Numerical Study of Shock Wave Structure Based on Quasigasdynamic Equations with Rotational Nonequilibrium

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1   Introduction

The quasigasdynamic (QGD) equation system, obtained in the late 80's, is a model for the description of viscous gas flows. Computer modeling and theoretical investigations showed the validity of this equation system to describe viscous heat-conductive flows and confirmed also some advantages of it compared with the Navier-Stokes system [1]. This work presents the generalization of the QGD system to flows of non-monoatomic gases with a difference between translational and rotational temperatures. This new system is referred to as QGDR.

A molecule is considered as a rigid rotator, possessing only kinetic energy. This description is valid if the temperature of gas not very high (vibrational degrees of freedom are not excited) and not very low (distribution by quantum levels can be approximated classically [2]).

To obtain the QGDR system the same procedure as described in [1] was used. The form of this system depends on the number of degrees of freedom of the molecule. The systems for three and two rotational degrees of freedom were obtained in arbitrary 3-dimensional space coordinates. Examples of numerical calculations are also presented.

2   Distribution functions

The gas system consisting of rigid rotators can be described by the one particle distribution function $f(t, \vec{x}, \vec{\xi}, \vec{\omega})$, depending on time t, coordinate $\vec{x}$, velocity of the center of mass $\vec{\xi} = \vec{u} + \vec{c}$ ($\vec{u}$ is the macroscopic velocity, $\vec{c}$ is the thermal velocity) and vector of angular velocities $\vec{\omega}$. It can be

normalized as $d\rho = f d\vec{\xi} d\vec{\omega}$.

Let f_{0r} be the local equilibrium Maxwellian two-temperature distribution function [2], p.109 :

$$f_{0r} = f_0 \cdot f_r, \qquad \text{where}$$

$$f_0 = \rho (2\pi \frac{\mathcal{R}}{\mathcal{M}} T_T)^{-3/2} \exp(-\frac{\vec{c}^2}{2(\mathcal{R}/\mathcal{M})T_T})$$

is the Maxwellian distribution function. f_r is Hinshelwood's distribution function for rotational energy [3]. Describing a molecule as a dumbbell rigid rotator (two internal degrees of freedom, 2R - case), we have

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

If the molecule has three rotational degrees of freedom, 3R - case), we have:

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

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 the Avogadro number, I is the principal moment of inertia of dumbbell molecule, I_α is the principal moments of inertia of arbitral molecule, ω_α are angular velocities, T_T is the translational temperature, T_r is the rotational temperature.

Translational pressure and temperature are defined as

$$p_T = \frac{1}{3} \int \vec{c}^2 f \, d\vec{\xi} d\vec{\omega} = \frac{1}{3} \int \vec{c}^2 f_{0r} \, d\vec{\xi} d\vec{\omega} = \rho \frac{\mathcal{R}}{\mathcal{M}} T_T.$$

Rotational pressure and temperature that are connected with rotational energy of the particles have the form

$$\rho \frac{\mathcal{R}}{\mathcal{M}} T_r = p_r = \int \varepsilon_\omega^{2R} f \, d\vec{\xi} d\vec{\omega} = \int \varepsilon_\omega^{2R} f_{0r} \, d\vec{\xi} d\vec{\omega} \quad \text{for the 2R case and}$$

$$\rho \frac{\mathcal{R}}{\mathcal{M}} T_r = p_r = \frac{2}{3} \int \varepsilon_\omega^{3R} f d\vec{\xi} d\vec{\omega} = \frac{2}{3} \int \varepsilon_\omega^{3R} f_{0r} d\vec{\xi} d\vec{\omega} \quad \text{for the 3R case,}$$

where the rotational energy for a particle is calculated as

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

for 2R and 3R gases, respectively.

The total energy is equal to

$$E = \int (\frac{\vec{\xi}^2}{2} + \varepsilon_\omega) f \, d\vec{\xi} d\vec{\omega} = \int (\frac{\vec{\xi}^2}{2} + \varepsilon_\omega) f_{0r} \, d\vec{\xi} d\vec{\omega} = E_T + E_r, \quad \text{where}$$

$$E_T = \frac{1}{2} \int \vec{\xi}^2 f \, d\vec{\xi} d\vec{\omega} = \frac{1}{2} \int \vec{\xi}^2 f_{0r} \, d\vec{\xi} d\vec{\omega} = \frac{\rho \vec{u}^2}{2} + \frac{3}{2} p_T,$$

