Quasi-Gasdynamic Equations and Their Possibilities in Rarefied Gas Flow Simulations

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Abstract. The kinetically-based way of construction of the quasi-gasdynamic equations is demonstrated. The advantages of these equations for rarefied gas flow simulations are discussed and illustrated.

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MODEL KINETIC EQUATION AND CONSTRUCTION OF QUASI-GASDYNAMIC SYSTEM

In recent time a number of attempts were undertaken to generalize the Navier-Stokes (NS) equations in order to extend their domain of validity when simulating moderate rarefied gas flows, see, e.g. [1] – [6]. But the constructed mathematical models are rather complicated, and far from practical applications.

The quasi-gasdynamic (QGD) model which generalizes the possibilities of the NS system, was first obtained in 1982 based on the kinetic model consisting in a cyclic process of free-scattering – instantaneous maxwellization. The development of this model is reflected in the RGD proceedings [7] – [12], and in other publications, e.g. [13] – [18].

The model kinetic equation to derive the QGD system can be presented as

$$\frac{\partial f}{\partial t} + (\vec{\xi}\cdot\vec{\nabla}) f^{(0)} - (\vec{\xi}\cdot\vec{\nabla})\tau(\vec{\xi}\cdot\vec{\nabla}) f^{(0)} = \frac{f^{(0)} - f}{\tau}, \tag{1}$$

where $f = f(\vec{x},\vec{\xi},t)$ is the one-particle distribution function, $f^{(0)}$ is the locally-equilibrium Maxwell distribution function, τ is the Maxwell relaxation time, that is close to the mean-free time between successive molecular collisions. Equation (1) can formally be obtained by the BGK equation

$$\frac{\partial f}{\partial t} + (\vec{\xi}\cdot\vec{\nabla}) f = \frac{f^{(0)} - f}{\tau}, \tag{2}$$

where the distribution function in the convective term is replaced by its approximation in the form of a Taylor expansion

$$f = f^{(0)} - \tau(\vec{\xi}\cdot\vec{\nabla}) f^{(0)}. \tag{3}$$

For stationary flows it was shown in [14] that if f satisfies Eq. (2), then it satisfies eq. (1) with the accuracy of $O(\tau^2)$ and vice-versa. For eq.(1), an analog of the Boltzmann H-theorem was proved.

Averaging the model kinetic Eq. (1) successively with the summation invariants 1, $\vec{\xi}$, $\xi^2/2$ we get the QGD system in vector form as

$$\frac{\partial \rho}{\partial t} + div(\rho\vec{u}) = div\left\{\tau\left[div(\rho\vec{u}\otimes\vec{u}) + \vec{\nabla}p\right]\right\}, \tag{4}$$

$$\frac{\partial(\rho\vec{u})}{\partial t} + div(\rho\vec{u}\otimes\vec{u}) + \vec{\nabla}p = div\left\{\tau\left[div(\rho\vec{u}\otimes\vec{u}\otimes\vec{u}) + (\vec{\nabla}\otimes p\vec{u}) + (\vec{\nabla}\otimes p\vec{u})^T\right]\right\} + \vec{\nabla}\left\{\tau[div(p\vec{u})]\right\}, \tag{5}$$

$$\frac{\partial}{\partial t}\left[\rho\left(\frac{\vec{u}^2}{2}+\varepsilon\right)\right] + div\left[\rho\vec{u}\left(\frac{\vec{u}^2}{2}+\varepsilon\right) + p\vec{u}\right] = div\left\{\tau\left\{div\left[\rho\left(\frac{\vec{u}^2}{2}+\varepsilon+2\frac{p}{\rho}\right)\vec{u}\otimes\vec{u}\right] + \vec{\nabla}\left[p\left(\frac{\vec{u}^2}{2}+\varepsilon+\frac{p}{\rho}\right)\right]\right\}\right\}. \tag{6}$$

System (4)–(6) corresponds to a hard-sphere gas, with $\gamma = 5/3$, $Pr = 1$, and $p = \rho RT$.

