

Model Kinetic Equations and the Description of Gas Flows at Various Relaxation Stages

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Abstract—Various relaxation stages in high-velocity and high-temperature gases with physicochemical processes are considered on the basis of model kinetic equations. Macroscopic equations are derived in the zero approximation of the modified Chapman–Enskog method and expressions for the flow members of gas-dynamic equations in terms of intensive and extensive parameters are deduced. A formula for the velocity of sound (as the velocity of propagation of small perturbations) is derived using the parameter α , which is not a constant under the considered conditions.

Keywords: model kinetic equations, various relaxation stages, extensive and intensive parameters.

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INTRODUCTION

The mathematical description of transport processes in high-velocity and high-temperature gases is generally conducted using kinetic equations that generalize the Boltzmann equations (see, e.g., [1–3]). The greatest difficulties in solving kinetic equations are associated with the presence of integral collision-operators in them. To simplify the solution of the problems, we can use model kinetic equations. Such equations for the kinetic description of a simple monoatomic gas are proposed in [4, 5]. In later works, the BGK (Bhatnagar–Gross–Krook) model is generalized for the case of gas mixtures and gases with internal degrees of freedom (see, e.g., [6, 7]).

It is known (see, e.g., [1–3]) that the collisions of molecules, accompanied by transitions of energy of internal degrees of freedom from one kind to another and by chemical reactions, have various frequencies. In many cases, two groups can be specified: in the first group are “fast” microscopic processes and the second group are “slow” ones (the speed of fast processes is much higher and the speed of slow processes is comparable to the characteristic rate of the change of macroparameters). In the case where all collisions belong to the first group, we have equilibrium distributions of molecules. If the first group includes only some collisions, we obtain nonequilibrium distributions over certain internal degrees of freedom, along with equilibrium distributions over other internal and translational degrees of the freedom of molecules. The gas relaxation stages are determined by a group of fast microscopic processes and corresponding statistical distributions. For the solution of kinetic equations at various relaxation stages, the modified Chapman–Enskog method (MCEM) [2] can be used.

In [8], the BGK model for approximation of part of the integral operator of kinetic equations was proposed; this part corresponds to fast microscopic processes. In this case, the model equations allow us to obtain closed systems of equations for the minimum number of extensive parameters or intensive ones associated with them in the study of equilibrium and nonequilibrium flow regimes of gas mixtures with physicochemical processes.

1. GENERALIZATION OF THE BGK MODEL

The statistical distribution has a formation time that is conditioned by collisions of a certain type: the relaxation time. In gas mixtures with internal degrees of freedom and chemical reactions, relaxation times satisfy a certain system of inequalities called the “hierarchy of relaxation times” [9].

Typically, these inequalities can be written as follows:

$$\tau_{TT} \leq \tau_{RT} \ll \dots \ll \tau_{VRT} \ll \dots \ll \tau_{eq}, \quad (1)$$

where the relaxation times τ_{TT} , τ_{RT} , and τ_{VRT} correspond to the establishment of equilibrium in the translational, rotational, and vibrational degrees of freedom of molecules; τ_{eq} is the time of the establishment of the complete thermodynamic and chemical equilibrium.

Suppose that θ is the characteristic time of changing macroscopic parameters and τ is the maximum relaxation time of fast microprocesses. We can introduce a small parameter $\varepsilon = \tau/\theta \ll 1$. Under this condition, the system of the kinetic equations can be written in the dimensionless form [2, 3, 10]

$$D_i f_i = \frac{1}{\varepsilon} J_i' + J_i'', \quad i = \overline{1, I}. \quad (2)$$

Here, the differential operator D_i characterizes the change of the distribution functions $f_i(\mathbf{r}, \mathbf{u}, t)$ when molecules move along phase trajectories; the integral operators J_i' and J_i'' describe their change due to collisions of molecules. Index i specifies the chemical grade of particles and a set of quantum numbers that characterize the internal-energy levels. It is assumed that the internal energy of a molecule is quantized and the translational energy is described quasi-classically. The J_i' operator corresponds to fast microscopic processes and the J_i'' operator describes slow microscopic processes; ε is an analog of the Knudsen number for collisions determined by the J_i' operator.

