2} p_r. \end{aligned}$$

In summary, we note that the total energy is given by $E = E_t + E_r$, the average temperature is related to the average pressure by the equation of state $p_{av} = \rho(\mathcal{R}/\mathcal{M})T_{av}$, and the average pressure is calculated as

$$p_{av} = \frac{3p_t + \zeta p_r}{3 + \zeta}, \quad \text{where } \zeta = 2, \text{ for the 2R gas and } \zeta = 3 \text{ for the 3R gas.}$$

3. COORDINATE SYSTEMS AND CERTAIN INTEGRALS

Let us introduce a Cartesian coordinate system (x, y, z) in the physical space and the corresponding radius vector \mathbf{R} . For a vector function $\mathbf{u}(\mathbf{R})$ of spatial coordinates, the quantities u_x , u_y , and u_z denote its x -, y -, and z -projections, respectively.

Let us introduce an arbitrary curvilinear coordinate system (η^1, η^2, η^3) . For the same vector function $\mathbf{u}(\mathbf{R})$, u_i denotes the covariant coordinate:

$$u_i = \mathbf{u} \cdot \mathbf{R}_i, \quad \text{where } \mathbf{R}_i = \partial \mathbf{R} / \partial \eta^i.$$

The contravariant coordinates have the form $u^i = g^{ij} u_j$, where $g^{ij} = \mathbf{R}^i \cdot \mathbf{R}^j$ is the metric tensor. The vectors \mathbf{R}^i satisfy the equations

$$\mathbf{R}_i \cdot \mathbf{R}^j = \delta_i^j, \quad \delta_i^j = 1(0), \quad i = (\neq) j.$$

Moreover, we have

$$u^i = \mathbf{u} \cdot \mathbf{R}^i, \quad u_i = g_{ij}u^j, \quad g_{ik}g^{jk} = \delta_i^j, \quad g_{ij} = \mathbf{R}_i \cdot \mathbf{R}_j.$$

In terms of Cartesian coordinates, u^i can be expressed as

$$u^i = \mathbf{u} \cdot \mathbf{R}^i = u_x R_x^i + u_y R_y^i + u_z R_z^i, \quad (3.1)$$

where R_x^i , R_y^i , and R_z^i are, respectively, the x -, y -, and z -projections of \mathbf{R}^i . The metric tensor can be expressed as

$$g^{ij} = \mathbf{R}^i \cdot \mathbf{R}^j = R_x^i R_x^j + R_y^i R_y^j + R_z^i R_z^j. \quad (3.2)$$

Let us also introduce two velocity spaces, the space of linear velocities and the space of angular velocities. The radius vector in the space of linear velocities is denoted by ξ . In terms of spatial coordinates, it can be treated as a constant vector field ξ^i :

$$\nabla_j \xi^i = 0, \quad (3.3)$$

where ∇_j is the covariant derivative [9]. In the space of linear velocities, we introduce a Cartesian coordinate system (ξ_x, ξ_y, ξ_z) whose axes are aligned with the axes of the Cartesian coordinate in the space of \mathbf{R} .

In the space of angular velocities, we introduce a Cartesian coordinate system $(\omega_1, \omega_2, \omega_3)$ whose axes are aligned with the principal axes of a molecule treated as a rigid body. These coordinate axes differ for different molecules.

Below, we calculate integrals in the space of linear velocities ξ and in the space of angular velocities ω with respect to the corresponding Cartesian coordinates. A set of moment equations is constructed in the curvilinear coordinate system (η^1, η^2, η^3) .

Let us evaluate certain integrals useful for further analysis, using (3.1) and (3.2):

$$\int c^i f_0 d\mathbf{c} = \int (c_x R_x^i + c_y R_y^i + c_z R_z^i) f_0 d\mathbf{c} = R_x^i \int \int \int c_x f_0 d c_x d c_y d c_z + \dots = 0, \quad (3.4)$$

$$\int c_i f_0 d\mathbf{c} = g_{ik} \int c^k f_0 d\mathbf{c} = 0, \quad (3.5)$$

$$\begin{aligned} \int c^i c^j f_0 d\mathbf{c} &= \int (c_x R_x^i + c_y R_y^i + c_z R_z^i)(c_x R_x^j + c_y R_y^j + c_z R_z^j) f_0 d\mathbf{c} \\ &= R_x^i R_x^j \int c_x^2 f_0 d\mathbf{c} + R_y^i R_y^j \int c_y^2 f_0 d\mathbf{c} + R_z^i R_z^j \int c_z^2 f_0 d\mathbf{c} = (\mathbf{R}^i \cdot \mathbf{R}^j) p_t = g^{ij} p_t, \end{aligned} \quad (3.6)$$

$$\int c^i c^j c^k f_0 d\mathbf{c} = 0, \quad (3.7)$$

$$\int c_x^4 f_0 d\mathbf{c} = \int c_y^4 f_0 d\mathbf{c} = \int c_z^4 f_0 d\mathbf{c} = 3 \frac{p_t^2}{\rho}, \quad (3.8)$$