Replacing $5/3$ by the specific heat ratio γ, we obtain

$$\varepsilon = \frac{p}{\rho(\gamma-1)}, \qquad E = \rho(\frac{u^2}{2} + \varepsilon). \tag{7}$$

QUASI-GASDYNAMIC EQUATIONS IN THE FORM OF CONSERVATION LAWS

According to [14], the QGD equations (4) – (7) can be presented as a system of three partial-derivative equations accounting for conservation of mass (equation of continuity)

$$\frac{\partial \rho}{\partial t} + \nabla_i J_m^i = 0, \tag{8}$$

conservation of momentum

$$\frac{\partial(\rho u^k)}{\partial t} + \nabla_i J_m^i u^k + \nabla^k p = \nabla_i \Pi^{ik}, \tag{9}$$

and conservation of total energy

$$\frac{\partial E}{\partial t} + \nabla_i \frac{J_m^i}{\rho}(E+p) + \nabla_i q^i = \nabla_i(\Pi^{ik}u^k), \tag{10}$$

where the mass flux vector J_m^i, the shear-stress tensor Π^{ik}, and the heat flux vector q^i are expressed as functions of macroscopic flow quantities in the following form

$$J_m^i = \rho u^i - \tau\left(\nabla_j(\rho u^i u^j) + \nabla^i p\right), \tag{11}$$

$$\Pi^{ik} = \Pi_{NS}^{ik} + \tau u^i\left(\rho u^j \nabla_j u^k + \nabla^k p\right) + \tau g^{ik}\left(u_j \nabla^j p + \gamma p \nabla_j u^j\right), \tag{12}$$

$$q^i = q_{NS}^i - \tau\rho u^i\left(u^j \nabla_j \varepsilon + p u_j \nabla^j(\frac{1}{\rho})\right). \tag{13}$$

Here q_{NS}^i and Π_{NS}^{ik} are the Navier-Stokes heat flux and shear-stress tensor, while g^{ik} is the metric tensor.

In the above presentation we obtain that the viscosity coefficient μ, the bulk viscosity ζ and the heat conductivity κ are related through the parameter τ as

$$\mu = \tau p, \quad \zeta = \tau p\left(\frac{5}{3} - \gamma\right), \quad \kappa = \tau p \frac{\gamma R}{\gamma - 1}. \tag{14}$$

In this form the coefficients μ and κ were derived in constructing the NS system by the Chapman-Enskog method based on BGK model for the hard-sphere gas, see, for example [19]. The bulk viscosity coefficient ζ in the form (14) was obtained in [19] by the BGK approximation for non-monoatomic gas with rotational degrees of freedom.

As for the NS system obtained by the BGK approximation, the dissipative coefficients (14) can be generalized. Introducing a Prandtl number $Pr \neq 1$ we can write the coefficient of the heat conductivity in the usual form

$$\kappa = \mu \frac{\gamma R}{\gamma - 1}\frac{1}{Pr}.$$

Introducing the Schmidt number Sc (close to unity in gases) we obtain

$$\tau = \frac{\mu}{pSc}.$$

The bulk viscosity coefficient can also be generalized. For example, by introducing the numerical factor B to adjust it to a case of translational-rotational non-equilibrium

$$\zeta = \mu B\left(\frac{5}{3}-\gamma\right), \qquad \text{where} \qquad B=(\gamma-1)\sqrt{\frac{\pi}{2}}\frac{3}{2}\sqrt{\frac{\pi}{8}}Z_{rot}, \tag{15}$$

and Z_{rot} is the coefficient of the energy exchange between translational and rotational degrees of freedom. The last one may be estimated by Parker's formula [20].

The QGD system is closely related to the NS system. For the QGD equations in the form (8) – (10), mass, momentum, ungular momentum, total energy conservation laws, and the entropy theorem, are valid as for the classic NS system.

Formally, QGD and NS systems differ from one another (terms contained τ) in the order of $O(\tau)$. But for stationary flows it was proved that these terms have the asymptotic order of $O(\tau^2)$ for $\tau \to 0$, or in the dimensionless form of the equations, the order of $O(Kn^2)$ for $Kn \to 0$.

The boundary layer approximation for the QGD equations leads to the classical Prandtl equation system. The same approximation is valid for the NS system. From the definitions of the shear stress tensor (12) and heat flux vector (13) it follows that on the unpenetrated boundaries ($u^i = 0$) the shear-stresses and the heat fluxes for the QGD and NS models coincide, namely $\Pi = \Pi_{NS}$ and $q = q_{NS}$. So the definitions for the friction forces and the heat flux on the boundaries for the QGD and NS models are the same. The barometric Laplace formula is the common exact solution for both the QGD and NS models. The other exact solution for both models is the solution of the classical Couette problem [14].