Many works (see, e.g., [1–3, 8, 10, 11]) have been devoted to the solution of Eq. (2) when $\varepsilon \rightarrow 0$. The present paper uses distribution functions in the following form [6]:

$$f_i^{(0)} = s_i \frac{m_i^3}{h^3} \exp \left(\gamma_0 \left(\frac{m_i c^2}{2} + \tilde{\varepsilon}_i \right) + \sum_{\lambda=1}^{\Lambda} \gamma_\lambda \Psi_i^{(\lambda)} \right), \quad (3)$$

where h is the Planck constant; m_i , s_i , and \mathbf{c} is the mass, the statistical weight, and the velocity of the i th molecule ($\mathbf{c} = \mathbf{u} - \mathbf{v}$, \mathbf{u} is the velocity of microparticles in a fixed coordinate system, and $\mathbf{v}(\mathbf{r}, t)$ is the mean mass velocity of a gas); $\tilde{\varepsilon}_i$ is the part of the internal energy of a molecule (this part exchanges incoming energy in collisions described by the operator J_i'); $\Psi_i^{(\lambda)}$ ($\lambda = \overline{1, \Lambda}$) are the additive invariants of collisions of this operator; and γ_λ ($\lambda = \overline{0, \Lambda}$) are parameters that can depend only on coordinates and time.

Functions (3) coincide with the distribution functions in the zero approximation for the MCEM in the solution of Eqs. (2). The conditions of the normalization of these functions can be presented as follows:

$$\psi_0 = \tilde{\varepsilon} = \sum_i \int f_i^{(0)} \left(\frac{m_i c^2}{2} + \tilde{\varepsilon}_i \right) d\mathbf{c} = -\frac{3}{2} \frac{n^{(0)}}{\gamma_0} + \sum_i n_i^{(0)} \tilde{\varepsilon}_i, \quad (4)$$

$$\psi_\lambda = \sum_i \int f_i^{(0)} \Psi_i^{(\lambda)} d\mathbf{c} = \sum_i n_i^{(0)} \Psi_i^{(\lambda)}, \quad \lambda = \overline{1, \Lambda}. \quad (5)$$

Here, $\psi_0 = \tilde{\varepsilon}$ and ψ_λ are the densities of determining extensive parameters that correspond to the total values of the invariants of collisions $\psi_i^{(0)} = m_i c^2 / 2 + \tilde{\varepsilon}_i$ and $\psi_i^{(\lambda)}$ per unit volume,

$$n_i^{(0)} = \int f_i^{(0)} d\mathbf{c} = s_i \exp \left(\gamma_0 \tilde{\varepsilon}_i + \sum_{\lambda=1}^{\Lambda} \gamma_\lambda \Psi_i^{(\lambda)} \right) \left(\frac{-2\pi m_i}{\gamma_0 h^2} \right)^{3/2}, \quad n^{(0)} = \sum_i n_i^{(0)}. \quad (6)$$

We compare the right-hand side of relation (4) with the known results of thermodynamics and obtain the equality

$$\gamma_0 = -\frac{1}{kT} \quad (7)$$

(k is the Boltzmann constant and T is the gas temperature).

In order to avoid the difficulties associated with the complex form of integral collision-operators, we can use the following system of model kinetic equations [8]:

$$D_i f_i = \frac{f_i^{(0)} - f_i}{\tau} + J_i'', \quad i = \overline{1, I}. \quad (8)$$

System (8) has the same advantages and disadvantages as the BGK model and can be used for describing weak deviations from equilibrium and nonequilibrium quasi-stationary distribution functions (3).

One criterion for the adequacy of the proposed kinetic model is the validity of the Boltzmann H-theorem. For model Eqs. (8), this theorem is proved in [8]. In the present paper, it is proposed to use the system of kinetic equations (8) in order to study the transport processes at different relaxation stages of gases with physicochemical processes.

