Theoretical and Numerical Analysis of Quasi-Gasdynamic and Quasi-Hydrodynamic Equations

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Abstract—The results obtained by the authors in developing new efficient mathematical models, systems of quasi-gasdynamic and quasi-hydrodynamic equations, are presented in a systematic form. A phenomenological interpretation of these systems is discussed, and their relation to the Navier–Stokes equations is investigated. The results of numerical simulations of some compressible and incompressible flows are compared with those based on other mathematical models.

1. INTRODUCTION

In [1–4], efficient algorithms were proposed for the mathematical modeling of gasdynamic flows. In those studies, kinetically consistent finite-difference schemes (KCFDS) and closely related quasi-gasdynamic equations were constructed. Quasi-gasdynamic equations differ from Navier–Stokes equations by their additional terms written in conservative form with a small parameter as a coefficient. In numerical simulations of viscous flows, these additional terms behave as efficient regularizers.

In this paper, we systematically expand on our theoretical and numerical results obtained by examining and applying the systems of quasi-gasdynamic (QGD) and quasi-hydrodynamic (QHD) equations in numerical experiments. We propose a phenomenological interpretation demonstrating that these schemes are consistent with basic conservation laws, analyze their relation to Navier–Stokes equations, and construct a QHD model for a viscous incompressible fluid. The results of numerical simulations of gas and fluid flows based on QHD and QGD equations are compared with analogous results obtained by applying other approaches.

The first of the QHD systems, the quasi-gasdynamic system, was derived in [2–4] from the well-known model of a free-molecular gas outflow followed by instant maxwellization. This approach was also used in [5–7] to develop numerical methods for problems in gas dynamics. The second, QHD system was introduced in [8]. A phenomenological interpretation of these systems and their representation in the form of integral conservation laws were proposed in [9]. In [8–11], entropy balance equations were obtained for both systems, properties of their solutions having the form of stationary shock waves were examined, and laminar boundary-layer approximations equivalent to the Prandtl equations were constructed. It was shown that time-independent QHD and QGD systems differ form Navier-Stokes equations by the additional conservative terms of the second order with respect to the Knudsen number. In [8, 9, 12], the Boussinesq approximation was constructed, a procedure of transition to mass Lagrangian coordinates was substantiated, and some exact solutions were found for the quasi-hydrodynamic equations. A version of the second QHD system designed for numerical simulation of the isothermal viscous incompressible flows a fluid was originally proposed in [13]. For this version, a theorem on the dissipation of the total kinetic energy in bounded domains was also proved, and exact solutions were constructed that are equivalent to the corresponding solutions to the Navier-Stokes equations. These solutions describe laminar pipe and plane Poiseuille flows and the Couette flows between coaxial cylinders rotating at constant angular velocities. Algorithms constructed based on the QHD and QGD equations were successfully used in numerical simulations of gas [14, 15] and fluid [16–18] flows.

The quasi-gasdynamic system was introduced in the context of an analysis of the differential approximations of KCFDS. The results of numerical studies of gasdynamic flows based on these schemes were presented in [19]. Note also that the QHD and QGD systems differ from the other systems similar in structure proposed in [20–23].

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2. PHENOMENOLOGICAL INTERPRETATION OF QUASI-HYDRODYNAMIC EQUATIONS

In this section, we discuss a phenomenological interpretation of the QHD system of equations originally published in [8] and check the fulfillment of basic conservation laws for this system. To this end, we follow the phenomenological derivation of the classical Navier–Stokes system [24, 25] that describes compressible viscous heat-conducting flows. The derivation is based on the postulates that express integral conservation laws for mass, momentum, angular momentum, total energy, and entropy for a moving material volume.

We define an inertial Cartesian coordinate system $\mathbf{x} = (x_1, x_2, x_3)$ in the Euclidean space \mathbb{R}^3 with an orthonormal basis ($\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$) and denote time by *t*. We use the following notation for macroscopic flow variables: $\rho = \rho(\mathbf{x}, t)$ is density, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is velocity, $p = p(\mathbf{x}, t)$ is pressure, $\varepsilon = \varepsilon(\mathbf{x}, t)$ is the specific internal energy, $T = T(\mathbf{x}, t)$ is temperature, and $s = s(\mathbf{x}, t)$ is the specific entropy. We assume that only two of the five thermodynamic variables ρ , *p*, ε , *T*, and *s* are independent. Three equations of state are given:

$$p = \Psi_1(\rho, T), \quad \varepsilon = \Psi_2(\rho, T), \quad s = \Psi_3(\rho, T).$$
 (2.1)

By **F**, we denote the body force per unit mass. For example, $\mathbf{F} = \mathbf{g}$ for a fluid in the gravitational field, where **g** is the acceleration of gravity.

The first postulate is the mass conservation law written in the form

$$\partial \rho / \partial t + \operatorname{div} \mathbf{j}_m = 0.$$
 (2.2)

We assume that the vector $\mathbf{j}_m = \mathbf{j}_m(\mathbf{x}, t)$ called the mass flux is defined at each point \mathbf{x} of the flow domain at each moment *t*. We do not specify its form at this point.

In the flow domain, we single out a moving material volume V = V(t) bounded by a smooth surface $\Sigma = \Sigma(t)$, which is oriented by a field of outward unit normal vectors **n**. We suppose that the volume V(t) evolves from a volume $V_0 = V(t_0)$, where t_0 is an initial moment, through the continuous deformation induced by the movement of particles from V_0 along the trajectories determined by the vector field \mathbf{j}_m/ρ . Using the well-known Liouville theorem on the derivative of an integral over a moving material volume [24], we represent the mass conservation law (2.2) as

$$\frac{d}{dt} \int_{V} \rho dV = 0.$$
(2.3)

The momentum conservation law is the second postulate:

$$\frac{d}{dt} \int_{V} (\rho \mathbf{u}) dV = \int_{V} \rho \mathbf{F} dV + \iint_{\Sigma} (\mathbf{n} \cdot P) d\Sigma.$$
(2.4)

The rate of momentum variation in the volume V equals the sum of forces applied to this volume. The first integral on the right-hand side of (2.4) is the body force induced by the external field, and the second integral determines the pressure and internal viscous friction forces applied to the surface Σ . The quantity $P = P(\mathbf{x}, t)$ is the internal stress tensor. By $(\mathbf{n} \cdot P)$, we denote a convolution (inner product) of the vector \mathbf{n} and the second-rank tensor P performed with respect to the first index of P. Accordingly, $(P \cdot \mathbf{n})$ is the convolution of P and \mathbf{n} with respect to the second index of P. In the case of a symmetric tensor P, $(\mathbf{n} \cdot P) = (P \cdot \mathbf{n})$. The total energy conservation law is the third postulate:

$$\frac{d}{dt} \int_{V} \rho \left(\frac{\mathbf{u}^{2}}{2} + \varepsilon \right) dV = \int_{V} (\mathbf{j}_{m} \cdot \mathbf{F}) dV + \iint_{\Sigma} (\mathbf{A} \cdot \mathbf{n}) d\Sigma - \iint_{\Sigma} (\mathbf{q} \cdot \mathbf{n}) d\Sigma.$$
(2.5)

Hereinafter, the square of an arbitrary vector is defined as $\mathbf{a}^2 = (\mathbf{a} \cdot \mathbf{a}) = |\mathbf{a}|^2$.

The first integral on the right-hand side of (2.5) is equal to the power of the external mass forces applied to the volume *V*, and the second integral is interpreted as the power of the surface pressure forces and internal viscous friction. The last term in (2.5) describes the energy flux across the surface Σ due to heat conduction. We write out the expressions for the vector fields $\mathbf{A} = \mathbf{A}(\mathbf{x}, t)$ and $\mathbf{q} = \mathbf{q}(\mathbf{x}, t)$ in what follows.

The next postulate expresses the conservation of angular momentum:

$$\frac{d}{dt} \int_{V} [\mathbf{x} \times (\mathbf{\rho} \mathbf{u})] dV = \int_{V} [\mathbf{x} \times \mathbf{\rho} \mathbf{F}] dV + \iint_{\Sigma} [\mathbf{x} \times (\mathbf{n} \cdot P)] d\Sigma.$$
(2.6)

It is represented in the classical form [24]. Internal torques and couples distributed over the volume and the surface are not taken into account.