The QGD system differs from the Burnett equations – the QGD system has additional terms in the form of the second space derivatives, while the Burnett equations have the additional third space derivative terms.

The QGD system can be regarded as an example of a model with non-classical continuity equation, or as a "two-velocities" gasdynamic model. The velocity u_i is related with the momentum transfer and frictions forces on the boundaries, while the J^i_m/ρ velocity describes the mass flow. One of the first variant of the "two-velocities" model was presented in 1951 [1]. Recently models of this type are widely proposed and investigated, e.g. [2] – [6]. Nevertheless, the QGD system differs significantly from the mentioned systems.

The advantages of the QGD model compared with the NS system are found for strongly non-stationary flows and for moderate rarefied flows, where terms contained τ are not negligible.

RAREFIED FLOW SIMULATIONS

Microchannel flows. Experiments of Knudsen, carried out in 1900, show the existence of the minimum of normalized flow-rate in long isothermal microchannels for $Kn \sim 1$. The possibilities of describing this phenomenon is a present-day problem for rarefied flow simulations in the framework of continuum models. The NS equation system with Maxwell-type slip boundary conditions fails to describe this effect. Using the NS system the Knudsen effect may be obtained by introducing artificial second order slip boundary conditions, e.g. [21]. Some results were obtained, for example, by 13-moment regularized Grad equations by a rather difficult mathematical technique together with enhanced boundary conditions [22]. Based on the BGK model for hard-sphere molecules the Knudsen effect has been described by a complex mathematical procedure in [23].

The QGD system complemented by the classic Maxwell-type slip boundary conditions allows to obtain the mass-flow rate formula describing the Knudsen effect in a simple way.

We analyze a gas flow in a plane channel of length L in x–direction and width H in y–direction. The pressures at the entrance and the exit of a channel are p_1 and p_2, where $p_1 > p_2$. We look for the solution of the system (8)–(10) in the form $u_x = u(y)$, $u_y = 0$, $p = p(x)$, $T = T_0$. In this case the NS and QGD systems reduce to the same equation

$$\frac{dp(x)}{dx} = \mu\frac{d^2u(y)}{dy^2}, \quad \text{where} \quad \frac{dp}{dx} = \frac{p_2-p_1}{L}.$$

Using Maxwell velocity-slip boundary conditions for both systems we get the classical modified Poiseuille formula for the velocity distribution

$$u_x(y) = -\frac{1}{2\mu}\frac{dp(x)}{dx}\left[y(H-y)+\frac{2-\sigma}{\sigma}\lambda H\right].$$

Here σ is the coefficient of accommodation for velocity, and λ is the mean free-path calculated as $\lambda = A\mu\sqrt{RT}/p$, where $A = \sqrt{\pi/2}$ for Chapman formula, or $A = 2(7-2\omega)(5-2\omega)/(15\sqrt{2\pi})$ for Bird formula [20].

In the the QGD formulation the flow-rate is calculated using the mass flux (11) $J_{mx} = \rho(u_x - w_x)$, as

$$J = \int_0^H J_{mx} dy, \quad \text{where} \quad w_x = -\frac{\tau}{\rho}\frac{dp}{dx} = -\frac{\mu}{pSc}\frac{1}{\rho}\frac{dp}{dx}.$$

So the normalized flow rate becomes

$$Q_{xy} = \frac{J}{J_0^{xy}} = \frac{3\sqrt{\pi}A}{8\sqrt{2}}\Big[\frac{Kn^{-1}}{6} + \frac{2-\sigma}{\sigma} + \frac{2}{A^2 Sc}Kn\Big]. \tag{16}$$

The first term in (16) describes the mass flow-rate for non-slip Poiseuille flow, the second one accounts for the flow-rate increased because of velocity-slip conditions, the third one explains the flow-rate increased because of self-diffusion. It does not depend on σ. The importance of the self-diffusion for rarefied flows in microchannels is pointed out in, e.g. [23]. This last term has the order of $O(\tau \cdot \mu)$ or $O(Kn^2)$, where $Kn = \lambda/H$. For stationary flows this fact corresponds to the difference between QGD and NS models in stationary cases. The minimum of Q_{xy} takes place for

$$Kn_m = \frac{A}{2}\sqrt{\frac{Sc}{3}}.$$

This value does not depend from σ. For $Sc = 1$, $A = \sqrt{\pi/2}$, $Kn_m = 0.36$. The results obtained together with the results e.g.[12], [16] show, that the QGD model increases for this problem the domain of validity of the continuum approach up to $Kn \sim 0.5$.

