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Quasi-gasdynamic equations and computer simulation of rarefied gas flows

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1 Introduction

Quasi-gasdynamic (QGD) equations were constructed in [1], [2] starting from kinetical model for distribution function. Computational algorithms, based on QGD model were called kinetical-consistent finite-difference (KCFD) schemes. This schemes were successively used for creating stable numerical methods for viscous supersonic flows [1], [2]. Now we consider QGD model as a specific mathematical model for simulations of rarefied gas flows. The validity of QGD approach is examined by numerical simulation of the static shock-wave structure.

2 Quasi-gasdynamic model

QGD equations may be constructed by averaging the following model kinetical equation for distribution function [3]

$$f_t + (\vec{\xi}\nabla)f - (\vec{\xi}\nabla)\tau(\vec{\xi}\nabla)f = \mathcal{J}(f, f') \tag{1}$$

where $f(\vec{x}, \vec{\xi}, t)$ is the distribution function for a monoatomic gas, $\mathcal{J}(f, f')$ is the collision integral, τ is a characteristic time of the evolution toward equilibrium (characteristic time for relaxation) in a gas with macroparameters defined by function f.

An equation like Eq.1 was first constructed by the authors[1] using the known kinetical model for the behavior of distribution function in a cyclically recurring process of the following type: Assume that at the time layer $t = t^j$ the distribution function is the locally- Maxwellian one as $f(\mathbf{x}, \vec{\xi}, t) = f^0$. Then during time interval τ collision-free scattering of gas molecules occurs, followed by instantaneous Maxwellization. Free-scattering step may be defined with the help of the expression

$$f^{j+1}(\vec{x}, \vec{\xi}, t) = f_0{}^j(\vec{x} - \vec{\xi}\tau, \vec{\xi}, t) \tag{2}$$

Expanding (2) into a Taylor series in the parameter $\xi\tau$ we obtain a model kinetical equation close to Eq.1. Successively multiplying it by the summation invariants $\varphi(\vec{\xi}) = 1, \vec{\xi}, 0.5\vec{\xi}^2$ and integrating over all molecular velocities $\vec{\xi}$ we obtain the system of differential equations for the macroparameters - QGD model [1], [2] . Note that, in obtaining the high-order moments to close the system, we had to suppose that the distribution function is equal to a locally-Maxwellian one f^0.

In invariant form QGD system was written in [3] as

$$\rho_t + div(\rho\vec{u}) = div\tau(div(\rho\vec{u} \otimes \vec{u}) + \vec{\nabla}p) \tag{3}$$

$$(\rho\vec{u})_t + div(\rho\vec{u}\otimes\vec{u}) + \vec{\nabla}p = \\ = div\tau(div(\rho\vec{u}\otimes\vec{u}\otimes\vec{u}) + (\vec{\nabla}\otimes p\vec{u}) + (\vec{\nabla}\otimes p\vec{u})^T) + \nabla\tau div(p\vec{u}), \tag{4}$$

$$E_t + div((E+p)\vec{u}) = div\tau(div((E+2p)\vec{u}\otimes\vec{u}) + \vec{\nabla}(p(E+p)/\rho)). \tag{5}$$

By adding to Eqs. (3) - (5) the equation of state of an ideal gas

$$E = \rho(\vec{u}^2/2 + \varepsilon),\ \varepsilon = p/\rho(\gamma - 1) \tag{6}$$

and, also, adding the initial and boundary conditions, we obtain a closed system of equations which describes the space-time evolution of the macroscopic parameters of the gas: $\vec{u}$ - velocity, ρ - density, p - pressure, E - energy. As discussed in [4], the transport phenomena appear in the equations through the characteristic time τ.

In the papers of Sloskin [5], Vallander [6], Alexeev [7], Klimontovich, [8] new equations of gas-dynamical type, usually called generalized NS equations, were constructed based on different hypotheses. These models differ from NS model and from Eqs.(3) - (5) by the structure of the second order differential terms.