The second law of thermodynamics serves as the fifth postulate:

$$\frac{d}{dt} \int_{V} (\rho s) dV = -\iint_{\Sigma} \frac{(\mathbf{q} \cdot \mathbf{n})}{T} d\Sigma + \int_{V} X dV.$$
(2.7)

The surface integral on the right-hand side of (2.7) is the rate of entropy variation in the volume V due to heat flux. It can be either positive or negative. The last integral in (2.7) is strictly nonnegative and describes the rate of entropy production due to internal irreversible processes.

The specific entropy s is defined by the well-known differential Gibbs identity

$$Tds = d\varepsilon + pd(1/\rho). \tag{2.8}$$

Again, to pass from integral relations (2.3)–(2.7) to corresponding differential equations, we use Liouville's volume theorem. We assume, in so doing, that all basic macroscopic variables are sufficiently smooth functions of coordinates and time. Since it was mentioned above that the motion of V is determined by the vector field \mathbf{j}_m/ρ , the Liouville theorem takes the form

$$\frac{d}{dt} \int_{V} \varphi dV = \int_{V} [D\varphi + \varphi \operatorname{div}(\mathbf{j}_{m}/\rho)] dV.$$
(2.9)

Here, $\varphi = \varphi(\mathbf{x}, t)$ is a continuously differentiable scalar or vector field, and $D = \partial/\partial t + (\mathbf{j}_m/\rho) \cdot \nabla$ is a differential operator.

Applying formula (2.9) to (2.3)–(2.7) and taking into account the arbitrariness of V, we obtain differential balance equations for mass,

$$\partial \rho / \partial t + \operatorname{div} \mathbf{j}_m = 0;$$
 (2.10)

momentum,

$$\partial(\rho \mathbf{u})/\partial t + \operatorname{div}(\mathbf{j}_m \otimes \mathbf{u}) = \rho \mathbf{F} + \operatorname{div} P;$$
 (2.11)

total energy,

$$\frac{\partial}{\partial t} \left[\rho \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) \right] + \operatorname{div} \left[\mathbf{j}_m \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) \right] = (\mathbf{j}_m \cdot \mathbf{F}) + \operatorname{div} \mathbf{A} - \operatorname{div} \mathbf{q}; \qquad (2.12)$$

angular momentum,

$$\frac{\partial}{\partial t} [\mathbf{x} \times \rho \mathbf{u}] + \operatorname{div}(\mathbf{j}_m \otimes [\mathbf{x} \times \mathbf{u}]) = [\mathbf{x} \times \rho \mathbf{F}] + \frac{\partial}{\partial x_i} [\mathbf{x} \times P_{ij} \mathbf{e}_j]; \qquad (2.13)$$

and entropy,

$$\partial(\rho s)/\partial t + \operatorname{div}(\mathbf{j}_m s) = -\operatorname{div}(\mathbf{q}/T) + X.$$
 (2.14)

Here, $(\mathbf{j}_m \otimes \mathbf{u})$ is the second-rank tensor obtained as the direct product of \mathbf{j}_m and \mathbf{u} . To calculate the divergence of a second-rank tensor, the convolution is performed with respect to its first index. In Eq. (2.13), the symbol P_{ij} denotes the components of P in the basis (\mathbf{e}_1 , \mathbf{e}_2 , \mathbf{e}_3), and summation is performed over the repeated indices *i* and *j*.

System (2.10)–(2.14) is not closed. The closure problem can be solved in different ways. To this end, the quantities \mathbf{j}_m , P, \mathbf{A} , \mathbf{q} , and X must be represented as functions of macroscopic flow variables and their derivatives.

The following expressions for these quantities correspond to the Navier–Stokes equations:

$$\mathbf{j}_m = \mathbf{\rho} \mathbf{u},\tag{2.15}$$

$$P = \Pi - pI, \tag{2.16}$$

$$\mathbf{A} = (\Pi \cdot \mathbf{u}) - p\mathbf{u}, \tag{2.17}$$

$$\mathbf{q} = -\kappa \nabla T, \tag{2.18}$$

$$X = \kappa \left(\frac{\nabla T}{T}\right)^2 + \frac{(\Pi : \Pi)}{2\eta T}.$$
(2.19)

In formulas (2.15)–(2.19), *I* denotes the unit tensor,

$$\Pi = \eta[(\nabla \otimes \mathbf{u}) + (\nabla \otimes \mathbf{u})^{\mathrm{T}} - (2/3)I\mathrm{div}\mathbf{u}]$$
(2.20)

is the Navier–Stokes viscous stress tensor, and $(\Pi : \Pi) = \sum_{i, j=1}^{3} \prod_{ij} \prod_{ij} \prod_{ij} a$ double inner product. The positive absolute viscosity η and heat conductivity κ are assumed to be given functions of density and temperature. In (2.20), the term corresponding to bulk viscosity is disregarded.

Formulas (2.15)–(2.19) can be used to show that the entropy balance equation (2.14) follows from Eqs. (2.10)–(2.12). Note that, for a moderately rarefied monatomic gas, expressions (2.18) and (2.20) can be derived from the Boltzmann kinetic equation by the Chapman–Enskog and Grad methods in the first approximation by expanding, in terms of the Knudsen small parameter [26, 27].

In the Navier–Stokes theory, density, velocity, and temperature are defined by averaging over a set of physically infinitesimal volumes in \mathbb{R}^3 at a fixed moment *t*. In changing from one inertial coordinate system to another, an instantaneous spatial average is transformed according to a certain law. Identity (2.15) can be proved for instantaneous spatial averages (see [27]).

Let us assume an alternative definition of gas flow variables that differs from the classical one and relies on a spatiotemporal averaging rather than on a spatial one. Such a procedure of smoothing over a set of physically infinitesimal four-dimensional parallelepipeds in the phase space $\mathbb{R}^3 \times \mathbb{R}_t$ was described in detail in [12]. In this procedure, the choice of \mathbf{j}_m , P, \mathbf{A} , \mathbf{q} , and X is not limited to the classical expressions (2.15)– (2.19) under the assumption that \mathbf{j}_m is not equal to $\rho \mathbf{u}$.

If we disregard the requirements (2.15)–(2.19), then the combined system of equations and variables generally loses its original physical meaning. However, it admits formal closures of at least two types. Since the starting postulates (2.10)–(2.14) hold as basic conservation laws, we preserve the corresponding notation for all variables in the equations. General considerations suggest that spatiotemporal and spatial averages are close for weakly nonequilibrium flows, differing by quantities containing a small parameter that plays the role of a regularizer in a numerical computation.

One closure of system (2.10)–(2.14) corresponding to the QGD system of equations is presented in the next section. Another closure, which leads to the QHD system, was discussed in detail in [9]. For QHD equations, the expressions analogous to (2.15)–(2.19) have the form

$$\mathbf{j}_m = \mathbf{\rho}(\mathbf{u} - \mathbf{w}),\tag{2.21}$$

$$P = \Pi - pI + \rho \mathbf{u} \otimes \mathbf{w} = \Pi_Q - pI, \qquad (2.22)$$

$$\mathbf{A} = (\mathbf{\Pi} \cdot \mathbf{u}) - p(\mathbf{u} - \mathbf{w}) + \rho \mathbf{u}(\mathbf{w} \cdot \mathbf{u}), \qquad (2.23)$$

$$\mathbf{q} = -\kappa \nabla T, \tag{2.24}$$

$$X = \kappa \left(\frac{\nabla T}{T}\right)^2 + \frac{(\Pi:\Pi)}{2\eta T} + \frac{\rho w^2}{\tau T}.$$
(2.25)

In (2.21)–(2.15), w is the vector defined as

$$\mathbf{w} = \frac{\tau}{\rho} [\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p - \rho \mathbf{F}], \qquad (2.26)$$

and Π is the Navier–Stokes viscous stress tensor. As in the classical case, when *P* is defined by (2.22), the angular momentum equation (2.13) is a Corollary of the momentum conservation law (2.11). The entropy balance equation is also derived by combining the Gibbs identity (2.8) with the mass, momentum, and energy conservation laws.