$$\int c_x^2 c_y^2 f_0 d\mathbf{c} = \int c_x^2 c_z^2 f_0 d\mathbf{c} = \int c_y^2 c_z^2 f_0 d\mathbf{c} = \frac{p_t^2}{\rho}, \quad (3.9)$$

$$\int c^i c^j c^2 f_0 d\mathbf{c} = 5 \frac{p_t^2}{\rho} g^{ij}. \quad (3.10)$$

The limits of integration in all of these integrals are infinite. The following relations are used here:

$$\int_{-\infty}^{\infty} \exp(-y^2) dy = \sqrt{\pi}, \quad \int_{-\infty}^{\infty} y^2 \exp(-y^2) dy = \frac{1}{2} \sqrt{\pi}, \quad \int_{-\infty}^{\infty} y^4 \exp(-y^2) dy = \frac{3}{4} \sqrt{\pi}.$$

4. CONSTRUCTION OF MOMENT EQUATIONS

The behavior of the distribution function f is described by the Boltzmann equation

$$\partial f / \partial t + (\xi \nabla) f = \mathcal{F}, \quad (4.1)$$

where \mathcal{F} is the collision integral. The conventional way to derive moment equations for viscous gas flows is as follows. The function f is approximated by an expansion in powers of a small parameter about its equilibrium value, and the resulting kinetic equation is averaged with summation invariants [4, 5].

To construct equations that take into account translational–rotational nonequilibrium (the so-called QGDR system), we replace f by its approximate value f^{QGDR} , which is an expansion in powers of a small parameter (gradient expansion) having the form

$$f^{QGDR} = f_{0r} - \tau(\xi \nabla) f_{0r}.$$

Here, τ is the Maxwellian relaxation time:

$$\tau = \mu / p_t,$$

where $\mu \sim T_i^s$ is the gas viscosity calculated for the translational temperature of particles [8] and s is determined by the law of intermolecular interaction [4].

The formal substitution

$$f \longrightarrow f^{QGDR}$$

in the convective term of the Boltzmann equation (4.1) results in the approximate equation

$$\partial f / \partial t + (\xi \nabla) f_{0r} - (\xi \nabla) \tau (\xi \nabla) f_{0r} = \mathcal{I}. \quad (4.2)$$

A similar approximate equation was used previously to construct the QGD equations [1, 2].

The macroscopic QGDR equations are derived by moment averaging of (4.2) over the velocity space. The derivation procedure for these equations is similar to that described in [9].

Using (3.3), we rewrite (4.2) in indexed form as

$$\partial f / \partial t + \nabla_i \xi^i f_{0r} - \nabla_i \tau \nabla_j \xi^i \xi^j f_{0r} = \mathcal{I}. \quad (4.3)$$

Integrating (4.3) with weight 1 and using (2.4), (3.4), and (3.6), we obtain

$$\begin{aligned} \int \frac{\partial f}{\partial t} d\xi d\omega &= \frac{\partial}{\partial t} \int f d\xi d\omega = \frac{\partial}{\partial t} \rho, \\ \int \nabla_i \xi^i f_{0r} d\xi d\omega &= \nabla_i \int (u^i + c^i) f_0 d\mathbf{c} \int f_r d\omega = \nabla_i \rho u^i, \\ \int \nabla_i \tau \nabla_j \xi^i \xi^j f_{0r} d\xi d\omega &= \nabla_i \tau \nabla_j \int (u^i + c^i)(u^j + c^j) f_0 d\mathbf{c} \\ &= \nabla_i \tau \nabla_j (\rho u^i u^j + \int c^i c^j f_0 d\mathbf{c}) = \nabla_i \tau \nabla_j (\rho u^i u^j + g^{ij} p_t). \end{aligned}$$

Since unity is a summation invariant for the Boltzmann collision integral, the integral on the right-hand side vanishes:

$$\int \mathcal{I} d\xi d\omega = 0.$$

Thus, we obtain the continuity equation

$$\frac{\partial}{\partial t} \rho + \nabla_i \rho u^i = \nabla_i \tau \nabla_j (\rho u^i u^j + g^{ij} p_t). \quad (4.4)$$

To derive the momentum equation, we integrate (4.3) with weight ξ^k , using (2.5), (3.4), (3.6), and (3.7):

$$\begin{aligned} \int \frac{\partial f}{\partial t} \xi^k d\xi d\omega &= \frac{\partial}{\partial t} \rho u^k, \\ \int \nabla_i \xi^i f_{0r} \xi^k d\xi d\omega &= \nabla_i (\rho u^i u^k + g^{ik} p_t), \\ \int \nabla_i \tau \nabla_j \xi^i \xi^j f_{0r} \xi^k d\xi d\omega &= \rho u^i u^j u^k + p_t (u^k g^{ij} + u^j g^{ik} + u^i g^{jk}). \end{aligned}$$

Since ξ^k is a summation invariant, we have

$$\int \mathcal{I} \xi^k d\xi d\omega = 0.$$

Combining the above relations yields the following equation for ρu^k :

$$\frac{\partial}{\partial t} \rho u^k + \nabla_i (\rho u^i u^k + g^{ik} p_t) = \nabla_i \tau \nabla_j [\rho u^i u^j u^k + p_t (u^k g^{ij} + u^j g^{ik} + u^i g^{jk})]. \quad (4.5)$$