For a monoatomic gas the numerous relations between QGD and Navier-Stokes equations have been established in [3] and [10]. It was shown [3] that in stationary form QGD system of equations differs from NS one by the additional terms, having the orders of $O(\tau^2)$ accuracy. The boundary layer approach for QGD system coincides with Prandtl's one with viscosity and heat conductivity coefficients in the form

$$\mu = p\tau \text{ and } \kappa = c_p p\tau = c_p\mu. \tag{7}$$

For QGD system the entropy equation was constructed in [3], [10], the suggestion about a rise of full thermodynamic entropy function for adiabatically isolated systems was proved. Moreover, in [9] it was proved that the full increase of entropy function in a shock wave is strongly positive.

If the second-order differential terms in Eqs.(3) - (5) are dropped, QGD equations reduce to NS equations and τ now receives a physical meaning. By identification, it can be related to the usual viscosity coefficient by $\tau = \mu/p$ or to the thermal conductivity by $\tau = \kappa/(c_p p)$. Both definitions are consistent only for a Prandtl number equal to unity ($Pr = 1$).

3 Shock-wave problem

For plane 1D case QGD system writes

$$\frac{\partial\rho}{\partial t} + \frac{\partial\rho u}{\partial x} = \frac{\partial}{\partial x}\tau\frac{\partial}{\partial x}(\rho u^2 + p) \tag{8}$$

$$\frac{\partial\rho u}{\partial t} + \frac{\partial}{\partial x}(\rho u^2 + p) = \frac{\partial}{\partial x}\tau\frac{\partial}{\partial x}(\rho u^3 + 3pu) \tag{9}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}u(E+p) = \frac{\partial}{\partial x}\tau\frac{\partial}{\partial x}u^2(E + \frac{5}{2}p) + \frac{\gamma}{\gamma-1}(\frac{\partial}{\partial x}\frac{p}{\rho}\tau\frac{\partial p}{\partial x}) + \frac{\gamma Pr^{-1}}{\gamma-1}(\frac{\partial}{\partial x}p\tau\frac{\partial}{\partial x}\frac{p}{\rho}) \tag{10}$$

To ensure consistency with the actual gas viscosity, τ should be taken equal to μ/p (Eq.7). In energy equation (Eq.10), the NS-like term responsible for heat-conductivity, has been corrected by introducing Prandtl number Pr.

Using Bird's relation between viscosity and mean free path [12]

$$\lambda = \frac{\mu}{\rho\sqrt{2\pi RT}} \times \frac{2(7-2\omega)(5-2\omega)}{15} \tag{11}$$

and the equation of state $p = \rho RT$, we get

$$\tau = \frac{\lambda}{\sqrt{RT}} \times \frac{15\sqrt{2\pi}}{2(7-2\omega)(5-2\omega)} \tag{12}$$

Eq.11 is a generalization of the usual expression for a hard-sphere gas ($\mu \propto T^{1/2}$) to a Variable Hard Sphere (VHS) gas whose viscosity law is $\mu \propto T^{\omega}$. Realistic values of ω fall between 0.5 and 1.

To solve the system of Eqs. (8) - (10) it is convenient to rewrite it in a non-dimensional form by introducing scaling quantities for all dimensional variables. The corresponding scaling quantities are taken in the free stream region: mean free path λ_1, density ρ_1, sound velocity $a_1 = \sqrt{\gamma RT_1}$, temperature T_1. As a mean free path we chose the mean free path for the hard-sphere gas $\omega = 0.5$ as it is accepted in shock-structure computations

$$\lambda_1 = \frac{\mu_1}{\rho_1\sqrt{2\pi RT_1}} \times \frac{16}{5} \tag{13}$$

So we have the following relations between adimensional and dimensional variables ("tilda" refers to dimensionless quantities)

$$\rho = \tilde{\rho}\rho_1,\ p = \tilde{p}\rho_1 {a_1}^2,\ T = \tilde{T}T_1,\ a = \tilde{a}a_1,\ x = \tilde{x}\lambda_1,$$

$$t = \tilde{t}\lambda_1/a_1,\ u = \tilde{u}a_1,\ \tau = \tilde{\tau}\lambda_1/a_1,\ E = \tilde{E}\rho_1 {a_1}^2 \tag{14}$$