In (2.26), the positive parameter τ , having the dimension of time, is assumed to be a prescribed function of density and temperature. To compute τ , the formula

$$\tau = \frac{\gamma}{\mathrm{Sc}} \frac{\mathrm{v}}{c_s^2}$$

was proposed in [9], where $v = \eta/\rho$ is the kinematic viscosity, γ is the ratio of specific heat, c_s is the sonic velocity, and $Sc = \eta/(\rho D)$ is the Schmidt number. The fluid self-diffusion coefficient *D* can be measured experimentally. For gases, the Schmidt number is close to unity. By virtue of Laplace's formula $c_s^2 = \gamma p/\rho$, the expression for τ can be transformed into $\tau = \eta/(pSc)$. Thus, τ is close in the order of magnitude to the mean free path of atoms in a gas.

Substituting (2.21)–(2.25) into (2.10)–(2.14), we arrive at the system of QHD equations

$$\partial \rho / \partial t + \operatorname{div}(\rho \mathbf{u}) = \operatorname{div}(\rho \mathbf{w}),$$
 (2.27)

$$\partial(\rho \mathbf{u}/\partial t) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \rho \mathbf{F} + \operatorname{div}\Pi + \operatorname{div}[(\rho \mathbf{w} \otimes \mathbf{u}) + (\rho \mathbf{u} \otimes \mathbf{w})], \quad (2.28)$$

$$\frac{\partial}{\partial t} \left[\rho \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) \right] + \operatorname{div} \left[\rho \mathbf{u} \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) + p \mathbf{u} \right] + \operatorname{div} \mathbf{q}$$

$$= \rho \mathbf{F} \cdot (\mathbf{u} - \mathbf{w}) + \operatorname{div} (\Pi \cdot \mathbf{u}) + \operatorname{div} \left[\rho \mathbf{w} \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) + p \mathbf{w} + \rho \mathbf{u} (\mathbf{w} \cdot \mathbf{u}) \right].$$
(2.29)

System (2.27)–(2.29) becomes closed if it is supplemented by analogues of the equations of state (2.1) and by expressions for the coefficients

$$\eta = \Psi_4(\rho, T), \quad \kappa = \Psi_5(\rho, T), \quad \tau = \Psi_6(\rho, T).$$
 (2.30)

We represent the entropy balance equation (2.14) as

$$\frac{\partial(\rho s)}{\partial t} + \operatorname{div}(\rho \mathbf{u} s) = \operatorname{div}(\rho \mathbf{w} s) + \operatorname{div}\left(\kappa \frac{\nabla T}{T}\right) + \kappa \left(\frac{\nabla T}{T}\right)^2 + \frac{\Phi}{T},$$
(2.31)

where

$$\Phi = \frac{(\Pi:\Pi)}{2\eta} + \frac{\rho \mathbf{w}^2}{\tau}$$
(2.32)

is a nonnegative dissipation function. It can be included into the system instead of the energy equation.

As $\tau \rightarrow 0$, the additional terms in (2.21)–(2.23), (2.25) (i.e., those containing the vector **w**) tend to zero; expressions (2.21)–(2.25) reduce to (2.15)–(2.19); and the system of QHD equations (2.27)–(2.29), including the equations of state, becomes the classical system of Navier–Stokes equations. General considerations naturally suggest that, in this limit, the spatiotemporal averages behave as follows: $\rho \rightarrow \rho_{NS}$, $\mathbf{u} \rightarrow \mathbf{u}_{NS}$, and $T \rightarrow T_{NS}$, where classical instantaneous spatial averages—density, velocity, and temperature—are denoted by ρ_{NS} , \mathbf{u}_{NS} , and T_{NS} , respectively.

Formulation of boundary conditions for the proposed equations is a complicated task connected to the existence, uniqueness, stability and physical adequacy of their solutions. Therefore, this task should be considered separately for each particular problem. The system of differential equations (2.27)–(2.29) is of a higher order, as compared to the Navier–Stokes system, due to the terms containing second-order partial derivatives of pressure with respect to spatial coordinates. Therefore, the number of boundary conditions for the QHD equations must be larger than in the classical case. Consider a fluid motion in a closed, adiabatically insulated volume V_0 bounded by a stationary smooth surface Σ_0 oriented by a field of outward unit normal vectors **n**. The following boundary conditions can be set on the boundary Σ_0 :

$$\mathbf{u}|_{\Sigma_0} = 0, \quad (\mathbf{w} \cdot \mathbf{n})|_{\Sigma_0} = 0, \quad \partial T / \partial \mathbf{n}|_{\Sigma_0} = 0. \tag{2.33}$$

The first condition in (2.33) is the no-slip condition on the walls of a vessel, the second condition combined with the first one ensures the absence of mass flux across the boundary, and the third condition implies that the normal component of the heat flux **q** vanishes on Σ_0 . Integrating Eq. (2.31) over V_0 and using boundary conditions (2.33) and the fact that the dissipation function (2.32) is nonnegative, we find that the total thermodynamic entropy of the fluid, $S = \int_{V_0} (\rho s) d\mathbf{x}$, cannot decrease in the volume in question. The Navier–Stokes system possesses a similar property [28]. Joule's principle of equivalence of mechanical work and heat for an adiabatically insulated volume with moving rigid walls can be obtained as a direct consequence of the QHD equations. The well-known barometric formula is also a consequence of system (2.27)–(2.29).

It is shown in [8] that classical Prandtl equations [25] provide the laminar boundary-layer approximation of the QHD equations. In the case of steady flows, the divergence terms in the QHD equations formally behave as $O(\tau^2)$ quantities as $\tau \longrightarrow 0$. However, these terms are on the order of $O(\tau)$ for unsteady flows, and their influence may be significant.

Finally, we note that small divergence terms that distinguish the QHD equations from the Navier–Stokes equations play the role of regularizers ensuring the efficiency of finite-difference algorithms, which is verified by numerous computations of complex gas and fluid flows.

3. SYSTEM OF QUASI-GASDYNAMIC EQUATIONS

This system was derived in [2, 4] in the form

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = \operatorname{div}\tau[\operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p], \qquad (3.1)$$

$$\partial(\rho \mathbf{u})/\partial t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p$$
(3.2)

$$= \operatorname{div} \tau[\operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} \otimes \mathbf{u}) + (\nabla \otimes p \mathbf{u}) + (\nabla \otimes p \mathbf{u})^{\mathrm{T}}] + \nabla \tau[\operatorname{div}(\rho \mathbf{u})],$$

$$\frac{\partial}{\partial t} \left[\rho \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) \right] + \operatorname{div} \left[\rho \mathbf{u} \left(\frac{\mathbf{u}^2}{2} + \varepsilon \right) + p \mathbf{u} \right]$$

$$= \operatorname{div} \tau \left\{ \operatorname{div} \left[\rho \left(\frac{\mathbf{u}^2}{2} + \varepsilon + 2\frac{p}{\rho} \right) \mathbf{u} \otimes \mathbf{u} \right] + \nabla \left[p \left(\frac{\mathbf{u}^2}{2} + \varepsilon + \frac{p}{\rho} \right) \right] \right\}.$$
(3.3)

The system is closed by the equations of state for a perfect polytropic gas

$$p = \rho RT, \quad \varepsilon = c_v T, \tag{3.4}$$

where R is the gas constant, and c_v is the specific heat at a constant volume.

When deriving (3.1)–(3.3), the authors used the well-known phenomenological model of free-molecular gas flow followed by instant maxwellization, which was employed in several studies to construct numerical methods in fluid dynamics [1–7].

The QGD equations can be derived as moment equations by averaging the products of the summation invariants 1, v, and $v^2/2$ with a model kinetic equation of the form [29]

$$\frac{\partial f}{\partial t} + (\mathbf{v} \cdot \nabla) f^{(0)} = (\mathbf{v} \cdot \nabla) \tau (\mathbf{v} \cdot \nabla) f^{(0)} + \frac{f^{(0)} - f}{\tau}, \qquad (3.5)$$

where $f = f(\mathbf{x}, \mathbf{v}, t)$ is a one-particle distribution function, and $f^{(0)}$ is a locally equilibrium Maxwellian function with macroscopic parameters determined by the function f. The parameter τ on the right-hand side of (3.5) is interpreted as the characteristic time of molecular relaxation to the locally equilibrium distribution and is close in the order of magnitude to the mean free path of molecules in a gas. The macroscopic parameters in the formula for τ are also quadratures of f.