$$E_r^{2R} = \int \varepsilon_\omega^{2R} f \, d\vec{\xi} d\vec{\omega} = \int \varepsilon_\omega^{2R} f_{0r} \, d\vec{\xi} d\vec{\omega} = \rho \frac{\mathcal{R}}{\mathcal{M}} T_r = p_r,$$

$$E_r^{3R} = \int \varepsilon_\omega^{3R} f \, d\vec{\xi} d\vec{\omega} = \int \varepsilon_\omega^{3R} f_{0r} \, d\vec{\xi} d\vec{\omega} = \frac{3}{2} \rho \frac{\mathcal{R}}{\mathcal{M}} T_r = \frac{3}{2} p_r.$$

3 Moment equations (QGDR system)

For constructing the moment QGDR equations we approximate the actual distribution function f by its gradient expansion near the equilibrium point in the form:
$$f^{QGDR} = f_{0r} - \tau \xi^i \nabla_i f_{0r},$$

where τ is the Maxwellian relaxation time $\tau = \mu/p_T$, $\mu \propto T_T^s$ is viscosity, depending on the translational temperature [4], s is defined by the law of molecular interaction [3]. Formal substitution

$$f \to f^{QGDR}$$

in the convective term of Boltzmann equation $f_t + (\xi \vec{\nabla} f) = \mathcal{I}$ results in the approximation

$$\frac{\partial f}{\partial t} + \nabla_i \xi^i f_{0r} - \nabla_i \tau \nabla_j \xi^i \xi^j f_{0r} = \mathcal{I}.$$

A similar approximation was used to obtain the QGD equations (e.g.,[1]). Averaging the latter equation over velocity space after multiplication by adequate factors results in a system of macroscopic QGDR equations. Particularly, integrating with 1, we obtain the equation for density, integrating with ξ^k, we obtain the momentum equation and integrating with $\vec{\xi}^2$, we obtain the equation for translational energy:

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

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

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$$\frac{\partial}{\partial t}E_T + \nabla_i u^i (E_T + p_T) = \nabla_i \tau (\nabla_j (E_T + 2p_T) u^i u^j + \frac{1}{2}\nabla^i u_k u^k p_T) +$$

$$\frac{5}{2}\nabla_i \tau \frac{p_T}{\rho}\nabla^i p_T + Pr^{-1}\frac{5}{2}\nabla_i \tau p_T \nabla^i \frac{p_T}{\rho} + S_T.$$

For rotational energy, we have to take into account the number of internal degrees of freedom of the molecule: in the 2R case, integration is performed with ε^{2R}, in the 3R case, integration is performed with ε^{3R}. Below only the 2R case will be described. The equation for rotational energy in a 2R gas has the form

$$\frac{\partial}{\partial t}E_r + \nabla_i u^i E_r = \nabla_i \tau \nabla_j u^i u^j E_r + \nabla_i \tau \frac{p_r}{\rho}\nabla^i p_T + Pr^{-1}\nabla_i \tau p_T \nabla^i \frac{p_r}{\rho} + S_r.$$

The Prandtl number Pr does not appear in the above-described treatment. It has been introduced artificially into the conductive term in the right-hand side of the energy equations to make the sum of these equations coincide with the previous QGD set in the case $T_T = T_r$. For a 2R gas we use Eucken's approximation $Pr = 14/19$.

4 Calculation of the exchange terms

The exchange terms S_T and S_r in the right-hand side of energy equations are the moments of the collision integral. A simple way to calculate them is to use the relaxation form of the collision integral

$$\mathcal{I} = \frac{f_{0r}^0 - f}{\tau_r},$$

where f_{0r}^0 is the distribution function f_{0r} for the equilibrium case, when $T_T = T_r = T_{av}$, and $p_T = p_r = p_{av}$. Average pressure and temperature are defined as

$$p_{av} = (3\,p_T + 2\,p_r)/5 = \rho\,(\mathcal{R}/\mathcal{M})\,T_{av}.$$

τ_r is the rotational relaxation time, that can be estimated as $\tau_r = Z\tau_c$, where τ_c is the mean collisional time [3] and Z is so-called rotational collision number. More complicated models can be used, e.g. [4].
So one gets

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

Introducing the expression for p_{av} we get

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$$S_T = \frac{3}{5\tau_r}(p_r - p_T); \quad S_r = -S_T.$$

Note that $S_T + S_r = 0$, consistent with the conservation of total energy.