After introducing adimensional values the form of the Eqs. (8) - (10) will not be changed. Below we will drop the sign "tilda". State equation, sound velocity and relaxation time write respectively

$$p = \rho T/\gamma,\ a = \sqrt{T},\ \text{and}\ \tau = \frac{T^{\omega}}{\gamma p} \times \frac{5}{16}\sqrt{2\pi\gamma}. \tag{15}$$

As initial and boundary conditions we used Hugoniot relations.

A finite-difference scheme was constructed based on the dimensionless form Eqs.(8) - (10), (15) with space accuracy of the order $O(h^2)$ (centered scheme). The steady-state solution was been obtained as the limit of a time-evolving process. The time step was defined from the Courant stability condition $\Delta t = \alpha \min h/\max V$ where $V = a + \sqrt{\vec{u}^2}$. Coefficient α was chosen experimentally and was equal to ~ 0.01 in all computations with $h = 0.5$. The computation was stopped when the steady-state solution was achieved according to the criteria $\varepsilon \leq 0.01$ with $\varepsilon = \frac{1}{N}\sum \frac{\rho^{j+1}-\rho^j}{\Delta t}$.

Some results for this test-problem have already been presented in [11].

The computational space step was smaller than the mean free path ($h < 1$). Furthermore the condition for the time step results in $\Delta t \ll 1$, which means that the time step is much smaller than τ and the mean molecular collisional time (both of them being of the order of λ_1/a_1). This was not the case when kinetical-consistent finite-difference (KCFD) schemes were constructed [1],[2]. Although based on the same formalism, KCFD schemes did not aim at solving the same physical problem as the present GQD equations.

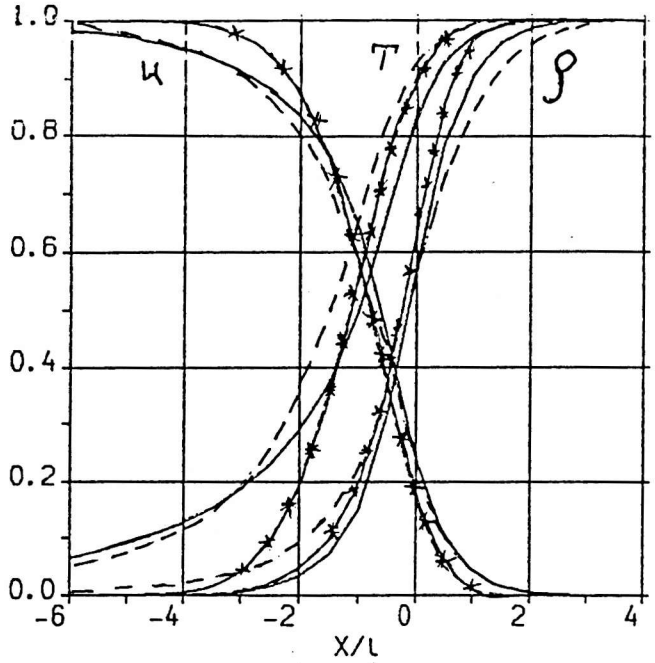

Fig. 1.

