

Description of Transport Processes in Intensive Parameters

Maria A. Rydalevskaya

*Saint-Petersburg State University,
Saint-Petersburg, Russia*

Abstract. This paper presents an extension of the research method which was named in [1] as “Nonextensive Gas Dynamics.” In [1] distribution functions and systems of gas dynamic equations in zero approximation of Chapman-Enskog method have been studied in terms of intensive parameters. In the present paper distribution functions in the first approximation and corresponding transport fluxes are expressed in terms of intensive parameters. The properties of these expressions are considered. Special attention is given to the connection of the volume (bulk) viscosity coefficient with the sound velocity.

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KINETIC EQUATIONS IN FIRST APPROXIMATION OF CHAPMAN-ENSKOG METHOD

Kinetic theory of the transport processes in reacting gases has been studied by many authors. Most of them used combinations of extensive and intensive parameters in the description of the transport fluxes. This approach allowed to obtain many interesting results [2]. Some researches used only extensive parameters. In this paper only intensive parameters are used.

Gas flows with physic-chemical processes are considered. Suppose some molecular processes are rapid and some are slow in comparison with macroscopic processes. Then the kinetic equations may be presented in the dimensionless form [2-4]

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

Here translational energy of the microscopic particles is considered in quasi classical approximation; all forms of their internal energy are assumed quantized; the subscript i characterizes their chemical sort and internal energy; the differential operators $D_i f_i$ have a standard form; J_i^I and J_i^II are the collision operators corresponding to the “rapid” and “slow” molecular processes; $\varepsilon = \tau_I / t_*$, τ_I is the average time between the collisions I , t_* is characteristic macroscopic time.

We assume that $\tau_I \ll t_*$ ($\varepsilon \ll 1$) and use modified Chapman – Enskog method [2–4] for the solution of the equations (1).

The distribution functions in zero approximation have the form [4]

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

where s_i is statistical weight; m_i is molecular mass; h is Plank's constant; $\mathbf{c} = \mathbf{u} - \mathbf{v}$ (\mathbf{v} is macroscopic gas velocity); ε_i is internal energy which may be transformed to translational energy by the collisions \mathbf{I} ; $\psi_i^{(\lambda)}$ are independent additive invariants under these collisions; intensive parameters γ_λ may depend on the coordinates and time.

Chapman – Enskog normalization conditions are

$$e = \psi_0 = \sum_i \int (m_i c^2 / 2 + \varepsilon_i) f_i^{(0)} d\mathbf{c} = -3n^{(0)} / 2\gamma_0 + \sum_i n_i^{(0)} \varepsilon_i; \quad (3)$$

$$\psi_\lambda = \sum_i \psi_i^{(\lambda)} \int f_i^{(0)} d\mathbf{c} = \sum_i n_i^{(0)} \psi_i^{(\lambda)}, \quad \lambda = \overline{1, \Lambda}. \quad (4)$$

Here ψ_λ ($\lambda = \overline{0, \Lambda}$) are the densities of the basic extensive parameters.

Using the definition of the thermal energy and that of the pressure p , we obtained

$$\gamma_0 = -1/(kT), \quad p = -n^{(0)} / \gamma_0 = n^{(0)} kT, \quad n^{(0)} = \sum_i n_i^{(0)}, \quad (5)$$

where k is the Boltzmann constant, T is the gas temperature and $n^{(0)}$ is the particle (atoms and molecules) number density calculated in zero approximation.

$\gamma_\lambda(\mathbf{r}, t)$ are the functions that define the dependence of the parameters ψ_λ and the pressure p on the coordinates and time. As it was demonstrated in [4], γ_λ ($\lambda = \overline{0, \Lambda}$) are intensive parameters, conjugated to the extensive parameters ψ_λ . In the zero approximation of Chapman – Enskog method the gas dynamic systems can be written in terms of extensive parameters and intensive ones.

The equations for the basic extensive parameters densities have the form [2-4]

$$d\mathbf{v}/dt = \mathbf{F} - \nabla p / \rho, \quad (6)$$

$$de/dt + (e + p) \operatorname{div} \mathbf{v} = \Delta e, \quad (7)$$

$$d\psi_\lambda/dt + \psi_\lambda \operatorname{div} \mathbf{v} = \Delta \psi_\lambda, \quad \lambda = \overline{1, \Lambda}, \quad (8)$$

where \mathbf{F} is an exterior force and ρ is mass density,

$$\Delta e = \sum_i \int (m_i c^2 / 2 + \varepsilon_i) J_i^{\Pi} (f^{(0)}) d\mathbf{c}, \quad \Delta \psi_\lambda = \sum_i \int \psi_i^{(\lambda)} J_i^{\Pi} (f^{(0)}) d\mathbf{c}.$$

Mass-conservation equation

$$d\rho/dt + \rho \operatorname{div} \mathbf{v} = 0 \quad (9)$$

follows from the equations (8).