To derive an equation for E_t , we average (4.3) with weight $\xi^2/2$, using (3.4)–(3.10):

$$\begin{aligned} \int \frac{\partial f}{\partial t} \frac{\xi^2}{2} d\xi d\omega &= \frac{\partial}{\partial t} E_t, \\ \int \nabla_i \xi^i f_{0r} \frac{1}{2} \xi^2 d\xi d\omega &= \nabla_i \frac{1}{2} \int (u^i + c^i) f_0 \xi^2 d\mathbf{c} = \nabla_i u^i (E_t + p_t), \\ \int \nabla_i \tau \nabla_j \xi^i \xi^j f_{0r} \frac{\xi^2}{2} d\xi d\omega &= \nabla_i \tau \nabla_j \left(u^i u^j E_t + 2u^i u^j p_t + \frac{1}{2} u_k u^k g^{ij} p_t + \frac{5}{2} \frac{p_t}{\rho} g^{ij} \right). \end{aligned}$$

For the collision integral \mathcal{F} , a $\xi^2/2$ is not a summation invariant, because the translational and rotational degrees of freedom may exchange energy. Thus, the last integral does not vanish. It is called the exchange term and denoted as follows:

$$\int \mathcal{F} \frac{\xi^2}{2} d\xi d\omega = S_t.$$

Combining the above expressions and differentiating by parts the last term (with pressure squared), we obtain

$$\frac{\partial}{\partial t} E_t + \nabla_i u^i (E_t + p_t) = \nabla_i \tau \nabla_j \left(u^i u^j E_t + 2u^i u^j p_t + \frac{1}{2} u_k u^k g^{ij} p_t \right) + \frac{5}{2} \nabla_i \tau \frac{p_t}{\rho} \nabla_j p_t g^{ij} + \frac{5}{2} \nabla_i \tau p_t \nabla_j \frac{p_t}{\rho} g^{ij} + S_t. \quad (4.6)$$

To derive an equation for E_r , we average (4.3) with weight ε_ω^{2R} [see (2.6)] for the 2R gas and with weight ε_ω^{3R} [see (2.7)] for the 3R gas, using relations (2.8), (2.9), (3.4), and (3.5). In the former case, we obtain

$$\begin{aligned} \int \frac{\partial f}{\partial t} \varepsilon_\omega d\xi d\omega &= \frac{\partial}{\partial t} E_r, \\ \int \nabla_i \xi^i f_{0r} \varepsilon_\omega d\xi d\omega &= \nabla_i \int \xi^i f_0 d\mathbf{c} \int \varepsilon_\omega f_r d\omega = \nabla_i u^i E_r, \\ \int \nabla_i \tau \nabla_j \xi^i \xi^j f_{0r} \varepsilon_\omega d\xi d\omega &= \nabla_i \tau \nabla_j (\rho u^i u^j + g^{ij} p_t) \frac{E_r}{\rho} = \nabla_i \tau \nabla_j \left(E_r u^i u^j + g^{ij} \frac{p_t E_r}{\rho} \right). \end{aligned}$$

The exchange term is denoted as follows:

$$\int \mathcal{F} \varepsilon_\omega d\xi d\omega = S_r.$$

Combining these expressions and differentiating by parts the term containing the product of pressures, we obtain the following equation for the rotational energy of a 2R gas:

$$\frac{\partial}{\partial t} E_r + \nabla_i u^i E_r = \nabla_i \tau \nabla_j u^i u^j E_r + \nabla_i \tau \frac{p_r}{\rho} \nabla_j p_t g^{ij} + \nabla_i \tau p_t \nabla_j \frac{p_r}{\rho} g^{ij} + S_r. \quad (4.7)$$

The equation for the 3R gas is derived in a similar way, but has a different right-hand side:

$$\frac{\partial}{\partial t} E_r + \nabla_i u^i E_r = \nabla_i \tau \nabla_j u^i u^j E_r + \frac{3}{2} \nabla_i \tau \frac{p_r}{\rho} \nabla_j p_t g^{ij} + \frac{3}{2} \nabla_i \tau p_t \nabla_j \frac{p_r}{\rho} g^{ij} + S_r. \quad (4.8)$$

This method of deriving moment equations leads to expressions for the heat flux in which the Prandtl number is equal to unity. To extend the equations to the case of an arbitrary Prandtl number, the next to last terms in the translational and rotational energy equations should be multiplied by Pr^{-1} [2]. The Prandtl number can be determined by invoking Aiken's approximation [10]:

$$\text{Pr} = (4\gamma)/(9\gamma - 5).$$

Here, γ is the specific-heat ratio. For a perfect gas, we have [4]

$$\gamma = (5 + \zeta)/(3 + \zeta),$$

where ζ is the number of internal degrees of freedom of a molecule. Thus, $\gamma = 7/5$ and $\text{Pr} = 14/19$ for the 2R gas, and $\gamma = 8/6$ and $\text{Pr} = 16/21$ for the 3R gas.