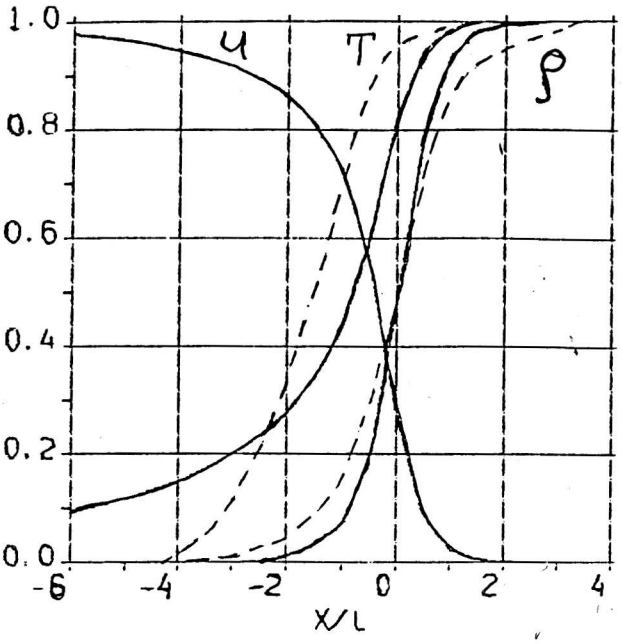

Fig. 2.

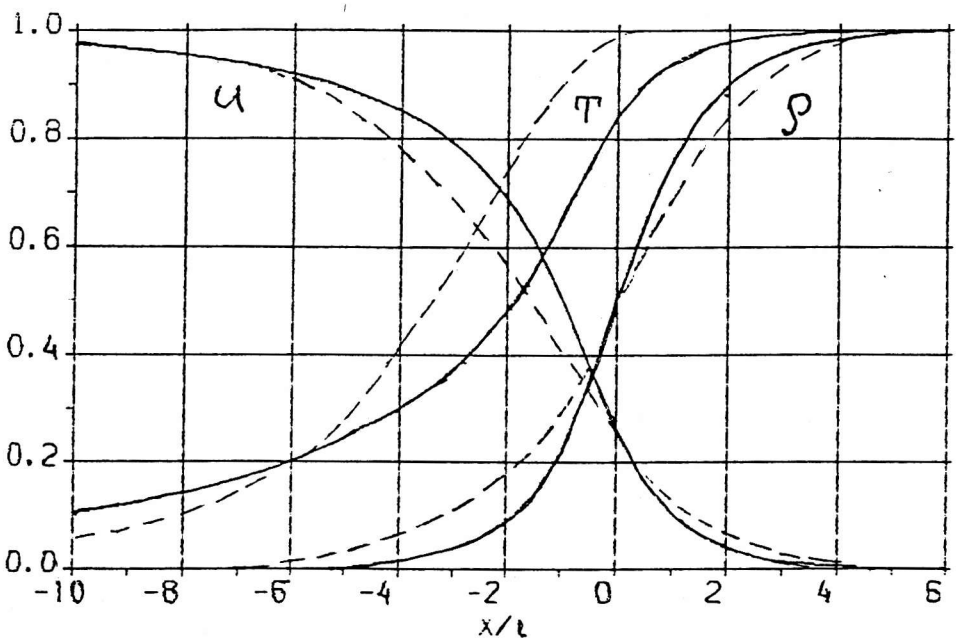

Fig. 3.

4 Numerical results

It is known that the solutions of shock-structure problems based on Navier-Stokes equations and others moment models disagree with experimental data and with the results of direct statistical model calculations (DSMC) for Mach numbers $M \geq 2$. Particularly, NS equations result in the shock width and the distance between density and temperature profiles being too small. The shock-structure problem is a severe test for macroscopic approaches because of large Knudsen numbers ($Kn \sim 0.3$).

Figure 1 shows normalized density, temperature and velocity profiles for the case $M = 3$, $\gamma = 5/3$, $\omega = 0.5$ for QGD (solid line) in comparison with S-model simulations (dashed line) [13].