Closed systems of equations for intensive parameters γ have the form [1]:

$$\frac{d\mathbf{v}}{dt} = \mathbf{F} + \frac{1}{\gamma_0} \left(H \nabla \gamma_0 + \sum_{\lambda=1}^{\Lambda} \Psi_\lambda \nabla \gamma_\lambda \right), \quad (10)$$

$$\frac{d\gamma_\lambda}{dt} = -\frac{\det_\lambda}{\det} \operatorname{div} \mathbf{v} + \frac{\det_\lambda^{\Pi}}{\det}, \quad \lambda = \overline{0, \Lambda}. \quad (11)$$

Here $H = (e + p) / \rho$ and $\Psi_\lambda = \psi_\lambda / \rho$ are specific values of enthalpy and summarized additive invariants ψ_λ , $\det = D(\psi_0, \psi_1, \dots, \psi_\Lambda) / D(\gamma_0, \gamma_1, \dots, \gamma_\Lambda)$ is the Jacobian of the transition from the parameters ψ_λ to γ_λ (the inequality $\det > 0$ is valid in [4]), \det_λ (\det_λ^{Π}) corresponds to the determinant \det where the column of the derivatives on γ_λ is substituted by the column of coefficients in front of $\operatorname{div} \mathbf{v}$ (by right sides in equations (7), (8)).

The properties of the equations (10), (11) were investigated in [1]. Analytical formula for sound velocity in non barotropic gas with physical and chemical processes was obtained. This formula has a traditional form

$$a^2 = \kappa(p/\rho), \quad (12)$$

but coefficient κ is not always constant. It was obtained the following expression for κ :

$$\kappa = \langle e + p \rangle \frac{\det_0}{\det} + \sum_{\lambda=1}^{\Lambda} \langle \psi_{\lambda} \rangle \frac{\det_{\lambda}}{\det}. \quad (13)$$

Here $\langle e + p \rangle$ and $\langle \psi_{\lambda} \rangle$ are the average values of enthalpy and additive invariants (calculated for one molecule).

In the first approximation of Chapman-Enskog method for the distribution function $f_i^{(1)} = f_i^{(0)} \Phi_i$ we get the equations:

$$J_i^I(f_i^{(0)} \Phi_i) = D_i^{(1)} f_i^{(0)} - J_i^{\Pi}(f^{(0)}), \quad (14)$$

$D_i^{(1)} f_i^{(0)}$ have traditional form [5,6]. Using (2), (10) and (11) and supposing $\mathbf{F}_i = 0$, we obtain

$$\begin{aligned} D_i^{(1)} f_i^{(0)} = f_i^{(0)} & \left[(m_i c^2 / 2 + \varepsilon_i - \hat{m}_i \langle e + p \rangle) \mathbf{c} \cdot \nabla \gamma_0 + \sum_{\lambda=1}^{\Lambda} (\psi_i^{(\lambda)} - \hat{m}_i \langle \psi_{\lambda} \rangle) \mathbf{c} \cdot \nabla \gamma_{\lambda} - \right. \\ & \left. - \gamma_0 m_i \mathbf{c}^{\circ} \mathbf{c} : \nabla \mathbf{v} - ((m_i c^2 / 2 + \varepsilon_i) \frac{\det_0}{\det} + \sum_{\lambda=1}^{\Lambda} \psi_i^{(\lambda)} \frac{\det_{\lambda}}{\det} + \gamma_0 m_i c^2 / 3) \operatorname{div} \mathbf{v} \right], \end{aligned} \quad (15)$$

where $\hat{m}_i = m_i / \langle m \rangle$, $\langle m \rangle = \rho / n^{(0)}$.