Note that the procedure employed here to construct moment equations can be used to develop a model allowing for nonequilibrium with respect to rotational and three translational degrees of freedom of molecules simultaneously.

5. CALCULATION OF EXCHANGE TERMS

The exchange terms on the right-hand sides of (4.6), (4.7), and (4.8) are moments of the collision integral of the Boltzmann equation (4.1). These terms can be calculated by employing the conventional relaxation model of the collision integral:

$$\mathcal{F} = (f_{0r}^0 - f)/\tau_r.$$

where f_{0r}^0 is the distribution function f_{0r} for equilibrium gas (i.e., when $T_t = T_r = T_{av}$ and $p_t = p_r = p_{av}$); and τ_r is the mean rotational relaxation time, which is usually several times as large as the Maxwell relaxation time τ (see [4, 8]).

Substituting the expression for the collision integral into the definition of the exchange term, we obtain, for the 2R gas

$$S_t = \int \frac{1}{\tau_r} (f_{0r}^0 - f) \frac{1}{2} \xi^2 d\xi d\omega = \frac{3}{2\tau_r} (p_{av} - p_t).$$

The second exchange term is

$$S_r = \int \frac{1}{\tau_r} (f_{0r}^0 - f) \varepsilon_\omega^{2R} d\xi d\omega = \frac{1}{\tau_r} (p_{av} - p_r).$$

For the 2R gas, substituting the expressions for the average pressures yields

$$p_{av} = \frac{1}{5}(3p_t + 2p_r), \quad S_t = \frac{3}{5\tau_r}(p_r - p_t), \quad S_r = -S_t.$$

For the 3R gas, a similar calculation gives

$$p_{av} = \frac{1}{2}(p_t + p_r), \quad S_t = \frac{3}{4\tau_r}(p_r - p_t), \quad S_r = -S_t.$$

Note that $S_t + S_r = 0$ by the energy conservation.

6. EQUATIONS FOR A GAS WITH TWO OR THREE ROTATIONAL DEGREES OF FREEDOM

Raising indices in the resulting equations by means of the metric tensor (where possible), we obtain the final QGDR equations for diatomic (2R) and polyatomic (3R) gases in a form invariant with respect to the frame of reference:

$$\frac{\partial}{\partial t} \rho + \nabla_i \rho u^i = \nabla_i \tau (\nabla_j \rho u^i u^j + \nabla^i p_t), \quad (6.1)$$

$$\frac{\partial}{\partial t} \rho u^k + \nabla_i \rho u^i u^k + \nabla^k p_t = \nabla_i \tau \nabla_j \rho u^i u^j u^k + \nabla_i \tau (\nabla^i p_t u^k + \nabla^k p_t u^i) + \nabla^k \tau \nabla_i p_t u^i, \quad (6.2)$$

$$\frac{\partial}{\partial t} E_t + \nabla_i u^i (E_t + p_t) = \nabla_i \tau \left(\nabla_j (E_t + 2p_t) u^i u^j + \frac{1}{2} \nabla^i u_k u^k p_t \right) + \frac{5}{2} \nabla_i \tau \frac{p_t}{\rho} \nabla^i p_t + \text{Pr}^{-1} \frac{5}{2} \nabla_i \tau p_t \nabla^i \frac{p_t}{\rho} + S_t. \quad (6.3)$$

For the 2R gas, the rotational energy equation and exchange terms are

$$\frac{\partial}{\partial t} E_r + \nabla_i u^i E_r = \nabla_i \tau \nabla_j u^i u^j E_r + \nabla_i \tau \frac{p_r}{\rho} \nabla^i p_t + \text{Pr}^{-1} \nabla_i \tau p_t \nabla^i \frac{p_r}{\rho} + S_r, \quad (6.4)$$

$$S_t = \frac{3}{5\tau_r} (p_r - p_t), \quad S_r = -S_t, \quad E_t = \frac{\rho \mathbf{u}^2}{2} + \frac{3p_t}{2}, \quad E_r = p_r,$$

where $\gamma = 7/5$ and $\text{Pr} = 14/19$.

For the 3R gas, the rotational energy equation and exchange terms are

$$\frac{\partial}{\partial t} E_r + \nabla_i u^i E_r = \nabla_i \tau \nabla_j u^i u^j E_r + \frac{3}{2} \nabla_i \tau \frac{p_r}{\rho} \nabla^i p_t + \text{Pr}^{-1} \frac{3}{2} \nabla_i \tau p_t \nabla^i \frac{p_r}{\rho} + S_r, \quad (6.5)$$

$$S_t = \frac{3}{4\tau_r} (p_r - p_t), \quad S_r = -S_t, \quad E_t = \frac{\rho \mathbf{u}^2}{2} + \frac{3p_t}{2}, \quad E_r = \frac{3}{2} p_r,$$

where $\gamma = 8/6$ and $\text{Pr} = 16/21$.