2. MACROSCOPIC EQUATIONS IN THE MCEM ZERO APPROXIMATION

We multiply each of Eqs. (8) by the collision invariants $m_i \mathbf{c}$ and $\psi_i^{(\lambda)}$ ($\lambda = \overline{0, \Lambda}$), integrate the result over space of the velocities \mathbf{c} , sum over i , and obtain the macroscopic equations for \mathbf{v} and ψ_λ (see (4) and (5)):

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\varrho} \nabla \cdot \mathbf{P}, \quad (9)$$

$$\frac{d\psi_0}{dt} = \frac{d\tilde{\epsilon}}{dt} = -\tilde{\epsilon} \nabla \cdot \mathbf{v} - \mathbf{P} : \nabla \mathbf{v} - \nabla \cdot \mathbf{q}_0 + r_0, \quad (10)$$

$$\frac{d\psi_\lambda}{dt} = -\psi_\lambda \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q}_\lambda + r_\lambda, \quad \lambda = \overline{1, \Lambda}. \quad (11)$$

Here, it is assumed for simplicity that external forces are absent; $d/dt = \partial/\partial t + \mathbf{v} \cdot \nabla$, and the pressure tensor is determined by the formula

$$\mathbf{P} = \sum_i \int f_i m_i \mathbf{c} \mathbf{c} d\mathbf{c}, \quad (12)$$

the energy transfer vector $m_i \mathbf{c}^2 / 2 + \tilde{\epsilon}_i$ has the form

$$\mathbf{q}_0 = \sum_i \int f_i \psi_i^{(0)} \mathbf{c} d\mathbf{c} = \sum_i \int f_i \left(\frac{m_i \mathbf{c}^2}{2} + \tilde{\epsilon}_i \right) \mathbf{c} d\mathbf{c}, \quad (13)$$

the transfer vector of any invariants $\psi_i^{(\lambda)}$ ($\lambda = \overline{1, \Lambda}$) is written as

$$\mathbf{q}_\lambda = \sum_i \int f_i \psi_i^{(\lambda)} \mathbf{c} d\mathbf{c}, \quad \lambda = \overline{1, \Lambda}, \quad (14)$$

and the relaxation terms are presented as follows:

$$r_0 = \sum_i \int \left(\frac{m_i \mathbf{c}^2}{2} + \tilde{\epsilon}_i \right) J_i'' d\mathbf{c}, \quad r_\lambda = \sum_i \int \psi_i^{(\lambda)} J_i'' d\mathbf{c}, \quad \lambda = \overline{1, \Lambda}. \quad (15)$$

Note that the continuity equation

$$\frac{d\varrho}{dt} + \varrho \nabla \cdot \mathbf{v} = 0 \quad (16)$$

is a consequence of Eqs. (11), because among them are equations associated with the conservation of certain indivisible particles.

The macroscopic parameters $\psi_0 = \tilde{\epsilon}$ and ψ_λ ($\lambda = \overline{1, \Lambda}$) represent the densities of main extensive parameters, the knowledge of which specifies the nature of the flow of a gas mixture under the considered conditions.

In the zero approximation, where $f_i = f_i^{(0)}$, we obtain

$$\mathbf{P}^{(0)} = p \mathbf{I}, \quad \mathbf{q}_\lambda^{(0)} = 0, \quad \lambda = \overline{0, \Lambda}, \quad (17)$$

$$p = -\frac{n^{(0)}}{\gamma_0} = n^{(0)} k T, \quad (18)$$

where p is pressure and \mathbf{I} is a unit tensor.

In this case, gas-dynamic Eqs. (9)–(11) can be presented as follows:

$$\frac{d_0 \mathbf{v}}{dt} = -\frac{1}{\varrho} \nabla p, \quad (19)$$

$$\frac{d_0 \Psi_0}{dt} = \frac{d_0 \tilde{\epsilon}}{dt} = -(\tilde{\epsilon} + p) \nabla \cdot \mathbf{v} + r_0^{(0)}, \quad (20)$$

$$\frac{d_0 \Psi_\lambda}{dt} = -\psi_\lambda \nabla \cdot \mathbf{v} + r_\lambda^{(0)}, \quad \lambda = \overline{1, \Lambda}. \quad (21)$$

These equations include the relaxation terms

$$r_\lambda^{(0)} = \sum_i \int \psi_i^{(\lambda)} J_i''(f^{(0)}) d\mathbf{c}, \quad \lambda = \overline{0, \Lambda}. \quad (22)$$

Note that $\psi_0 = \tilde{\epsilon}$ and ψ_λ ($\lambda = \overline{1, \Lambda}$) are related to the parameters γ_λ ($\lambda = \overline{0, \Lambda}$) included in distribution functions (3). Here, γ_λ ($\lambda = \overline{0, \Lambda}$) are intensive parameters conjugate to the densities of the extensive parameters Ψ_λ ($\lambda = \overline{0, \Lambda}$).