Remark 1: The above equation for rotational energy E_r can be simplified and approximated as

$$\frac{\partial}{\partial t}T_r + u^i \nabla_i T_r = (T_{av} - T_r)/\tau_r,$$

which is the form frequently used in the investigation of relaxation processes (see [3], p. 117).

Remark 2: In the case of temperature equilibrium ($p_T = p_r = p_{av} = p$), the QGDR system turns into the one-temperature QGD system with the adequate value of the specific heat ratio γ for a non-monoatomic gas ($\gamma = (5 + \zeta)/(3 + \zeta)$, where ζ is the number of internal degrees of freedom of the molecule). The equation for energy writes then

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

Other details can be found in [5].

5 Computational results

The present QGDR model can be applied to 3-D flows. In this work, however, it is used to investigate 1-D problems. For 1D plane flows equations simplifies:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r}\rho u = \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}\rho u^2 + \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}p_T,$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial r}\rho u^2 + \frac{\partial}{\partial r}p_T = \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}\rho u^3 + 2\frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}p_T u + \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}p_T u,$$

$$\frac{\partial E_T}{\partial t} + \frac{\partial}{\partial r}u(E_T + p_T) = \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}(E_T + 2p_T)u^2 + \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}\frac{1}{2}u^2 p_T +$$
$$\frac{5}{2}\frac{\partial}{\partial r}\tau\frac{p_T}{\rho}\frac{\partial}{\partial r}p_T + Pr^{-1}\frac{5}{2}\frac{\partial}{\partial r}\tau p_T \frac{\partial}{\partial r}\frac{p_T}{\rho} + S_T,$$

$$\frac{\partial E_r}{\partial t} + \frac{\partial}{\partial r}u E_r = \frac{\partial}{\partial r}\tau\frac{\partial}{\partial r}u^2 E_r + \frac{\partial}{\partial r}\tau\frac{p_r}{\rho}\frac{\partial}{\partial r}p_T + Pr^{-1}\frac{\partial}{\partial r}\tau p_T \frac{\partial}{\partial r}\frac{p_r}{\rho} + S_r.$$

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The above QGDR equations were used for the simulation of a rotational relaxation problem and for the shock-wave problem in nitrogen (2R gas, $Z = 5, s = 0.75$) For the numerical realization an explicit finite–difference method of the second order in space was used.

Relaxation problem. We consider a stationary one-dimensional gas flow ($Ma_1 = 3.571$) with initial non-equilibrium at $x = 0$, characterized by temperatures $T_{T1} \neq T_{r1}$, density ρ_1 and velocity u_1. It evolves toward equilibrium as x increases.

ρ, u and T_T and T_r are normalized by reference quantities (1) respectively, that are taken at $x = 0$ and corresponds to DSMC results. $T_1 = T_{av}$ at $x = 0$, x is normalized by the mean free path λ_1, where

$$\lambda_1 = \frac{\mu(T_1)}{\rho_1 \sqrt{2(\mathcal{R}/\mathcal{M})T_1}} \times \frac{2(7-s)(5-s)}{15\sqrt{\pi}}.$$

Reference DSMC calculations were carried out using the DISIRAF computer code [6]. In these calculations, the Borgnakke-Larsen restricted energy exchange model was used for rotation-translation exchanges, with a restriction factor $f = 0.2$, that is approximately consistent with $Z = 5$. The presence of a temperature gradient causes a difficulty when setting the upstream boundary conditions in DSMC calculations. Molecules from a gas in translational equilibrium at T_T and rotational equilibrium at T_r were injected at some negative value of abscissa x. The values of temperatures and other flow parameters found at $x = 0$ in the DSMC calculation were taken as boundary conditions for the QGDR calculations. The results obtained by both methods are shown in Figs.1 and 2. The agreement between the two methods is found, particularly, if one remembers that the parameters f and Z involved in the models are not strictly equivalent.