For one-dimensional flows, these equations are simplified to

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^\nu} \frac{\partial}{\partial r} r^\nu \rho u = \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{\partial}{\partial r} r^\nu \rho u^2 + \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau r^\nu \frac{\partial}{\partial r} p_t, \quad (6.6)$$

$$\frac{\partial \rho u}{\partial t} + \frac{1}{r^\nu} \frac{\partial}{\partial r} r^\nu \rho u^2 + \frac{\partial}{\partial r} p_t = \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{\partial}{\partial r} r^\nu \rho u^3 + 2 \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau r^\nu \frac{\partial}{\partial r} p_t u - 2\nu \frac{\tau}{r^2} p_t u + \frac{\partial}{\partial r} \tau \frac{\partial}{\partial r} r^\nu p_t u, \quad (6.7)$$

$$\begin{aligned} \frac{\partial E_t}{\partial t} + \frac{1}{r^\nu} \frac{\partial}{\partial r} r^\nu u (E_t + p_t) &= \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{\partial}{\partial r} r^\nu (E_t + 2p_t) u^2 + \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau r^\nu \frac{\partial}{\partial r} \frac{1}{2} u^2 p_t \\ &+ \frac{5}{2} \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{p_t}{\rho} r^\nu \frac{\partial}{\partial r} p_t + \text{Pr}^{-1} \frac{5}{2} \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau p_t r^\nu \frac{\partial}{\partial r} \frac{p_t}{\rho} + S_t. \end{aligned} \quad (6.8)$$

For the 2R gas, we have

$$\frac{\partial E_r}{\partial t} + \frac{1}{r^\nu} \frac{\partial}{\partial r} r^\nu u E_r = \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{\partial}{\partial r} r^\nu u^2 E_r + \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{p_r}{\rho} r^\nu \frac{\partial}{\partial r} p_t + \text{Pr}^{-1} \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau p_t r^\nu \frac{\partial}{\partial r} \frac{p_t}{\rho} + S_r. \quad (6.9)$$

For the 3R gas,

$$\frac{\partial E_r}{\partial t} + \frac{1}{r^\nu} \frac{\partial}{\partial r} r^\nu u E_r = \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{\partial}{\partial r} r^\nu u^2 E_r + \frac{3}{2} \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau \frac{p_r}{\rho} r^\nu \frac{\partial}{\partial r} p_t + \text{Pr}^{-1} \frac{3}{2} \frac{1}{r^\nu} \frac{\partial}{\partial r} \tau p_t r^\nu \frac{\partial}{\partial r} \frac{p_t}{\rho} + S_r. \quad (6.10)$$

Here, $\nu = 0$ corresponds to planar flow; $\nu = 1$, to cylindrically symmetric flow; and $\nu = 2$, to spherically symmetric flow.

When supplemented with boundary conditions, these sets of equations constitute a closed model for computing flows of moderately rarefied gases with possible nonequilibrium between translational and rotational degrees of freedom.

When the gas is in translational and rotational equilibrium, (i.e., when $T_t = T_r = T$ and $p_t = p_r = p$), the total energy per unit volume is

$$E = E_t + E_r = \frac{\rho \mathbf{u}^2}{2} + \frac{p}{\gamma - 1}.$$

The equation for E is obtained by summing the equations for E_t and E_r . The continuity and momentum equations remain unchanged:

$$\frac{\partial}{\partial t} \rho + \nabla_i \rho u^i = \nabla_i \tau (\nabla_j \rho u^i u^j + \nabla^i p), \quad (6.11)$$

$$\frac{\partial}{\partial t} \rho u^k + \nabla_i \rho u^i u^k + \nabla^k p = \nabla_i \tau \nabla_j \rho u^i u^j u^k + \nabla_i \tau (\nabla^i p u^k + \nabla^k p u^i) + \nabla^k \tau \nabla_i p u^i. \quad (6.12)$$

The equation for total energy takes the form

$$\frac{\partial}{\partial t} E + \nabla_i u^i (E + p) = \nabla_i \tau \left(\nabla_j (E + 2p) u^i u^j + \frac{1}{2} \nabla^i u_k u^k p \right) + \frac{\gamma}{\gamma - 1} \nabla_i \tau \frac{p}{\rho} \nabla^i p + \text{Pr}^{-1} \frac{\gamma}{\gamma - 1} \nabla_i \tau p \nabla^i \frac{p}{\rho}. \quad (6.13)$$

Note that this equation can be obtained directly by averaging the approximate equation (4.3) with summation invariant $\xi^2/2 + \epsilon_\omega$ and by extending the resulting equation to the case $\text{Pr} \neq 1$.

System (6.11)–(6.13) coincides with the QGD system (see, e.g., [3]), which was constructed for a monatomic gas and was then formally extended to the case $\gamma \neq 5/3$.