DISTRIBUTION FUNCTIONS AND TRANSPORT PROCESSES IN FIRST APPROXIMATION OF CHAPMAN-ENSKOG METHOD

Taking into account (15) and traditional normalization conditions of Chapman-Enskog method, we obtain the following solution of the systems (14):

$$\Phi_i = - \sum_{\lambda=0}^{\Lambda} A_{\lambda,i} \mathbf{c} \cdot \nabla \gamma_{\lambda} - B_i \mathbf{c}^{\circ} \mathbf{c} : \nabla \mathbf{v} - D_i \operatorname{div} \mathbf{v} - G_i. \quad (16)$$

Coefficients $A_{\lambda,i}$, B_i , D_i and G_i must satisfy the corresponding integral equations and the relations:

$$\sum_i \int f_i^{(0)} A_{\lambda,i} m_i c^2 d\mathbf{c} = 0, \quad \lambda = \overline{0, \Lambda}, \quad (17)$$

$$\sum_i f_i^{(0)} D_i (m_i c^2 / 2 + \varepsilon_i) d\mathbf{c} = 0, \quad \sum_i \psi_i^{(\lambda)} \int f_i^{(0)} D_i d\mathbf{c} = 0, \quad \lambda = \overline{1, \Lambda}, \quad (18)$$

$$\sum_i f_i^{(0)} G_i (m_i c^2 / 2 + \varepsilon_i) d\mathbf{c} = 0, \quad \sum_i \psi_i^{(\lambda)} \int f_i^{(0)} G_i d\mathbf{c} = 0, \quad \lambda = \overline{1, \Lambda}, \quad (19)$$

When any “slow” molecular processes are absent in gas flow, collision operators J_i^{Π} in the equations (1) are absent. In this case in distribution functions (16) scalar terms G_i are absent.

If we consider a simple gas without internal degrees of freedom and chemical reactions, the expressions in round brackets (15) in front of $\operatorname{div} \mathbf{v}$ and D_i in (16) are equal to zero.

In this approximation gas dynamic equations contain the fluxes of energy and others additive invariants under collisions I. Using (16), we obtain transport fluxes as linear combinations of the gradients of intensive parameters:

$$\mathbf{q}_0 = \sum_i \int f_i^{(0)} \Phi_i (m_i c^2 / 2 + \varepsilon_i) \mathbf{c} d\mathbf{c} = \sum_{v=0}^{\Lambda} \lambda_{0,v} \nabla \gamma_v = \lambda_{0,0} \nabla T / (kT^2) + \sum_{v=1}^{\Lambda} \lambda_{0,v} \nabla \gamma_v, \quad (20)$$

$$\mathbf{q}_{\lambda} = \sum_i \psi_i^{(\lambda)} \int f_i^{(0)} \Phi_i \mathbf{c} d\mathbf{c} = \sum_{v=0}^{\Lambda} \lambda_{\lambda,v} \nabla \gamma_v = \lambda_{\lambda,0} \nabla T / (kT^2) + \sum_{v=1}^{\Lambda} \lambda_{\lambda,v} \nabla \gamma_v, \quad \lambda = \overline{1, \Lambda}. \quad (21)$$

The pressure tensor \mathbf{P} in present approximation has the form

$$\mathbf{P} = (p - p_{rel})\mathbf{I} - 2\eta\mathbf{S} - \zeta \operatorname{div} \mathbf{v} \mathbf{I}, \quad (22)$$

where \mathbf{I} is the unit tensor, \mathbf{S} is the tensor of shear velocities, p_{rel} is the relaxation pressure, η, ζ are the shear and volume (bulk) viscosity coefficients.

Integral equations for $A_{\lambda,i}$, B_i and D_i and the normalization conditions (17), (18) allow us to get the following:

$$\begin{aligned} \lambda_{\lambda,\nu} &= [A_\nu \mathbf{c}, A_\lambda \mathbf{c}] = \sum_i \int A_{\nu,i} \mathbf{c} \cdot J_i^1(A_{\lambda,i} \mathbf{c}) d\mathbf{c}, \quad \lambda, \nu = \overline{0, \Lambda}, \\ \eta &= -1/(10\gamma_0) [B\mathbf{c}^\circ \mathbf{c}, B\mathbf{c}^\circ \mathbf{c}] = -1/(10\gamma_0) \sum_i \int B_i \mathbf{c}^\circ \mathbf{c} : J_i^1(B_i \mathbf{c}^\circ \mathbf{c}) d\mathbf{c}, \\ \zeta &= -1/\gamma_0 [D, D] = -\sum_i \int D_i J_i^1(D_i) d\mathbf{c}. \end{aligned} \quad (23)$$

It is easy to see that Onsager's reciprocal relations hold:

$$\lambda_{\lambda,\nu} = \lambda_{\nu,\lambda}, \quad \lambda, \nu = \overline{0, \Lambda}, \quad (24)$$

In [7] it was claimed that in chemical equilibrium regime the matrix of transport coefficients (the element diffusion matrix) does not appear directly in the framework of Onsager's reciprocal relations. In contrast we have obtained that in terms of intensive parameters the matrix of any transport coefficients (including transport element coefficients) satisfy Onsager's relations.