Taking into account relations (3)–(6), it is possible to present the left-hand sides of Eqs. (20) and (21) as follows:

$$\frac{d_0 \Psi_\lambda}{dt} = \sum_{\nu=0}^{\Lambda} \frac{\partial \Psi_\lambda}{\partial \gamma_\nu} \frac{d_0 \gamma_\nu}{dt}. \quad (23)$$

According to representation (23), we can consider Eqs. (20) and (21) as a system of linear algebraic equations for finding the unknowns $d_0 \gamma_\nu / dt$ ($\nu = \overline{0, \Lambda}$). The solution of this system can be presented as follows [11, 12]:

$$\frac{d_0 \gamma_\lambda}{dt} = -\chi_\lambda \nabla \cdot \mathbf{v} + \tilde{\chi}_\lambda, \quad \lambda = \overline{0, \Lambda}. \quad (24)$$

Here,

$$\chi_\lambda = \frac{\det_\lambda'^{(0)}}{\det}; \quad \tilde{\chi}_\lambda = \frac{\det_\lambda''^{(0)}}{\det}; \quad (25)$$

the determinant \det is the Jacobian of the transition from extensive to intensive parameters:

$$\det = \frac{D(\Psi_0, \Psi_1, \dots, \Psi_\Lambda)}{D(\gamma_0, \gamma_1, \dots, \gamma_\Lambda)} \quad (26)$$

(it is proved in [3] that $\det > 0$); $\det_\lambda'^{(0)}$ is obtained from (26) if the column of the γ_λ -derivatives is replaced by the column of coefficients for $\nabla \cdot \mathbf{v}$ in the right-hand sides of Eqs. (20) and (21); and $\det_\lambda''^{(0)}$ is obtained from (26) by replacing the same column with the column of relaxation terms (22).

Using relations (18) and (6), we can present Eq. (19) as follows [11]:

$$\frac{d_0 \mathbf{v}}{dt} = \frac{1}{\langle m \rangle} \frac{\langle \tilde{h} \rangle \nabla \gamma_0 + \sum_{\lambda=1}^{\Lambda} \langle \psi_\lambda \rangle \nabla \gamma_\lambda}{\gamma_0}, \quad (27)$$

where $\langle m \rangle = \varrho / n^{(0)}$, $\langle \tilde{h} \rangle = (\tilde{\epsilon} + p) / n^{(0)}$, and $\langle \psi_\lambda \rangle = \Psi_\lambda / n^{(0)}$ are average values of mass, enthalpy, and the invariants $\psi_i^{(\lambda)}$, which fall per one molecule.

According to (4)–(6) and (18), the expression in the right-hand side of Eq. (27) is determined by the parameters γ_λ ($\lambda = \overline{0, \Lambda}$) depending on the coordinates and time.

Equations (24) and (27) form a closed system for the velocity \mathbf{v} and the intensive parameters γ_λ ($\lambda = \overline{0, \Lambda}$) in the MCEM zero approximation. This system describes flows of a nonviscous and thermally non-conductive gas.

3. INTEGRALS OF MOTION AND THE VELOCITY OF PROPAGATION OF SMALL PERTURBATIONS

In fluid mechanics, the velocity of sound is associated with the velocity of propagation of small perturbations in a nonviscous and thermally nonconductive fluid.