The relation between the QGD and Navier–Stokes equations for a monatomic gas with $\text{Pr} = 1$ was analyzed in [9, 11]. In particular, the QGD equations were represented in [11] as balance equations for mass, momentum, and total energy in local form:

$$\frac{\partial}{\partial t} \rho + \nabla_i j^i = 0, \quad \frac{\partial}{\partial t} \rho u^k + \nabla_i j^i u^k = \nabla_i P^{ik}, \quad \frac{\partial}{\partial t} E + \nabla_i j^i E / \rho = \nabla_i (A^i - q^i).$$

Here,

$$j^i = \rho u^i - \tau (\nabla_j \rho u^i u^j + \nabla^i p),$$

is the mass flux density. The stress tensor P^{ik} , the heat flux q^i , and the vectors j^i and A^i are represented as sums of the corresponding variables in the Navier–Stokes representation with additional terms whose asymptotic order is $O(\tau^2)$ for steady flows. It can be shown that these results remain valid for polyatomic gases with $Pr \neq 1$ if the bulk viscosity η in the Navier–Stokes model [12, p. 72] is approximated by the expression

$$\eta = \mu(5/3 - \gamma), \text{ where } \mu = p\tau.$$

This simple approximation is consistent with the well-known properties of bulk viscosity [5, p. 188; 6, p. 97]: it is always positive, is finite for gases of molecules with internal degrees of freedom, and is zero for monatomic gases.

7. NUMERICAL ALGORITHM AND EXAMPLES OF COMPUTATIONS

The numerical solution of the QGDR equations is demonstrated by solving the one-dimensional system (6.6)–(6.10) for planar flow ($v = 0$).

The Maxwellian relaxation time $\tau = \mu/p$ contained in the dissipative terms of the QGDR equations is calculated with the expression for viscosity taken from [4]:

$$\mu = \frac{\lambda\rho\sqrt{2\pi(\mathcal{R}/\mathcal{M})T}}{4}\Omega(s) = \mu_{\text{ref}}\left(\frac{T}{T_{\text{ref}}}\right)^s, \quad \Omega(s) = \frac{30}{(7-2s)(5-2s)},$$

where λ is the mean free path. In these relations, the temperature is set equal to T_t , because the translational temperature determines the mean free time mean free path [8].

The rotational relaxation time τ_r contained in the expressions for S_t and S_r can be calculated as

$$\tau_r = Z \times \tau_c, \text{ where } \tau_c = \tau \times \Omega^{-1}(s),$$

here, τ_c is the mean free time and Z^{-1} is the relative frequency of inelastic collisions [see 4, p. 117; 8]. For example, $Z = 5$ for nitrogen. However, more accurate formulas for this quantity can be found in the literature, which allow for its dependence on T_t and T_r (see, e.g., [13; 4, p. 413]). We set $\tau_r = Z\tau$ in the calculations described below.

To solve the QGDR equations numerically, we nondimensionalize them, using the reference length λ_{ref} , reference density ρ_{ref} , and reference temperature T_{ref} . The last parameter is also used to calculate the sonic velocity $a_{\text{ref}} = \sqrt{\gamma(\mathcal{R}/\mathcal{M})T_{\text{ref}}}$, which is also in the nondimensionalization. The general form of the equations remains unchanged, whereas the relations between variables and parameters take the form

$$p_t = \rho T_t / \gamma, \quad p_r = \rho T_r / \gamma, \quad a_t = \sqrt{T_t}, \quad a_r = \sqrt{T_r},$$

$$\lambda = \frac{T_t^{s-1/2}}{\rho} = \frac{(\gamma p_t)^{s-1/2}}{\rho^{s+1/2}}, \quad \tau = \frac{\mu(T_t)}{p_t} = \frac{(\gamma p_t)^{s-1} \sqrt{2\pi\gamma}}{\rho^s} \Omega(s).$$

The QGDR equations are solved numerically by a finite difference method [14]. Specifically, all spatial derivatives are approximated by second-order accurate central differences on a uniform grid. The time derivatives are approximated by forward differences with first order accuracy. A steady-state solution is obtained by the relaxation method based on a finite-difference scheme that is explicit in time and conditionally stable. The time step Δt is set by the Courant-type condition

$$\Delta t = \alpha \frac{\min(h)}{\max[\max(a_t, a_r) + \sqrt{u^2}]},$$

where h is the mesh size. A solution is assumed to reach a steady state if

$$\max \frac{\rho^{n+1} - \rho^n}{\Delta t} \leq \epsilon_p, \text{ where } n \text{ is the time-step index.}$$

The problem of spatial relaxation. As a first example illustrating the use of the QGDR equations, we consider the spatial relaxation of a gas toward equilibrium. Consider the half-space $x \geq 0$ with a uniform gas flow across the left boundary, characterized by temperatures T_{t0} and T_{r0} , velocity u_0 , and density ρ_0 . On the right boundary, we set conditions ensuring free gas outflow across this boundary. For supersonic flow, it is sufficient to set the gradients of ρ , T_t , T_r , and u equal to zero to satisfy this requirement.

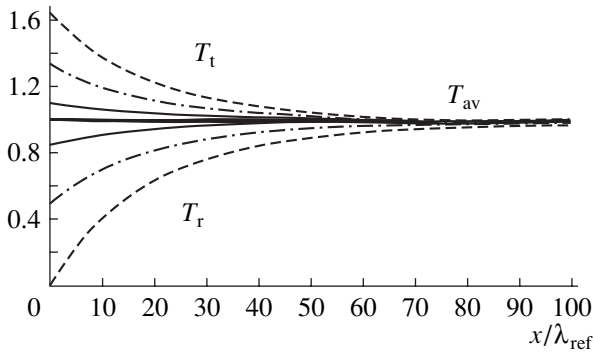


Fig. 1.