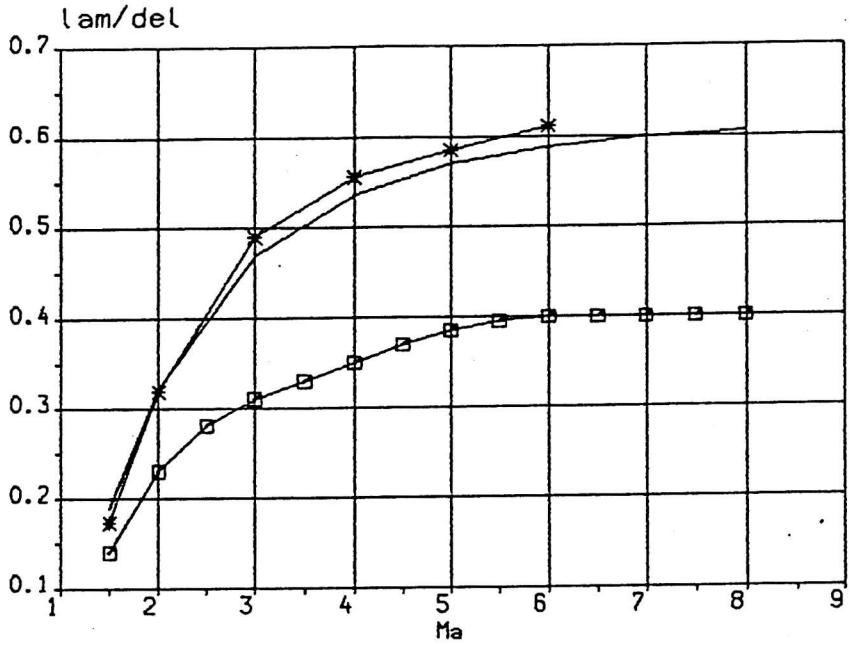

Fig. 4.

We have also plotted NS results (dashed line with stars) that we have obtained using the same numerical procedure as QGD results after removing the additional terms. It is known that for low Mach numbers, S-model computations concord well with the DSMC data. A rather good concordance is observed between QGD and NS density profiles and QGD and S-model velocity profiles.

Fig.2 shows the case $M = 8$, $\gamma = 5/3$, $\omega = 0.5$ for QGD (solid line) in comparison with computations based on conservative scheme in splitting form for kinetical equation (dashed line) [14]. In Fig.3 is shown the variant for $M = 8$, $\gamma = 5/3$, $\omega = 0.816$ for QGD and S-model [13] computations (dashed line). For high Mach numbers, QGD profiles do not concord well with the data obtained directly from kinetical models. Particularly, the temperature profile approaches its asymptotic value behind the shock more slowly than for refereed data. Better results have been obtained when we took τ in Eq.8 and in two terms in right hand of Eq.10 according with heat-conductivity k and in all other terms - according with viscosity μ. Unfortunately, this way may disturb the dissipative characteristics of QGD system.

Numerical experiments have shown that for a given explicit scheme, the number of time steps required for convergence was 3 - 4 times less for QGD equations, than for the same variant based on NS equations. For example the number of iterations to compute a $M = 3$ shock wave is 12.10^3 for QGD, and 82.10^3 for NS. For $M = 5$ the corresponding numbers are 40.10^3 and 143.10^3 respectively. In the latter case, oscillations in density profiles appear in NS calculations before the shock front. For M=8 we have not got the converged NS solution and could not compare it with QGD results.

Adimensional inverse shock thickness (λ_1/δ) vs Mach number is presented as a solid line in Fig.4 for $Pr = 2/3$, $\gamma = 5/3$, $\omega = 0.5$. For comparison the data for kinetical model [14] has been also plotted as $\square$, as well as the solution of NS equations (plotted as $*$) obtained by the authors after having removed additional terms from QGD equations. Shock thickness results obtained by GQD equations differ only little from those obtained by NS equations. We came to the same conclusion for a VHS-gas ($\omega = 0.72$).

The results obtained by QGD and NS models for small Mach numbers are particularly close to one another, (especially for density and velocity profiles). In other words in spite of the distinction in the structure of dissipative terms and the presence of self diffusion in QGD model, the QGD

and NS solutions are rather close not only for smooth functions as it was shown in [3], but also in the case of functions with sharp gradients.

In conclusion, QGD model, like NS one, approximately describes the profiles of gasdynamic parameters in a shock wave for low Mach numbers. For high Mach number flows, the results obtained by QGD and NS equations remain close to one another but computations based on QGD equations are much more stable. This is an important feature for the creation of numerical algorithms for 2D and 3D supersonic flow problems.

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