If we neglect J_i'' operators in Eqs. (2) and (8) and the relaxation terms $r_\lambda^{(0)}$ and $\tilde{\chi}_\lambda$ ($\lambda = \overline{0, \Lambda}$) in the right-hand sides of Eqs. (20) and (21), then according to the traditional methods (see, e.g., [13]) we can obtain integrals of motion. These integrals can be presented as follows [14]:

$$\frac{\Psi_\lambda}{\rho} = \text{const}, \tag{28}$$

$$\gamma_0 \frac{\tilde{e} + p}{\rho} + \sum_{\lambda=1}^{\Lambda} \gamma_\lambda \frac{\Psi_\lambda}{\rho} = \text{const}, \tag{29}$$

$$\frac{\partial \varphi}{\partial t} + \frac{v^2}{2} + \frac{\tilde{e} + p}{\rho} = 0. \tag{30}$$

Zero on the right-hand side of Lagrangian integral (30) is associated with a particular choice of the velocity potential φ .

In the case of small perturbations, the terms $(\mathbf{v} \cdot \nabla)\gamma_\lambda$ and $\tilde{\chi}_\lambda$ in Eq. (24) and the terms $v^2/2$ in Eq. (30) can also be neglected. Instead of (24), we obtain the equation

$$\frac{\partial \gamma_\lambda}{\partial t} = -\chi_\lambda \nabla \cdot \mathbf{v}, \quad \lambda = \overline{0, \Lambda} \tag{31}$$

and instead of (30), we have

$$\frac{\partial \varphi}{\partial t} + \frac{\tilde{e} + p}{\rho} = 0. \tag{32}$$

Equation (32), which was obtained from (30), we differentiate in time and obtain the relation

$$\frac{\partial^2 \varphi}{\partial t^2} = -\frac{\partial}{\partial t} \left(\frac{\tilde{e} + p}{\rho} \right). \tag{33}$$

Using integrals (28) and (29), we can present (33) as follows:

$$\frac{\partial^2 \varphi}{\partial t^2} = \frac{1}{\gamma_0} \left(\frac{\tilde{e} + p}{\rho} \frac{\partial \gamma_0}{\partial t} + \sum_{\lambda=1}^{\Lambda} \frac{\Psi_\lambda}{\rho} \frac{\partial \gamma_\lambda}{\partial t} \right). \tag{34}$$

Using expressions (25) and Eqs. (31), we have

$$\frac{\partial^2 \varphi}{\partial t^2} = -\frac{1}{\gamma_0 \rho} \left((\tilde{e} + p)\chi_0 + \sum_{\lambda=1}^{\Lambda} \Psi_\lambda \chi_\lambda \right) \nabla \cdot \mathbf{v}. \tag{35}$$

Taking into account the relation $\nabla \cdot \mathbf{v} = \nabla \cdot (\nabla \varphi) = \Delta \varphi$, expressions (18) for pressure, and the notation introduced in (27), we obtain the wave equation

$$\frac{\partial^2 \varphi}{\partial t^2} = \frac{p}{\rho} \left(\langle \tilde{h} \rangle \chi_0 + \sum_{\lambda=1}^{\Lambda} \langle \Psi_\lambda \rangle \chi_\lambda \right) \nabla \varphi. \tag{36}$$

The coefficient of the Laplace operator $\Delta \varphi$ in wave equation (36) can be associated with the squared velocity of sound [15]:

$$a^2 = \left(\langle \tilde{h} \rangle \chi_0 + \sum_{\lambda=1}^{\Lambda} \langle \Psi_\lambda \rangle \chi_\lambda \right) \frac{p}{\rho}. \tag{37}$$

Relation (37) can be presented in the traditional form

$$a^2 = \varkappa \frac{p}{\rho}; \quad \varkappa = \langle \tilde{h} \rangle \chi_0 + \sum_{\lambda=1}^{\Lambda} \langle \Psi_\lambda \rangle \chi_\lambda \tag{38}$$

is not a constant. Formulas (38) allow determining the dependence of the velocity of sound on the temperature T (or γ_0) and other intensive parameters. These formulas are used in [16] to study the effects of the vibrational excitation of molecules on the velocity of sound.