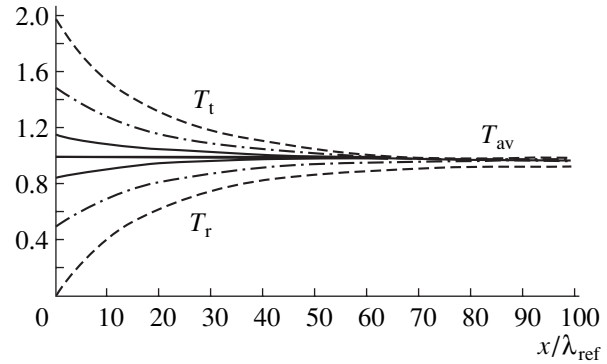


Fig. 2.

The basic reference parameters used to nondimensionalize equations (6.6)–(6.10) are the average inlet temperature,

$$T_{\text{ref}}^{2\text{R}} = \frac{3T_{t0} + 2T_{r0}}{5} \quad \text{and} \quad T_{\text{ref}}^{3\text{R}} = \frac{3T_{t0} + 3T_{r0}}{6},$$

for the 2R and 3R gases, respectively; density $\rho_{\text{ref}} = \rho_0$; and the sonic velocity and mean free path represented as

$$a_{\text{ref}} = \sqrt{\gamma(\mathcal{R}/\mathcal{M})T_{\text{ref}}}, \quad \lambda_{\text{ref}} = \frac{4\mu(T_{\text{ref}})}{\rho_{\text{ref}}\sqrt{2\pi(\mathcal{R}/\mathcal{M})T_{\text{ref}}}}\Omega(s)^{-1}.$$

Setting the initial dimensionless velocity $u_0 = 3$, we consider three cases of initial nonequilibrium for the 2R gas: $T_{t0} = 5/3$, $T_{r0} = 0$ (which corresponds to zero rotational energy on the inlet boundary), and two variants of a weaker inlet thermal nonequilibrium: $T_{t0} = 1.33$, $T_{r0} = 0.5$ and $T_{t0} = 1.1$, $T_{r0} = 0.85$. We set $Z = 5$ and $s = 0.75$. These values of Z and s were used in solving the problem of rotational temperature relaxation in nitrogen (see [4, 15], where the problem was solved in spatially uniform formulation).

Our computations were conducted on a 201-point grid with mesh size $h = 0.5$. The initial values of flow variables were set equal to those on the inlet boundary. The parameter α was set at 0.01 to ensure stability of the algorithm. The number of time steps required for relaxation was about 600000 for the admissible error $\varepsilon_p = 10^{-4}$. When the mesh size was reduced by a factor of two, the numerical results changed very slightly, which shows that the method is convergent.

Figure 1 shows relaxation curves for rotational and translational temperatures for the 2R gas in the above three cases of inlet nonequilibrium. The dashed, dot-and-dash, and solid curves correspond to the first, second, and third cases, respectively. The graphs of average temperature are also presented in the figure. It is evident that both temperatures slowly approach the equilibrium value $T_{\text{av}} = 1$. As the degree of initial nonequilibrium is increased, the relaxation slows down, which agrees with results presented in [4, 15]. An equilibrium is attained at a distance of about 100 times the mean free path, which corresponds to about 35 collisions and is in qualitative agreement with the results reported in [4, p. 233].

Figure 2 shows analogous curves calculated for the 3R gas. The initial values were $T_{t0} = 2$, $T_{r0} = 0$; $T_{t0} = 1.5$, $T_{r0} = 0.5$; and $T_{t0} = 1.15$, $T_{r0} = 0.85$. Here, the rotational and translational temperatures also monotonically approach the average value.

The problem of shock-wave structure. Another example illustrating the use of the proposed mathematical model is the problem of stationary shock-wave structure in nitrogen. For comparison, we use the results of Monte Carlo simulation reported in [4, 15].

The QGDR equations were nondimensionalized by the values of the flow variables for the incoming stream. The numerical solution of the QGDR equations was based on the algorithm described above. The Rankine–Hugoniot conditions for a stationary shock wave were set on the left- and right boundaries. The same values were used as initial conditions on the right and left of the shock front.

Our computations were carried out at the Mach number $M = 1.71$ ($Z = 5$ and $Z = 10$), which corresponds to [4], and at $M = 7$ and 12.9 ($Z = 5$), which corresponds to [15]. The problem was solved on a 201-points uniform grid with mesh size $h = 0.5$. The parameter α was set equal to 0.01 to ensure the stability of the algorithm. The number of time steps required for convergence varied from 20000 to 1000000, depending

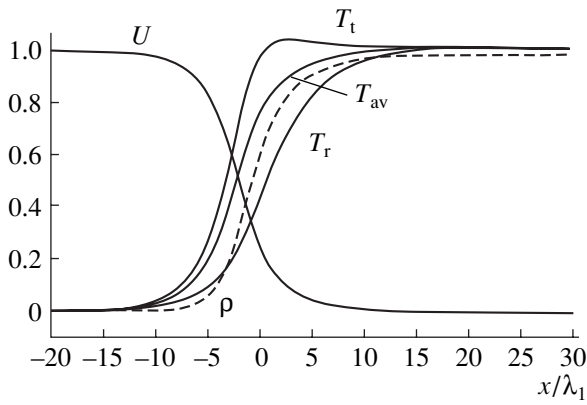


Fig. 3.