Shock-wave problem. The shock-wave problem is a widely used test to examine the mathematical models and numerical algorithms for rarefied flow simulations.

Below we compare the structure of shock wave fronts at different Mach numbers, modeled via NS and QGD equations, with experimental results from the literature. Monoatomic argon, and diatomic nitrogen, are considered. The molecular parameters are taken from [20]. In this modeling a finite-difference scheme with the second-order spatial accuracy is employed for both the NS and QGD equations [11].

In Fig. 1, left, the distributions of velocity, density and temperature in an argon shock wave are shown together with experimental data. The density thickness calculated via QGD and NS models ($\gamma = 5/3, \omega = 0.81, Sc = 0.752, Pr = 2/3$) are in a good agreement with each other, and with the experimental results. But velocity and temperature profiles in the upstream region differ – in the QGD formulation they are smoothed compared with the NS one. This effect is similar to that found for BGK modeling. The QGD-based algorithm converges to the steady state solution approximately 10 times faster than the NS-based algorithm due to the absence of numerical oscillations (Fig. 1, right). In Fig. 2, left, the reciprocal shock-wave thickness compared with the experiment is shown. For these distributions QGD and NS results are close one to each other, and both differ from the experiment by $\sim 30\%$ for $Ma > 2$.

Calculations for diatomic nitrogen in the NS and QGD formulations ($\gamma = 7/5, \omega = 0.74, Sc = 0.746, Pr = 14/19$) were performed taking into account the bulk viscosity in the form (15). The reciprocal shock wave thickness for $B = 0$ (line 1), $B = 1$ (line 2) and $B(Z_{rot})$ (line 3) are shown in Fig. 2, right.

Here again the QGD results for the density distributions are close to the NS. Both depend strongly on the value of the bulk viscosity. If the numerical factor B in (15) is taken according to translational-rotational exchange law, the calculated shock-wave densities differ moderately from experimental data even for $Ma > 2$.

Flat-plane flow and other examples. The comparison of the QGD, NS and DSMC calculations for the supersonic air flow near a flat plane is shown in Fig. 3. Parameters of the undisturbed flow are: Mach number $Ma = 2$, $\rho = 0.000169 kg/m^3, T = 167K, u = 518 m/s$. The surface temperature is $T_w = 300K$, the length of the plate is 12 cm. The slip velocity and temperature-jump conditions are imposed on the surface [18].

In this flow $Kn \sim 0.01$, and as it is seen from the Fig. 3, the velocity profiles calculated by the DSMC (reference data), NS and QGD systems, are extremely close one to each other, and the DSMC velocity distributions are always placed between the NS and the QGD lines. Comparison of the convergence rate shows that the computational time for the QGD algorithm is less than the NS computational time by a factor of 20. The difference arises from the smaller NS computational time step and the greater number of time steps to achieve convergence.

The QGD system was successfully used in other numerical simulations of rarefied gas flows, e.g. underexpanded jets and jet interaction [10], supersonic flows around infinitely thin disk [17], the orbiter flow simulations and others. The possibilities of extending the QGD model to thermal non-equilibrium flows and to binary gas mixtures are presented, e.g., in [8] and [9].