Shock wave problem. For the shock wave problem calculations were carried out for upstream Mach numbers $Ma = 1.71$ ($Z = 5$ and $Z = 10$), which corresponds to DSMC calculations by Bird [3] p.298, and for $Ma = 7$ and 12.9, which corresponds to DSMC calculations by Koura [7]. The profiles obtained are shown in Figs.$3 - 6$, where x is reduced by the upstream mean free path. Ordinates are reduced as usual, based on the Rankine-Hugoniot values upstream (1) and downstream (2) of the shock wave. On Fig.3 ($Z = 5$) one can see the characteristic features of the problem under consideration: the arrangement of the curves corresponds to the results of Bird. One can see the lag of the T_r profile compared with that of T_T, and the small extremum on the profile of T_T ($T_T = 1.021$). The inverse density thickness is $\lambda_1/\delta = 0.152$. When increasing Z, the width of shock profile increases ($\lambda_1/\delta = 0.136$ in Fig.4) and the overshoot of T_T increases is approximately twice larger ($T_T = 1.058$), as found by Bird [3].

Results for $Ma = 7.0$ and $Ma = 12.9$ are shown in Figs 5 and 6, respectively. They are very similar to those of Koura [7], particularly, the fact that the

profiles of ρ and T_r are close to one another. Moreover the values of maxima of T_T are in good agreement ($T_T = 1.068$ for $Ma = 7.0$, $T_T = 1.070$ for $Ma = 12.9$). The inverse density thicknesses λ_1/δ for these cases are 0.297 and 0.244, respectively. However in the region just upstream of the shock wave both T_T and T_r computed by QGDR equations are overestimated when compared with DSMC values.

The calculations confirmed the stability properties of the QGDR system with its associated computational algorithm.

6   Conclusion

A continuum model (QGDR) for the description of rarefied gas flows has been developed. It includes the treatment of nonequilibrium between translational and rotational temperatures. Results were obtained based on QGDR equations for space relaxation and for the shock wave problem in a wide range of Mach numbers. They show that these equations can be used in addition to approaches based on kinetic theory or DSMC method.

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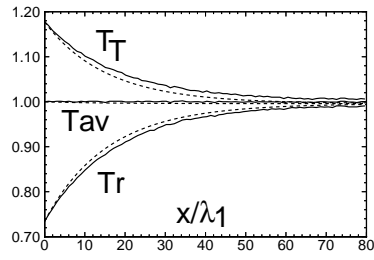
Figure 1: Profiles of reduced temperatures in space relaxation problem. Solid line corresponds to DSMC, dashed one corresponds to QGDR.
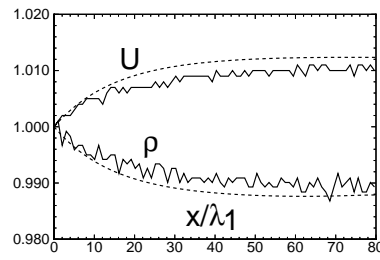
Figure 2: Profiles of reduced density and velocity in space relaxation problem. The same notations as in Fig.1.
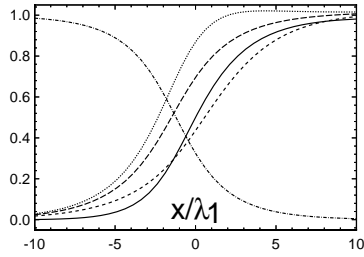

Figure 3: Shock wave problem, $Ma = 1.71, Z = 5$. Solid line corresponds to ρ, dashed one - to T_r, dotted one - to T_T, long-dashed - to T_{av} and dash-dot - to u.
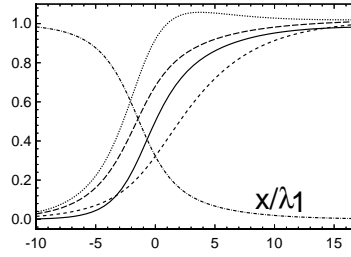
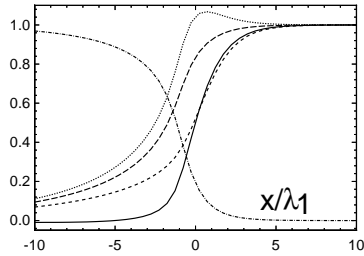Figure 4: Shock wave problem, $Ma = 1.71, Z = 10$. The same notations as in Fig. 3.

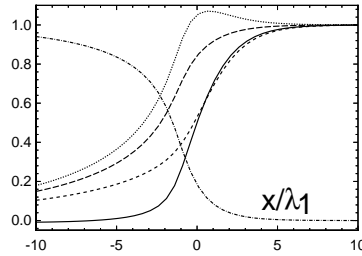Figure 5: Shock wave problem, $Ma = 7.0, Z = 5$. The same notations as in Fig. 3.

Figure 6: Shock wave problem, $Ma = 12.9, Z = 5$. The same notations as in Fig. 3.

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