It was shown in [9] that, when the external force **F** is negligible, Eqs. (3.1)–(3.3) for a polytropic perfect monatomic ($\gamma = 5/3$) gas can be derived from integral conservation laws (2.3)–(2.7) and represented in the form (2.10)–(2.12) with the following expressions for **j**_m, *P*, **A**, **q**, and *X*:

$$\mathbf{j}_m = \boldsymbol{\rho}(\mathbf{u} - \mathbf{w}), \tag{3.6}$$

$$P = \Pi - pI + \tau \mathbf{u} \otimes [\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p] + \tau I[(\mathbf{u} \cdot \nabla)p + \gamma p \operatorname{div} \mathbf{u}], \qquad (3.7)$$

$$\mathbf{A} = (\mathbf{\Pi} \cdot \mathbf{u}) - p(\mathbf{u} - \mathbf{w}) + \tau \mathbf{u} \Big[\rho(\mathbf{u} \cdot \nabla) \Big(\frac{\mathbf{u}^2}{2} \Big) + (\mathbf{u} \cdot \nabla) p \Big] + \tau \mathbf{u} [(\mathbf{u} \cdot \nabla) p + \gamma p \operatorname{div} \mathbf{u}],$$
(3.8)

$$\mathbf{q} = -\kappa \nabla T - \tau \rho T \mathbf{u} (\mathbf{u} \cdot \nabla) s, \qquad (3.9)$$

$$X = \kappa \left(\frac{\nabla T}{T}\right)^2 + \frac{(\Pi : \Pi)}{(2\eta T)} + \frac{p\tau}{\rho^2 T} [\operatorname{div}(\rho \mathbf{u})]^2 + \frac{\tau}{\rho T} [\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p]^2 + \frac{\tau}{\rho \varepsilon T} [\rho(\mathbf{u} \cdot \nabla)\varepsilon + p \operatorname{div}\mathbf{u}]^2, \quad (3.10)$$

where

$$\mathbf{w} = \frac{\tau}{\rho} [\operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p], \qquad (3.11)$$

and the absolute viscosity η and heat conductivity κ are calculated as $\eta = p\tau$ and $\kappa = c_p p\tau$, respectively. Note that these are the values of η and κ obtained when the Navier–Stokes system is derived from the well-known Bhatnager–Gross–Krook kinetic equation [26].

System (3.1)–(3.3) can be formally generalized to describe a polyatomic gas and also to the case of an arbitrary Prandtl number. To do this, one must use the true value of γ in expressions (3.6)–(3.11) and define the coefficients η and κ as $\eta = p\tau$ and $\kappa = c_p p\tau/Pr$, respectively. In (2.20), the terms corresponding to the bulk viscosity must also be taken into account.

By using (3.6)–(3.11), it can be shown that the momentum conservation law follows from the momentum balance equation. The entropy balance equation can also be derived from system (3.1)–(3.3) (see [9]). Note that this derivation fundamentally relies on the assumption that the gas is perfect and polytropic.

The time-independent quasi-gasdynamic equations differ from the corresponding Navier–Stokes equations by additional divergence terms that formally are $O(\tau^2)$ as $\tau \longrightarrow 0$ or, in a dimensionless form, $O(Kn^2)$ as $Kn \longrightarrow 0$ (see [10]). For this QGD system, the classical Prandtl system of equations serves as a laminar boundary-layer approximation. For Eqs. (3.1)–(3.3), the properties of stationary shock-wave solutions were analyzed in [11]. In the limit case of $\kappa = 0$ and $\eta \neq 0$, it was proved that entropy strictly increases across a shock wave with a positive derivative.

4. QHD MODEL OF VISCOUS INCOMPRESSIBLE FLOWS

In models of convective fluid flows in uniform gravitational fields, the simplified form of the Navier– Stokes system proposed by Boussinesq is widely used [28, 30]. The corresponding approximation of the QHD equations was derived in [9] in the form

$$\operatorname{div} \mathbf{u} = \operatorname{div} \mathbf{w}, \tag{4.1}$$

$$\partial \mathbf{u}/\partial t + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) + \frac{1}{\rho} \nabla p = \frac{1}{\rho} \operatorname{div} \Pi + \operatorname{div}[(\mathbf{w} \otimes \mathbf{u}) + (\mathbf{u} \otimes \mathbf{w})] - \beta \mathbf{g} T, \qquad (4.2)$$

$$\partial T/\partial t + \operatorname{div}(\mathbf{u}T) = \operatorname{div}(\mathbf{w}T) + \chi \operatorname{div}(\nabla T).$$
(4.3)

Here, the vector \mathbf{w} is defined by the expression

$$\mathbf{w} = \tau \left[(\mathbf{u} \cdot \nabla) \mathbf{u} + \frac{1}{\rho} \nabla p + \beta \mathbf{g} T \right].$$

The following standard notation is used in (4.1)–(4.3): $\rho = \text{const} > 0$ is the average density, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the fluid velocity, $p = p(\mathbf{x}, t)$ is the hydrodynamic pressure, and $T = T(\mathbf{x}, t)$ is the temperature deviation from its mean value $T_0 = \text{const} > 0$. The quantity $\rho \mathbf{u}$ is interpreted as the spatiotemporal mean momentum per unit volume of a fluid. Here, vector \mathbf{g} is the acceleration of gravity, $\Pi = \eta[(\nabla \otimes \mathbf{u}) + (\nabla \otimes \mathbf{u})^T]$ is the Navier–Stokes viscous stress tensor in the case of an incompressible fluid. In Eqs. (4.1)–(4.3), the thermal expansion coefficient β , thermal diffusivity χ , absolute viscosity coefficient η , and parameter τ are positive constants. A term containing the dissipation function is omitted in (4.3).

As $\tau \rightarrow 0$, system (4.1)–(4.3) becomes the classical Boussinesq system used in models of thermal convection. Exact solutions to Eqs. (4.1)–(4.3) that describe convection in plane vertical and plane horizontal layers were obtained in [9, 12].

In [13], a variant of system (4.1)–(4.3) describing an isothermal viscous flow was originally postulated, and the corresponding balance equation for kinetic energy was derived in the form

$$\frac{\partial}{\partial t} \left(\rho \frac{\mathbf{u}^2}{2} \right) + \operatorname{div} \left[(\mathbf{u} - \mathbf{w}) \left(\rho \frac{\mathbf{u}^2}{2} + p \right) - (\Pi_Q \cdot \mathbf{u}) \right] = -\Phi.$$
(4.4)

The nonnegative dissipation function Φ is calculated as

$$\Phi = \frac{(\Pi:\Pi)}{2\eta} + \frac{\rho \mathbf{w}^2}{\tau}.$$

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Integrating (4.4) over a bounded domain V_0 and using the boundary conditions

$$\mathbf{u}|_{\Sigma_0} = 0, \quad (\mathbf{w} \cdot \mathbf{n})|_{\Sigma_0} = 0,$$

one finds that the total kinetic energy $E = \int_{V_0} (\rho \mathbf{u}^2/2) d\mathbf{x}$ decreases with time elapsed. The analogous theorem on kinetic energy dissipation is true for the Navier-Stokes system [28].

Exact solutions to this system describing the well-known laminar pipe and plane channel Poiseuille flows and the Couette flows between two planes and two coaxial cylinders rotating at constant angular velocities were constructed in [13].

It was shown in [12, 31] that quasi-magnetohydrodynamic (QMHD) models can be constructed for flows of viscous electrically conducting media (both compressible and incompressible) by combining the quasihydrodynamic equations with the Maxwell equations. Exact solutions to the QMHD systems were obtained for analogues of the Hartmann and Gershuni–Zhukhovitskii problems.