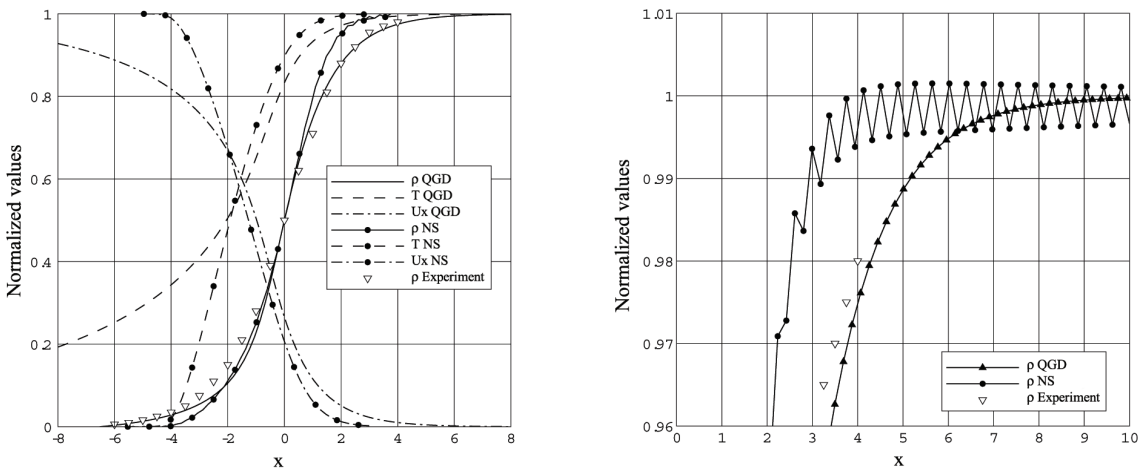

FIGURE 1. Density, velocity and temperature distributions in argon shock-wave, Ma=9 (left). Fragment for the density distribution (right) Comparison of the QGD and NS solutions with the experiment.

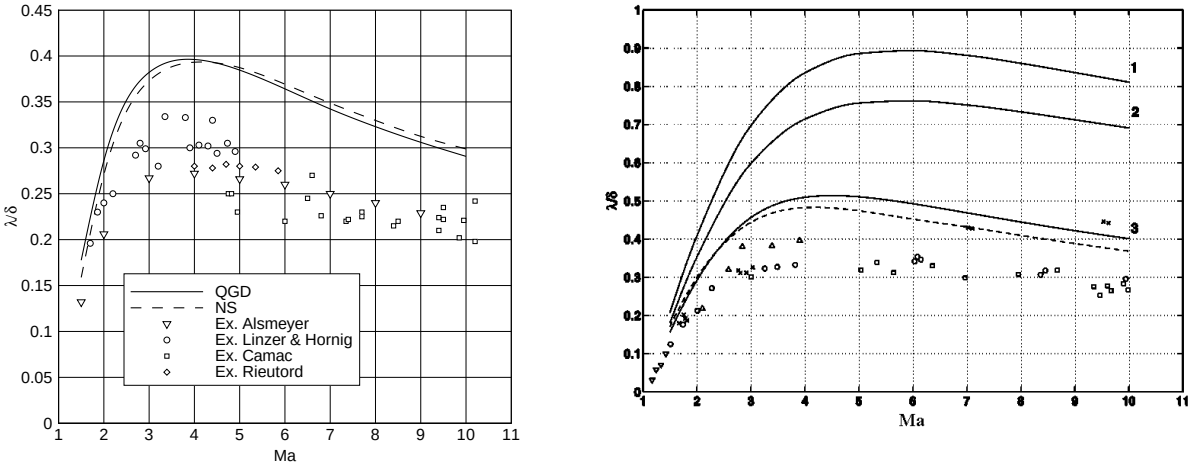

FIGURE 2. Reciprocal shock-wave thickness in argon (left) and nitrogen (right) compared with the experiment. Navier-Stokes computations - solid lines, QGD computations - dashed lines.

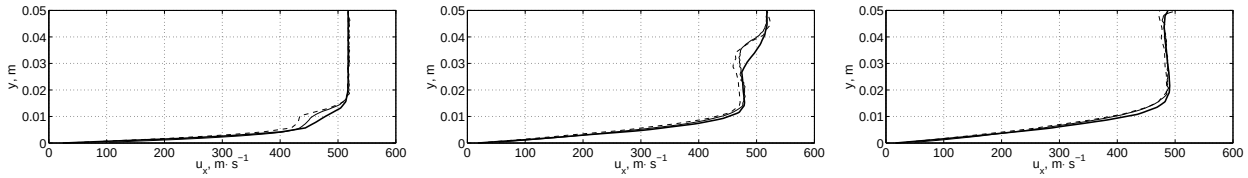

FIGURE 3. Longitudinal velocity profiles for the flow around flat plate at a distance from leading edge x = 4 cm, 7 cm and 10 cm respectively, from left to right. DSMC calculations - solid line, QGD - bold solid line, NS - dashed lines.

CONCLUSION

The quasi-gasdynamic equation system that generalizes the Navier-Stokes equations is presented together with its kinetic origin. The advantages of this model in rarefied gas dynamics are demonstrated for microchannels, shock-wave structure and various other flow computations.

For practical applications the form of quasi-gasdynamic equations allows to solve them with a better convergence rate than the Navier-Stokes equations.

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