A CONNECTION BETWEEN THE VOLUME VISCOSITY COEFFICIENT AND THE SOUND VELOCITY

The volume viscosity coefficient ζ is defined by the relation:

$$\zeta = 1/3 \sum_i \int f_i^{(0)} D_i(c^2) m_i c^2 d\mathbf{c}. \quad (25)$$

For the definition the functions $D_i(c^2)$ we have a system of integral equations:

$$J_i^1(D_i) = -f_i^{(0)} \left((m_i c^2 / 2 + \varepsilon_i) \frac{\det_0}{\det} + \sum_{\lambda=1}^{\Lambda} \psi_i^{(\lambda)} \frac{\det_\lambda}{\det} + \gamma_0 m_i c^2 / 3 \right). \quad (26)$$

In the right sides of equations (26) one can obtain the same expressions as those in front of $\nabla \gamma_\lambda$ in (15). As a result equations (26) take the form

$$\begin{aligned} J_i^1(D_i) &= -f_i^{(0)} \left(\hat{m}_i \left(\langle e + p \rangle \frac{\det_0}{\det} + \sum_{\lambda=1}^{\Lambda} \langle \psi_\lambda \rangle \frac{\det_\lambda}{\det} - 5/3 \right) + \right. \\ &\left. + (m_i c^2 / 2 + \varepsilon_i - \hat{m}_i \langle e + p \rangle) \frac{\det_0}{\det} + \sum_{\lambda=1}^{\Lambda} (\psi_i^{(\lambda)} - \hat{m}_i \langle \psi_\lambda \rangle) \frac{\det_\lambda}{\det} + 2/3 \gamma_0 (m_i c^2 / 2 + \hat{m}_i 5/(2\gamma_0)) \right). \end{aligned} \quad (27)$$

A comparison of (27) with (13) allows us to write

$$\begin{aligned} J_i^1(D_i) &= -f_i^{(0)} \left(\hat{m}_i (\kappa - 5/3) + (m_i c^2 / 2 + 5/(2\gamma_0) \hat{m}_i) (\det_0 / \det + 2/3 \gamma_0) + \right. \\ &\left. + (\varepsilon_i - \hat{m}_i \langle \varepsilon_{int} \rangle) \det_0 / \det + \sum_{\lambda=1}^{\Lambda} (\psi_i^{(\lambda)} - \hat{m}_i \langle \psi_\lambda \rangle) \det_\lambda / \det \right), \end{aligned} \quad (28)$$

where κ is the coefficient of proportionality in (12).

One can expand the solution of integral equations (27) or (28) in the series on modified Sonine and Waldmann-Trubenbacher polynomials. Retaining in these expansions only combinations of polynomials corresponding to right sides of (28) and using the normalization conditions (18) we obtain the following expression for D_i :

$$D_i = (5/3 - \kappa) \left(d \hat{m}_i + d_0 \left((m_i c^2 / 2 + 5/(2\gamma_0) \hat{m}_i) (2/3 \gamma_0 \det / \det_0 - 1) - (\varepsilon_i - \langle \varepsilon_{\text{int}} \rangle \hat{m}_i) \right) - \sum_{\lambda=1}^{\Lambda} d_{\lambda} \left(\psi_i^{(\lambda)} - \hat{m}_i \langle \psi_{\lambda} \rangle \right) \right). \quad (29)$$

Here d and d_{λ} ($\lambda = \overline{0, \Lambda}$) are defined from (18) and (28). The coefficient d is proportional to time.

Let us substitute (29) in (25). As a result we shall get

$$\zeta = p(5/3 - \kappa)d, \quad (30)$$

Relation (30) once again demonstrate that ζ is equal to zero in a simple gas when κ is equal to 5/3.

Taking into account an expression for sound velocity a (formula (12)), we can write the following:

$$\zeta/d = \rho(a_s^2 - a^2),$$

where a_s is the sound velocity in simple gas without internal degrees of freedom and chemical reactions.