CONCLUSIONS

The model Eqs. (8) considered in this paper allow us to obtain closed systems of equations for the minimum number of extensive or associated intensive parameters in the study of equilibrium and nonequilibrium regimes of gas mixture flows with physicochemical processes. Resulting macroscopic equations (24) and (27) represent a closed system of equations for the velocity \mathbf{v} and the intensive parameters γ_λ ; the system describes flows of a nonviscous and thermally nonconductive gas in the zero approximation of the MCEM. The squared velocity of sound is defined as the coefficient of the Laplace operator in wave equation (36). In this case, the parameter α is not fixed under the considered conditions, and formulas (38) can be used to study the dependence of the velocity of sound on the temperature T and on the intensive parameters γ_λ ($\lambda = \overline{1, \Lambda}$).

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REFERENCES

1. S. V. Vallander, E. A. Nagnibeda, and M. A. Rydalevskaya, *Some Questions of the Kinetic Theory of the Chemical Reacting Gas Mixture* (Leningr. Gos. Univ., Leningrad, 1977; US Air Force, FASTC–ID (RS) TO–0608–93).
2. E. A. Nagnibeda and E. V. Kustova, *Non-Equilibrium Reacting Gas Flows. Kinetic Theory of Transport and Relaxation Processes* (St.-Petersb. Gos. Univ., St. Petersburg, 2003; Springer-Verlag, Berlin, 2009).
3. M. A. Rydalevskaya, *Statistical and Kinetic Models in Physical–Chemical Gas Dynamics* (S.-Peterb. Gos. Univ., St. Petersburg, 2003) [in Russian].
4. P. L. Bhatnagar, Gross, E. P., and M. Krook, “A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems,” *Phys. Rev.* **94**, 511–525 (1954). <https://doi.org/10.1103/PhysRev.94.511>
5. E. P. Gross and M. Krook, “Model for collision processes in gases: Small-amplitude oscillations of charged two-component systems,” *Phys. Rev.* **102**, 593–604 (1956). <https://doi.org/10.1103/PhysRev.102.593>
6. F. B. Hanson and T. F. Morse, “Kinetic models for a gas with internal structure,” *Phys. Fluids* **10**, 345–353 (1967). <https://doi.org/10.1063/1.1762114>
7. T. F. Morse, “Kinetic model for gases with internal degrees of freedom,” *Phys. Fluids* **7**, 159–169 (1964). <https://doi.org/10.1063/1.1711128>
8. M. A. Rydalevskaya, “Hierarchy of relaxation times and the model kinetic equations,” *Vestn. St.-Petersb. Univ., Ser. 1: Mat., Mekh., Astron.*, No. 2, 55–62 (2010).
9. E. Stupochenko, S. Losev, and A. Osipov, *Relaxation in Shock Waves* (Nauka, Moscow, 1965; Springer-Verlag, Heidelberg, 1967).
10. D. Bruno and V. Giovangigli, “Relaxation of internal temperature and volume viscosity,” *Phys. Fluids* **23**, 093104 (2011). <https://doi.org/10.1063/1.3640083>
11. M. A. Rydalevskaya, “Modified Chapman–Enskog method in the terms of intensive parameters,” *Comput. Math. Math. Phys.* **50**, 1238–1248 (2010). doi 10.1134/S0965542510070122
12. M. A. Rydalevskaya, “Kinetic foundation of nonextensive gas dynamics,” *AIP Conf. Proc.* **762**, 1073–1078 (2005). <https://doi.org/10.1063/1.1941677>
13. S. V. Vallander, *Lectures on Hydroaeromechanics* (S.-Peterb. Gos. Univ., St. Petersburg, 2005) [in Russian].
14. M. A. Rydalevskaya and Yu. N. Voroshilova, *Hydromechanics of an Ideal Fluid. Statement of Problems and Basic Properties* (S.-Peterb. Gos. Univ., St. Petersburg, 2016) [in Russian].
15. L. I. Sedov, *A Course on Continuum Mechanics* (Wolters-Noordhoff, Groningen, 1971; Nauka, Moscow, 1973), Vol. 2.
16. Yu. N. Voroshilova and M. A. Rydalevskaya, “Effect of vibrational excitation of molecules on the velocity of sound in a high-temperature diatomic gas,” *J. Appl. Mech. Tech. Phys.* **49**, 369–374 (2008). <https://doi.org/10.1007/s10808-008-0051-1>

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