5. MODELS OF VISCOUS COMPRESSIBLE GAS FLOWS BASED ON THE QUASI-GASDYNAMIC EQUATIONS

Numerical analysis of supersonic gas flows based on the Navier-Stokes system presents certain difficulties. One of them is associated with the construction of special grid regularizers ensuring that a finite-difference solution is adequate, and computations are stable. For quasi-gasdynamic equations, this problem can be solved in a simple and efficient way. The regularizers are constructed on the basis of the additional divergence terms and allow the use of the second-order accurate approximations of all derivatives in spatial variables.

For plane or axially symmetric flows, the quasi-gasdynamic system (3.1)–(3.3) is

$$\begin{aligned} \frac{\partial \rho}{\partial t} &+ \frac{1}{r^{k} \partial r} (r^{k} \rho u_{k}) + \frac{\partial}{\partial z} (\rho u_{z}) = \frac{1}{r^{k} \partial r} \Big[\tau \frac{\partial}{\partial r} (r^{k} \rho u_{r}^{2}) \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial}{\partial z} (\rho u_{z}^{2}) \Big] \\ &+ \frac{1}{r^{k} \partial r} \Big(r^{k} \tau \frac{\partial \rho}{\partial r} \Big) + \frac{\partial}{\partial z} \Big(\tau \frac{\partial \rho}{\partial z} \Big) + \frac{1}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial}{\partial z} (\rho u_{r} u_{z}) \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r} u_{z}) \Big], \end{aligned}$$

$$\begin{aligned} & \frac{\partial (\rho u_{r})}{\partial t} + \frac{1}{r^{k} \partial r} (r^{k} \rho u_{r}^{2}) + \frac{\partial}{\partial z} (\rho u_{r} u_{z}) + \frac{\partial \rho}{\partial r} = \frac{1}{r^{k} \partial r} \Big[\tau \frac{\partial}{\partial r} (r^{k} \rho u_{r}^{3}) \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial}{\partial z} (\rho u_{r} u_{z}) \Big] \\ &+ 2 \frac{1}{r^{k} \partial r} \Big(r^{k} \tau \frac{\partial \rho u_{r}}{\partial r} \Big) - 2k \tau \frac{\rho u_{r}}{r^{2}} + \frac{\partial}{\partial r} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}) \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial \rho u_{r}}{\partial z} \Big] + \frac{1}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial}{\partial z} (\rho u_{r}^{2} u_{z}) \Big] \\ &+ \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2} u_{z}) \Big] + \frac{\partial}{\partial r} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2}) \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial \rho u_{r}}{\partial z} \Big] + \frac{1}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial \rho u_{r}}{\partial z} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2} u_{z}) \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial \rho u_{z}}{\partial r} \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial \rho u_{z}}{\partial z} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2} u_{z}) \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial \rho u_{z}}{\partial r} \Big] + \frac{\partial}{\partial z} \Big[\tau \frac{\partial \rho u_{z}}{\partial r} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\tau^{k} \frac{\partial \rho u_{z}}{\partial r} \Big] + \frac{\partial}{\partial z} \Big[\rho u_{z}^{2} \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2} u_{z}) \Big] + \frac{\partial}{\partial z} \Big[\tau^{k} \frac{\partial \rho u_{z}}{\partial r} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\tau^{k} \frac{\partial \rho u_{z}}{\partial r} \Big] + \frac{\partial}{\partial z} \Big[\rho u_{z}^{2} \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2} u_{z}) \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial \rho u_{z}}{\partial r} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\tau^{k} \frac{\partial \rho u_{z}}{\partial r} \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} (r^{k} \rho u_{r}^{2} u_{z}) \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial \rho u_{z}}{\partial r} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial \rho u_{z}}{\partial r} \Big] \\ \\ &+ \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} \Big[r^{k} \tau \frac{\partial \rho u_{z}}{\partial r} \Big] + \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} \Big] \\ &+ \frac{\partial}{\partial z} \Big[\frac{\tau}{r^{k} \partial r} \Big] \\ \\ &+$$

$$+\frac{1}{r^{k}\partial r}\left[r^{k}\tau\frac{\partial}{\partial r}\left(p\frac{u_{r}^{2}}{2}\right)\right] + \frac{\partial}{\partial z}\left[\tau\frac{\partial}{\partial z}\left(p\frac{u_{z}^{2}}{2}\right)\right] + \frac{1}{r^{k}\partial r}\left[r^{k}\tau\frac{\partial}{\partial r}\left(p\frac{u_{z}^{2}}{2}\right)\right] + \frac{\partial}{\partial z}\left[\tau\frac{\partial}{\partial z}\left(p\frac{u_{r}^{2}}{2}\right)\right] + \frac{\gamma}{\gamma-1}\frac{1}{r^{k}\partial r}\left(r^{k}\frac{p\tau\partial p}{\rho}\right) + \frac{\gamma}{r^{-1}}\frac{1}{r^{k}\partial r}\left[r^{k}p\tau\frac{\partial}{\partial r}\left(p\frac{p}{\rho}\right)\right] + \frac{\gamma}{\gamma-1}\frac{1}{\partial z}\left[p\tau\frac{\partial}{\partial z}\left(p\frac{p}{\rho}\right)\right]$$
(5.4)

+

$$+\frac{1}{r^{k}}\frac{\partial}{\partial r}\left[\tau r^{k}\frac{\partial}{\partial z}(u_{r}u_{z}(E+2p))\right]+\frac{\partial}{\partial z}\left[\frac{\tau}{r^{k}}\frac{\partial}{\partial r}(r^{k}u_{r}u_{z}(E+2p))\right].$$

The parameter k is zero in the plane case and unity in the axially symmetric case. The system is closed by the equations

$$E = \rho \frac{u_r^2 + u_z^2}{2} + \frac{p}{\gamma - 1}, \quad p = \rho RT, \quad \tau = \frac{\eta}{p}.$$
 (5.5)

In the formula for τ , the Schmidt number Sc is set equal to unity. System (5.1)–(5.5) should be supplemented by initial and boundary conditions.

For the normal and tangential velocity components u_n and u_t on a solid surface Σ , impermeability and slip conditions were set:

$$u_n|_{\Sigma} = 0, \quad u_t|_{\Sigma} = \left(\frac{\sqrt{\pi\eta}}{\rho\sqrt{2RT}}\frac{\partial u_t}{\partial \mathbf{n}}\right)|_{\Sigma}.$$

The temperature jump condition

$$T|_{\Sigma} - T_{w} = \frac{\sqrt{\pi}}{2R} \left(\frac{1}{\sqrt{2RT}} \frac{\kappa}{\rho} \frac{\partial T}{\partial \mathbf{n}} \right) \Big|_{\Sigma}$$

was also set, where T_w is the surface temperature. In the case of a plane surface, an additional boundary condition for pressure had the form

$$\partial p/\partial \mathbf{n}|_{\Sigma} = 0$$

and ensured zero mass flux across the boundary. The viscosity η was calculated as

$$\eta = \eta_1 (T/T_1)^{\omega}, \tag{5.6}$$

where η_1 is a tabular value of this coefficient at a temperature T_1 , and $\omega = 0.5$. The relation of η to the mean free path of molecules λ was determined by the expression

$$\eta = \lambda \rho \sqrt{2\pi RT} \frac{15}{2(7 - 2\omega)(5 - 2\omega)}.$$
(5.7)

We used an explicit finite-difference method to solve the above system of equations. Spatial derivatives were approximated by central differences, and the derivatives in time were approximated by first-order upwind differences. All quantities were computed at the grid points. To improve numerical stability at high flow velocities, the parameter τ was replaced by $\tau + \alpha h/c_s$ in some terms without mixed derivatives in spatial variables, where *h* is the mesh size, and $0 < \alpha < 1$. In all computations, the convergence and accuracy of the results were analyzed by reducing the mesh size.

In [15], system (5.1)–(5.5) was solved to compute a plane flow over a semi-infinite thin plate parallel to the incoming supersonic stream. The Mach number M was varied from 1.5 to 20. We analyzed the case of a monatomic gas of rigid spheres with Pr = 2/3 and $\gamma = 5/3$.