Notice that the pressure tensor (22) can be written in the form:

$$\mathbf{P} = (1 - d(5/3 - \kappa) \operatorname{div} \mathbf{v} - p_{\text{rel}}/p) p \mathbf{I} - 2\eta \mathbf{S}. \quad (31)$$

FLOWS OF DISSOCIATED DIATOMIC GASES

In [1] the foundations of non-extensive gas dynamics were illustrated on the example of local equilibrium flows of homo-nuclear diatomic gases with dissociation and recombination.

The distribution functions for atoms and molecules in zero approximation of Chapman-Enskog method are

$$f_1^{(0)} = (m_1^3 / h^3) \exp(\gamma_0 m_1 c^2 / 2 + \gamma_1), \quad (32)$$

$$f_{2vr}^{(0)} = s_{2r} (m_2^3 / h^3) \exp(\gamma_0 (m_2 c^2 / 2 + \varepsilon_{2r} + \varepsilon_{2v} - d_2) + 2\gamma_1), \quad (33)$$

where 1 and 2 denote the chemical sort of free atoms and diatomic molecules; ε_{2r} , ε_{2v} and d_2 are rotation, vibration and dissociation energies; s_{2r} and $s_{2v} = 1$ are the corresponding statistical weights; the coefficients in front of γ_1 correspond to additive invariants and are equal to the number of elements (indivisible atoms) in particles 1 and 2. Functions (32) and (33) are normalized on the total energy $\psi_0 = e$ (including all types of energy) and the number density of indivisible atoms $\psi_1 = \tilde{n}_1$.

In first approximation the functions (16) have the form

$$\Phi_1 = -A_{01} \mathbf{c} \cdot \nabla \gamma_0 - B_1 \mathbf{c}^\circ \mathbf{c} : \nabla \mathbf{v} - D_1 \operatorname{div} \mathbf{v}, \quad (34)$$

$$\Phi_{2vr} = -A_{0,2vr} \mathbf{c} \cdot \nabla \gamma_0 - B_{2vr} \mathbf{c}^\circ \mathbf{c} : \nabla \mathbf{v} - D_{2vr} \operatorname{div} \mathbf{v}. \quad (35)$$

Here the coefficients in front of $\nabla \gamma_1$ are equal to zero. In gas dynamics system there are transport fluxes:

$$\mathbf{q}_0 = \lambda_{00} \nabla \gamma_0 = \frac{\lambda_{00}}{kT^2} \nabla T, \quad (36)$$

$$\mathbf{P} = (p - \zeta \operatorname{div} \mathbf{v}) \mathbf{I} - 2\eta \mathbf{S}. \quad (37)$$

The coefficient ζ is defined by (30), where

$$\kappa = \langle e + p \rangle \det_0 / \det + \langle \tilde{n}_1 \rangle \det_1 / \det. \quad (38)$$

Here \det is Jacobian of transition from $\psi_0 = e$ and $\psi_1 = \tilde{n}_1$ to γ_0 and γ_1 .

The temperature dependence of the relation $\zeta/(pd)$ calculated by formulas (30) and (38) for nitrogen (when $\tilde{n}_1 = 2n_L$, n_L is Loschmidt's number) is shown on Fig.1. At not very high temperatures this relation is constant and equal to $4/15$, then it increases, and approximately at $6000K$ it begins to decrease. When temperature is equal approximately to $12000K$ and almost all molecules are dissociated, the value of $\zeta/(pd)$ is approaching zero.

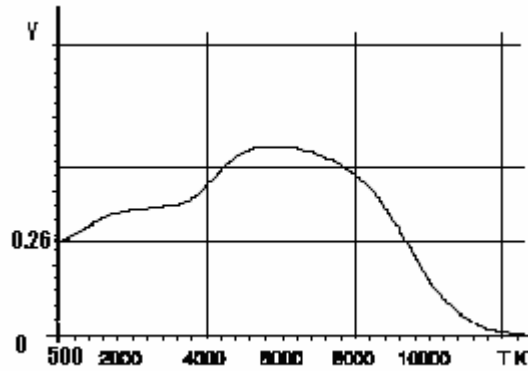


FIGURE 1. The Temperature Dependence $Y = \zeta/(pd)$ for Nitrogen.

In conclusion one may add that transition to intensive parameters in gas dynamic equations allows: (a) to obtain closed gas dynamic systems for viscose gas with internal degrees and chemical reactions and to investigate the transport processes; (b) to prove easily the correctness of Onsager's relations for different regimes of flow; and (c) to find the connection between the volume viscosity coefficient and the sound velocity.

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