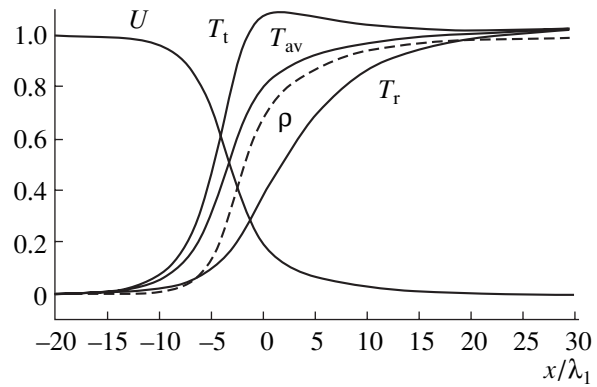


Fig. 4.

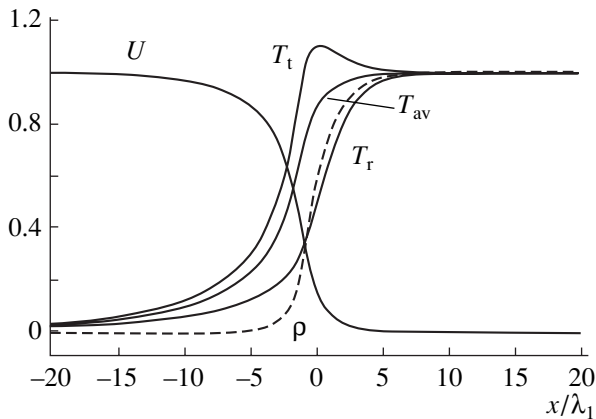


Fig. 5.

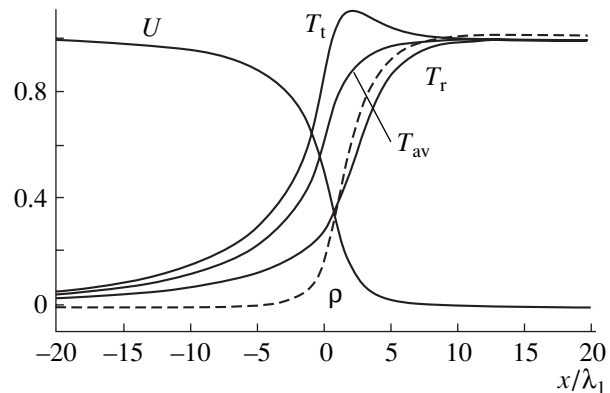


Fig. 6.

on the Mach number, for the error $\epsilon_p = 10^{-3}$. When the mesh size was reduced by a factor of two, the numerical results varied very slightly even at $M = 12.9$, which shows that the method is convergent.

Figures 3–6 show dimensionless flow variables (velocity; density; and translational, rotational, and average temperatures) in the shock waves obtained for the upstream and downstream Rankine–Hugoniot conditions. The coordinate x was nondimensionalized by the mean free path λ_1 for the incoming stream.

Figure 3 ($M = 1.71, Z = 5$) reveals typical features of the problem in question. Specifically, the relative positions of the curves for $T_t, T_{av}, \rho,$ and T_r agree with the results of [4]. It is seen that T_t is higher than T_r . A small maximum of translational temperature, $T_t = 1.042$, is observed in the figure. The solution to the same problem but for $Z = 10$ is shown in Fig. 4. The width of the shock wave is greater, its inverse width with respect to density is less by about 20%, and the maximum T_t increases is more than twice as high ($T_t = 1.087$), which exactly agrees with the results reported in [4, p.298].

Figures 5 and 6 show the numerical results obtained at $M = 7.0$ and 12.9 for $Z = 5$. The relative positions of all curves, in particular, the ρ and T_r profiles (the density curve is close to that of rotational temperature), as well as the peak values of translational temperature, agree well with the reference solution presented in [15]: the maximum is $T_t = 1.098$ at $M = 7$ and $T_t = 1.096$ at $M = 12.9$.

8. CONCLUSIONS

A system of quasi-gasdynamic equations making allowance for translational and rotational nonequilibrium (QGDR equations) has been constructed to describe gas flows. These equations were derived by representing the distribution function as a gradient expansion about its equilibrium value. The exchange terms were obtained by using the relaxation form of the collision integral.

In the equilibrium case, this system is identical with the QGD equations previously derived for a polyatomic gas.

The QGDR equations were used to compute spatial relaxation and shock-wave structure. The numerical results based on the QGDR equations are in good agreement with those obtained by direct simulation, which requires substantially larger computing resources as compared to moment methods. This suggests that the proposed model can be applied to compute multidimensional flows of moderately rarefied polyatomic gases.

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