In [32], simulation results were presented for supersonic gas flows around a thin disk set perpendicularly to the incoming supersonic stream. Comparisons with numerical results obtained by solving the Navier–Stokes equations and also with the results of direct numerical simulations by the Monte Carlo (DSMC) method performed in the framework of the kinetic model have demonstrated certain advantages of the QGD equations.

Let us discuss in more detail the numerical results obtained for the structure of a stationary shock wave in a monatomic polytropic gas on the basis of the quasi-gasdynamic equations. It is well known that, when the free-stream Mach number M lies in the interval (1, 2), the profiles of flow variables computed with the use of the Navier–Stokes model are in good agreement with experimental observations. However, there is a noticeable discrepancy when $M \ge 2$ [26]. In the framework of the costly kinetic approach, the shock-wave structure is adequately described in a broad range of Mach numbers.

The properties of the shock-wave solutions of quasi-gasdynamic equations were theoretically examined in [11]. In [14, 32], an explicit, conditionally stable algorithm was employed to compute these solutions, with all spatial derivatives in the one-dimensional Eqs. (5.1)–(5.5) approximated to the second order of









accuracy without additional regularizers. The Mach number M was set equal to 2, 5, and 10. In formulas (5.6) and (5.7), the parameter ω was 0.5 for a gas of rigid spheres and 1 for a gas of Maxwellian molecules.

When M = 2, the QGD models, the Navier–Stokes models, and the DSMC yielded close results consistent with experimental data. In Fig. 1, the profiles of density ρ , velocity **u**, and temperature *T* computed by using the QGD system (dot-and-dash curves) at M = 5 and ω = 0.5 are compared with analogous profiles obtained on the basis of the Navier–Stokes equations (dashed curves) and by the DSMC method (solid curves). One can conclude that, for the QGD model, the function u(x) in the whole computational domain and the function $\rho(x)$ for x > 0 are in a better agreement with the DSMC data than analogous dependences found by solving the Navier–Stokes system.

In Fig. 2, the distributions of a dimensionless heat flux across a shock wave computed for M = 5, $\omega = 0.5$, and 1 are presented. Here, $\rho_1 c_{s1}^2$ is used as a measurement unit, where ρ_1 and c_{s1} are the density and sonic velocities ahead of the shock wave. For the QGD and Navier–Stokes systems, the heat flux was calculated by using formulas (3.9) and (2.18), respectively. In the kinetic model, we used the expression

$$\mathbf{q} = 0.5 \rho \langle \mathbf{c}^2 \mathbf{c} \rangle$$

where $\mathbf{c} = \mathbf{v} - \mathbf{u}$ is the molecular thermal velocity, and $\langle \rangle$ means averaging over an ensemble of particles. It is clear that the values of this quantity computed by applying the QGD and DSMC approaches are very similar, whereas the Navier–Stokes model yields a result that is not quite satisfactory. Note that the last term in



(3.9) is an $O(Kn^2)$ quantity and substantially affects the heat flux, since the Knudsen number is not small in this problem.

Figure 3 shows the inverse wave thickness λ_1/δ as depending on the Mach number M for $\omega = 0.5$ and $\omega = 1$. Here, λ_1 is the mean free path of molecules in the incoming supersonic stream; $\delta = (\rho_2 - \rho_1)/\max(d\rho/dx)$; and ρ_1 and ρ_2 are the gas densities ahead of and behind shock wave, respectively. For $\omega = 1$, similar results were obtained by using both macroscopic models (curves 1, 2) in the range of the Mach number indicated above, whereas the QGD system was found to have a certain advantage when $\omega = 0.5$ (curves 2). All these advantages of the QGD system are more clearly visible at higher Mach numbers. Curves 3 were obtained by the DSMC method.

The problem of shock-wave structure was also solved by computing QHD system (2.27)–(2.29). It was found that the results of computations based on the quasi-gasdynamic system are more accurate than those obtained by using the QHD model.

6. NUMERICAL SIMULATION OF CONVECTIVE FLOWS

Convective flows in closed volumes have been widely investigated on the basis of Navier–Stokes equations written in the Oberbeck–Boussinesq approximation [30, 33, 34]. Various types of artificial grid regularizers or special finite-difference approximations have been used to obtain stable computational procedures.

Consider the problem of thermal convection of a fluid in a rectangular enclosure of height *H* and length L = AH. The relative temperatures T_1 and T_2 of the left (hot) and right (cold) walls are kept constant, $\Delta T = T_1 - T_2 > 0$. One can assume, without loss of generality, that $T_2 = 0$. Let *u* and *v* be the horizontal and vertical components of the velocity vector **u** in a Cartesian coordinate system (*x*, *y*). Measuring *x*, *y*, *t*, *u*, *v*, *p*, *T*, and $\tau \text{ in } H, H, H^2/v, \nu/H, \nu/H, \rho(\nu/H)^2, \Delta T/A$, and H^2/v , respectively, we represent system (4.1)–(4.3) written for plane unsteady flows in the dimensionless form:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = \frac{\partial}{\partial x} \left[\tau \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[\tau \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - \operatorname{Gr} T \right) \right], \tag{6.1}$$

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(u^2) + \frac{\partial}{\partial y}(uv) + \frac{\partial p}{\partial x} = 2\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial y \partial x}$$

$$+ 2\frac{\partial}{\partial x} \left[\tau u \left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x}\right)\right] + \frac{\partial}{\partial y} \left[\tau v \left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x}\right)\right] + \frac{\partial}{\partial y} \left[\tau u \left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - \operatorname{Gr} T\right)\right],$$
(6.2)

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$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial y}(v^{2}) + \frac{\partial}{\partial x}(uv) + \frac{\partial p}{\partial y} = 2\frac{\partial^{2} v}{\partial y^{2}} + \frac{\partial^{2} v}{\partial x^{2}} + \frac{\partial^{2} u}{\partial x \partial y} + 2\frac{\partial}{\partial y} \Big[\tau v \Big(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - \operatorname{Gr} T \Big) \Big] + \frac{\partial}{\partial x} \Big[\tau u \Big(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - \operatorname{Gr} T \Big) \Big] + \frac{\partial}{\partial x} \Big[\tau v \Big(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} \Big) \Big] + \operatorname{Gr} T,$$

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x} (uT) + \frac{\partial}{\partial y} (vT) = \frac{1}{\Pr} \Big(\frac{\partial^{2} T}{\partial x^{2}} + \frac{\partial^{2} T}{\partial y^{2}} \Big)$$

$$+ \frac{\partial}{\partial x} \Big[\tau T \Big(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} \Big) \Big] + \frac{\partial}{\partial y} \Big[\tau T \Big(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - \operatorname{Gr} T \Big) \Big].$$

$$(6.4)$$

Here, the Grashof number Gr and Prandtl number Pr are calculated as

$$\operatorname{Gr} = \frac{\beta g \Delta T H^4}{v^2 L}, \quad \operatorname{Pr} = \frac{v}{\chi}.$$

Let $G = \{(x, y) : 0 < x < A, 0 < y < 1\}$ be the flow domain. If the fluid does not slip past domain boundaries and the upper and lower walls are not heat-conducting, then system (6.1)–(6.4) must be supplemented by the following boundary conditions on the left, right, lower, and upper walls, respectively:

$$u = 0, \quad v = 0, \quad \partial p / \partial x = 0, \quad T = A, \tag{6.5}$$

$$u = 0, \quad v = 0, \quad \partial p / \partial x = 0, \quad T = 0,$$
 (6.6)

$$u = 0, \quad v = 0, \quad \partial p/\partial y = \operatorname{Gr} T, \quad \partial T/\partial y = 0,$$
 (6.7)

$$u = 0, \quad v = 0, \quad \partial p / \partial y = \operatorname{Gr} T, \quad \partial T / \partial y = 0.$$
 (6.8)

Conditions (6.5)–(6.8) are conservative and ensure that the integral laws of mass and momentum conservation hold. The unperturbed velocity and temperature fields are used as initial conditions:

$$u|_{t=0} = v|_{t=0} = 0, \quad T|_{t=0} = 0, \quad (x, y) \in G.$$
 (6.9)

The ambiguity in pressure is eliminated by the normalization

$$p(A, 1) = 1. (6.10)$$

To solve the initial-boundary value problem (6.1)–(6.10), we used the conditionally stable, conservative, and uniform computational algorithm described in [16–18]. The computational domain *G* was discretized by introducing a uniform $N_x \times N_y$ grid. The equations of motion (6.2) and (6.3) and heat equation (6.4) were approximated to the second order of accuracy in spatial variables and to the first order in time. The boundary conditions were automatically approximated by introducing fictitious cells along the domain boundaries. On each time layer, the computed velocity and temperature fields were used to determine the pressure field by solving the Poisson equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = \frac{1}{\tau} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - \frac{\partial}{\partial x} \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) - \frac{\partial}{\partial y} \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} - \operatorname{Gr} T \right),$$

which is an equivalent representation of (6.1). We applied a modified conjugate gradient method characterized by a high convergence rate. The pressure at the upper right grid point was kept equal to unity. Then, velocity and temperature were calculated on the next time layer by means of an explicit scheme. All terms depending on τ were regarded as the artificial regularizers required to stabilize the algorithm.

First, let us discuss the well-known test problem of thermal convection in a square (A = 1) heated on its left side. The problem was solved with moderate Grashof numbers varied within 10^3-10^5 for various values of τ within $10^{-5}-10^{-2}$. The Prandtl number was set equal to unity. Uniform $N \times N$ grids were used with N = 21, 41, and 81.

The streamfunction ψ was derived from the solenoidal field **u** – **w**:

$$u - w_x = \partial \psi / \partial y, \quad v - w_y = -\partial \psi / \partial x.$$

Here, w_x and w_y are the horizontal and vertical components of **w**, respectively. When τ is small, the vectors **u** and **u** – **w** differ insignificantly.



Fig. 4.



Fig. 5.





To compute the dimensionless heat flux across the left boundary (the Nusselt number Nu = Nu(y)), we used the expression

$$\operatorname{Nu}(y) = -\frac{1}{\Pr} \frac{\partial T(0, y)}{\partial x}.$$

The average Nusselt number was calculated as

$$\mathrm{Nu}_0 = \int_0^1 \mathrm{Nu}(y) dy.$$

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τ	Grid	Ref.	ψ _{max}	<i>u</i> _{max}	ν_{max}	Nu ₀	Nu _{max}	Nu _{min}
10-4	21×21	present	5.044	15.938	19.513	2.306	3.939	0.579
		[34]	5.277	16.144	19.363	2.253	3.615	0.591
10-4	41×41	present	5.099	16.005	19.663	2.281	3.708	0.591
		[34]	5.125	16.262	19.602	2.249	3.563	0.586
10-4	81×81	present	5.113	16.070	19.663	2.275	3.649	0.581
		[34]	5.086	16.219	19.648	2.247	3.541	0.585
		[33]	5.071	16.178	19.617	2.238	3.528	0.586
10^{-3}	21×21	present	5.195	15.587	18.565	2.431	4.318	0.529
10^{-2}	21×21	present	6.723	13.182	11.542	3.850	9.268	0.352

Table 1

Table 2

τ	Grid	Ref.	$ \psi _{mid}$	ψ _{max}	<i>u</i> _{max}	ν_{max}	Nu ₀	Nu _{max}	Nu _{min}
10 ⁻⁵	21×21	present	9.264	9.666	32.33	67.70	4.865	9.777	0.204
		[34]	10.259	10.860	40.30	65.07	4.532	8.123	0.762
10^{-5}	41 × 41	present	9.502	9.909	33.24	70.91	4.682	8.733	0.729
		[34]	9.388	9.918	36.63	68.11	4.554	7.968	0.730
		[33]	9.111	9.612	34.73	68.59	4.509	7.717	0.729
10^{-4}	21×21	present	9.358	9.754	32.20	66.71	4.906	9.931	-0.033
10 ⁻³	21×21	present	10.400	10.740	33.12	57.86	5.732	12.091	-0.611

The following notation was also employed: $|\psi|_{mid}$, the absolute value of the streamfunction at the domain center; $|\psi|_{max}$, the maximum of the stream function's absolute value over the computational domain; u_{max} , the maximum horizontal velocity in the median vertical cross section; v_{max} , the maximum vertical velocity in the median horizontal cross section; Nu_{max}, the maximum value of the Nusselt number at the left boundary; and Nu_{min}, the minimum value of the Nusselt number at the left boundary.

Figure 4 shows equidistant lines of constant streamfunction (a), isotherms (b) and isobars (c) of the steady flow computed for $Gr = 10^4$, $\tau = 10^{-4}$, and N = 41, which correspond to $\psi_i = \psi_{max} - i(\psi_{max} - \psi_{min})/15$, $T_i = T_{max} - i(T_{max} - T_{min})/15$, and $p_i = p_{max} - i(p_{max} - p_{min})/15$. In this computation, $\psi_{min} = -5.099$, $\psi_{max} = 0$, $T_{min} = 0$, $T_{max} = 1$, $p_{min} = -5065.8$, and $p_{max} = 1660.7$. The pressure minimum is reached in the left lower corner of the domain; the maximum, in its left upper corner. A similar flow pattern was observed both in experiments [33] and in computations based on the Navier–Stokes model [34].

In Tables 1 and 2, the numerical results are compared with analogous results obtained by using the Navier–Stokes model written in terms of streamfunction, vorticity, and temperature [34] and with the experimental data reported in [33]. In the range of Gr indicated above, the calculated values of the flow parameters are in good agreement with one another. The numerical accuracy improves when finer grids are used. It also improves with decreasing τ , i.e., as the time step is reduced. The influence of τ on the flow structure is illustrated by Fig. 5 (streamlines) and Fig. 6 (isotherms).

Numerical test results obtained for the thermal convection of a fluid with low Pr in rectangular enclosures are presented in [18].

Thus, the computations of the QFD systems performed in this study can serve as a basis for simulating real flows in a broad range of parameters.

7. CONCLUSIONS

The present study was an analysis of two interrelated mathematical models, the QGD one and the QHD one. Both models differ from the Navier–Stokes equations by small divergence terms and can be interpreted

as systems describing the evolution of spatiotemporal averages of density, velocity, and temperature. Each model is associated with a particular closure of Eqs. (2.10)-(2.14), which follow from the integral conservation laws for a fixed material volume. In the time-independent form, both systems differ from Navier–Stokes equations by divergent terms that formally behave as asymptotically small $O(Kn^2)$ quantities as $Kn \rightarrow 0$. The influence of additional terms is insignificant for steady and quasi-steady gas flows characterized by small Kundsen numbers. However, their contribution is essential for unsteady flows and at Kn close to unity. The advantages of the new models should be sought in this class of problems.

The derivation of these two systems presented in [35] is based on a finite-difference analysis and differs from the derivation in Section 2. In [35], the applicability conditions were also discussed for the new models. It was concluded that the QGD equations should be used in simulations of flows of perfect polytropic gas, whereas QHD models can describe the motions of real gases and fluids. The scope of these models is one of the most difficult questions. To provide an answer to this question, further long-term theoretical, numerical, and experimental studies are required.

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REFERENCES

- 1. Volchinskaya, M.I., Pavlov, A.N., and Chetverushkin, B.N., An Integration Scheme for Gasdynamics Equations, *Preprint of Inst. Appl. Math., Acad. Sci. USSR*, Moscow, 1983, no. 113.
- 2. Elizarova, T.G., Pavlov, A.N., and Chetverushkin, B.N., Application of a Kinetic Model in the Derivation of Gasdynamics Equations, *Preprint of Inst. Appl. Math., Acad. Sci. USSR*, Moscow, 1983, no. 144.
- Elizarova, T.G. and Chetverushkin, B.N., Application of Kinetic Models in Flow Computations in Gas Dynamics, *Matematicheskoe modelirovanie: Protsessy v nelineinykh sredakh* (Mathematical Modeling: Processes in Nonlin-ear Media), Samarskii, A.A., Kurdyumov, S.P., and Galaktionov, V.A., Eds., Moscow: Nauka, 1986, pp. 261–278.
- 4. Elizarova, T.G., Pavlov, A.N., and Chetverushkin, B.N., Application of a Quasi-Gasdynamic System of Equations in Computing a Flow around a Body with a Spike, *Dokl. Akad. Nauk SSSR*, 1987, vol. 292, no. 2, pp. 327–331.
- Reitz, R.D., One-Dimensional Compressible Gas Dynamic Calculations Using the Boltzmann Equation, J. Comput. Phys., 1981, vol. 42, no. 1, pp. 108–123.
- 6. Aristov, V.V. and Cheremisin, F.G., Solution of the Euler and Navier–Stokes Equations Based on Operator Splitting in the Boltzmann Kinetic Equation, *Dokl. Akad. Nauk SSSR*, 1983, vol. 272, no. 3, pp. 555–559.
- Deshpande, S.M. and Mandal, J.C., Kinetic Theory Based New Upwind Methods for Inviscid Compressible Flow, *Theor. Appl. Mech.* (Sofia), 1988, vol. 19, no. 3, pp. 32–38.
- Sheretov, Yu.V., A New Mathematical Model in Fluid Dynamics, *Primenenie funktsional'nogo analiza v teorii priblizhenii* (Application of Functional Analysis in Approximation Theory), Tver: Tver. Gos. Univ., 1996, pp. 124– 134.
- 9. Sheretov, Yu.V., Quasi-Hydrodynamic Equations as a Model of Compressible Viscous Heat-Conducting Flows, *Primenenie funktsional'nogo analiza v teorii priblizhenii* (Application of Functional Analysis in Approximation Theory), Tver: Tver. Gos. Univ., 1997, pp. 127–155.
- Elizarova, T.G. and Sheretov, Yu.V., Invariant Form and Asymptotic Properties of a Generalized Quasi-Gasdynamic System, *Zh. Vychisl. Mat. Mat. Fiz.*, 1991, vol. 31, no. 7, pp. 1042–1050.
- 11. Elizarova, T.G. and Sheretov, Yu.V., Properties of Shock-Type Solutions to Quasi-Gasdynamic Equations, *Preprint of Inst. Appl. Math., Acad. Sci. USSR*, Moscow, 1990, no. 156.
- 12. Sheretov, Yu.V., On the Exact Solutions of Quasi-Hydrodynamic Equations, *Primenenie funktsional'nogo analiza v teorii priblizhenii* (Application of Functional Analysis in Approximation Theory), Tver: Tver. Gos. Univ., 1998, pp. 213–241.
- 13. Sheretov, Yu.V., On the Uniqueness of Solutions to a Dissipative System of Equations of Quasi-Hydrodynamic Type, *Mat. Modelirovanie*, 1994, vol. 6, no. 10, pp. 35–45.
- 14. Graur, I.A., Elizarova, T.G., and Sheretov, Yu.V., Computation of the Structure of a Stationary Shock Wave Based on Quasi-Gasdynamic Equations, *Preprint of National Center for Mathematical Modeling, Russ. Acad. Sci.*, Moscow, 1992, no. 42.
- Elizarova, T.G., Graur, I.A., Lengrand, J.C., and Chpoun, A., Rarefied Gas Flow Simulation Based on Quasi-Gasdynamic Equations, AIAA J., 1995, vol. 33, no. 12, pp. 2316–2324.
- Gurov, D.B., Elizarova, T.G., and Sheretov, Yu.V., Numerical Simulation of Fluid Flow in a Cavity Based on the Quasi-Hydrodynamic System of Equations, *Mat. Modelirovanie*, 1996, vol. 8, no. 7, pp. 33–44.

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- Elizarova, T.G., Kalachinskaya, I.S., Klyuchnikova, A.V., and Sheretov, Yu.V., Application of the Quasi-Hydrodynamic System of Equations in Simulations of Heat-Conducting Flows, *Trudy IV Mezhdunarodnoi konferentsii "Matematika, komp'yuter, obrazovanie"* (Proc. IV Int. Conf. "Mathematics, Computer, Education"), Moscow, 1997, pp. 108–115.
- Elizarova, T.G., Kalachinskaya, I.S., Klyuchnikova, A.V., and Sheretov, Yu.V., Application of Quasi-Hydrodynamic Equations in the Modeling of Low-Prandtl Thermal Convection, *Zh. Vychisl. Mat. Mat. Fiz.*, 1998, vol. 38, no. 10, pp. 1732–1742.
- 19. Chetverushkin, B.N., *Kineticheski-soglasovannye skhemy v gazovoi dinamike* (Kinetically Consistent Schemes in Gas Dynamics), Moscow: Mosk. Gos. Univ., 1999.
- Slezkin, N.A., On Differential Equations of Gas Motion, *Dokl. Akad. Nauk SSSR*, 1951, vol. 77, no. 2, pp. 205–208.
- 21. Vallander, S.V., Equations of Motion for a Viscous Gas, Dokl. Akad. Nauk SSSR, 1951, vol. 58, no. 1, pp. 25–27.
- 22. Klimontovich, Yu.L., *Statisticheskaya teoriya otkrytykh sistem* (Statistical Theory of Open Systems), Moscow: YaNUS, 1995.
- 23. Alekseev, B.V., Generalized Boltzmann Physical Kinetics, Teplofiz. Vys. Temp., 1997, vol. 35, no. 1, pp. 129-146.
- 24. Sedov, L.I., Mekhanika sploshnoi sredy (Continuum Mechanics), Moscow: Nauka, 1976.
- 25. Loitsyanskii, L.G., Mekhanika zhidkosti i gaza (Fluid Mechanics), Moscow: Nauka, 1987.
- 26. Bird, G.A., *Molecular Gas Dynamics*, Oxford: Clarendon, 1976. Translated under the title *Molekulyarnaya* gazovaya dinamika, Moscow: Mir, 1981.
- 27. Lifshitz, E.M. and Pitaevskii, L.P., Fizicheskaya kinetika (Physical Kinetics), Moscow: Nauka, 1979.
- 28. Landau, L.D. and Lifshitz, E.M., Gidrodinamika (Fluid Mechanics), Moscow: Nauka, 1986.
- 29. Elizarova, T.G. and Sheretov, Yu.V., Invariant Form of the System of Quasi-Gasdynamic Equations and Its Relation to the Navier–Stokes Equations, *Preprint of Inst. Appl. Math., Acad. Sci. USSR*, Moscow, 1987, no. 230.
- 30. Gershuni, G.Z. and Zhukhovitskii, E.M., Konvektivnaya ustoichivost' neszhimaemoi zhidkosti (Convective Stability of Incompressible Fluids), Moscow: Nauka, 1972.
- Sheretov, Yu.V., Quasi-Hydrodynamic Model of Conducting Viscous Flow in Electromagnetic Field, *Primenenie funktsional'nogo analiza v teorii priblizhenii* (Application of Functional Analysis in Approximation Theory), Tver: Tver. Gos. Univ., 1997, pp. 155–169.
- 32. Elizarova, T.G., Graur, I.A., Chpoun, A., and Lengrand, J.C., Comparison of Continuum and Molecular Approaches for the Flow around a Perpendicular Disk, *Proc. of the 20th Int. Symp. on Shock Waves*, Sturtevand, B., *et al.*, Singapore: World Sci., 1997, pp. 795–800.
- 33. De Vahl Davis, G. and Jones, I.P., Natural Convection in a Square Cavity—a Comparison Exercise, *Int. J. Numer. Methods Fluids*, 1983, no. 3, pp. 227–248.
- 34. Vabishchevich, P.N., Makarov, M.M., Chudanov, V.V., and Churbanov, A.G., Numerical Simulation of Convective Flows in Terms of Streamfunction–Vorticity–Temperature Variables, *Preprint of Inst. Math. Modeling, Russ. Acad. Sci.*, Moscow, 1993, no. 28.
- 35. Sheretov, Yu.V., Finite-Difference Schemes For Fluid Dynamics in Eulerian and Lagrangian Coordinates Based on Quasi-Gasdynamic and Quasi-Hydrodynamic Equations, *Primenenie funktsional'nogo analiza v teorii priblizhenii* (Application of Functional Analysis in Approximation Theory), Tver: Tver. Gos. Univ., 1999, pp. 184–208.