Constitutive Relations for Stresses and Heat Flux.
Non-Newtonian Gasdynamics

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Abstract. The constitutive relations between stresses and heat fluxes in Couette flow and gradients of velocity and temperature, known for Maxwell molecules, are generalized for hard sphere molecules. These relations are the generalization of Newton-Fourier (Navier-Stokes) relations for shear flow with strong nonequilibrium. Similar relations are established for strong shock wave flow and for spherical expansion into vacuum for Maxwell and hard sphere molecules. General structure of constitutive relations for macroscopic description of gas flow with strong translational nonequilibrium outside the thin Knudsen boundary layers is established. Derivation is based on the hypothesis: on the solution of Boltzmann equation the stresses and heat flux depend only on velocity gradient and temperature gradient. Hamilton theorem on square dependence of arbitrary tensor function of second rank on symmetric tensor of second rank is generalized. Generalization of transport coefficients, - transport scalar function, - depends on molecular potential and on tensor invariants of symmetric and anti-symmetric parts of velocity gradient and of temperature gradient. The part of transport functions is determined by DSMC solutions of Boltzmann equation for one-dimensional flow problem.

INTRODUCTION

Essential feature of hypersonic rarefied gas flows past relatively cold bodies is the small thickness of boundary Knudsen layers. So it’s possible to hope to describe these flows with the help of macroscopic equations. In fact, for small values of viscous stresses (relative to pressure) the Navier-Stokes equations are true mathematical model. However in the hypersonic flows past cold bodies there are zones with high deviations from local equilibrium (in these zones the values of viscous stresses are of the order of pressure). These zones are: the flow in strong shock wave, the shear flow past side surface of thin bodies, the expansion flow in base zone and so on. For the flow with high values of local Knudsen number up to now there were used Boltzmann equation.

But there are some approaches to derivation of more general equations, than Navier-Stokes equations, for flows under high value of local Knudsen number. For example, in [1] there is modification of Burnett equations, in [2] the super-Burnett equations are constructed, in [3,4] Grad’s method is modified.

Present investigation is the extension to previous research of impulse and energy transport processes in two one-dimensional flows under special molecular model [5-9]. In paper [5] the structure of asymptotic series of Hilbert normal solution for shear flow corresponding to the plane Couette problem was obtained. There the one-component gas of Maxwell molecules was considered. It was shown that the terms of asymptotic series depend only on ratio \( a = p_{xy}^N / p \), this value is the measure of translational nonequilibrium. Here index \( k \) is the order of the term, \( p_{xy}^N, q_y^F \) are the stress and the heat flux in Navier-Stokes approximations, defined by Newton-Fourier relations, \( p \) is the pressure. Paper [6] develops these studies. It was shown (with the help of BGK kinetic equation) that the asymptotic series of the normal solution of the kinetic equation can be related to the function defined for any values of parameter \( a \). Moreover, it was proved that this function is the solution of the model kinetic equation for Couette problem. The general results of paper [6] are valid not only for BGK equation, but also for Boltzmann equation with Maxwell molecular model, as it was shown by DSMC method in papers [7,8]. Statements of Couette problem differ in [7,8] by the boundary conditions for Boltzmann equation. In paper [9] it was
shown, that it is possible to describe the strong shock wave flow by the macroscopic equations that are the generalization of Navier-Stokes equations. One of the purposes of this research is the determination of the applicability the results of papers [7-9] to the gas with another molecular models.

Basic hypothesis assumed in this paper is the generalization of dependences established for shear flow problem. Exactly, asymptotic forms of stress tensor and heat flux vector, derived as normal solutions of Boltzmann equation are degenerated. Outside the boundary Knudsen layers they are the nonlinear functions on symmetric part $u_{i,j}^{s}$ and anti-symmetric part $u_{i,j}^{as}$ of velocity gradient tensor and temperature gradient vector $T_{i,j}$. The derivation of constitutive relations for stress and heat flux is based on following statements. The arbitrary tensor function of second rank, depending on each of these arguments, in homogeneous isotropic space is a second order polynomial in $u_{i,j}^{s}$, $u_{i,j}^{as}$ and first order polynomial in $T_{i,j}$. The coefficients of these polynomials are the scalar functions of invariants of arguments. The arbitrary tensor function of second rank, depending on joint arguments, is the combinations of these polynomials (with taking into account the non-commutation of tensor product). The coefficients of these polynomials are the scalar functions in invariants. In this case the additional joint invariants must be added. The whole number of invariants is nine. These statements give the opportunity for formulation of general form of constitutive relation for symmetric stress tensor (accurate to scalar transport functions).

The analogous consideration of arbitrary vector function in the same arguments makes it possible to establish constitutive relation for heat flux vector. It is proportional to the product of temperature gradients and arbitrary tensor function of second rank in velocity gradient. In this case the polynomial coefficients (nonlinear transport functions) are the scalar functions in nine invariants of arguments above mentioned.

As the transport coefficients in Chapman-Enskog method must be determined from the solution of auxiliary problem, so as the nonlinear transport functions must be determined from the solutions of auxiliary one-dimensional problems on rarefied gas flows. For the determination the part of transport functions there were solved three one-dimensional problems by DSMC method: plane Couette flow, plane shock wave flow and expansion into vacuum.

## PLANE COUETTE FLOW

It was shown in [7,8] that the constitutive relations, established for a gas with Maxwell molecules, is approximately true also for a gas with hard sphere molecules. Here we’ll show that in more accurate statement the constitutive relations have more complex structure. The more elaborated transport functions are determined by the numerical results of DSMC solutions of Boltzmann equation.

### Problem Statement

The problem statement is the same as in [7]. The one-component monatomic gas flow between parallel flat plates moving with relative dimensionless velocity $S_{w}$ and equal temperatures $T_{w1} = T_{w2} = T_{w}$ is studied. The complete diffusion interaction molecules with the plates are applied. The hard sphere molecules (HS), Maxwell molecules (MM) and VHS model for Maxwell molecules (PMM) are chosen as molecular models. The DSMC method with majorant collision frequency is used. Time step, size of cells and other computational parameters are chosen to reduce the statistics error of calculation of hydrodynamic parameters to 0.1%. For the calculation Newton stress $(\sigma_{x,x})$ and Fourier heat flux $(q_{x,x})$ outside the boundary Knudsen layers the linear dependence of the velocity upon coordinate $s$ is used. This coordinate is introduced by equation $\frac{\partial}{\partial s} = \mu \frac{\partial}{\partial y}$, where $\mu$ is a viscosity coefficient.

Dimensionless variables are introduced: coordinate $y$ is related to distance between plates, density is related to average density $\rho_{av}$, temperature to $T_{w}$, velocity to $c_{w} = \sqrt{2RT_{w}}$, pressure to $0.5\rho_{av}c_{w}^{2}$, heat flux to $0.5\rho_{av}c_{w}^{3}$. Knudsen number is defined with the help of distance between the plates and mean free path $\lambda_{w} = \frac{16}{5\pi} \frac{\mu_{w}}{\rho_{av}} \sqrt{\frac{\pi}{2RT_{w}}} (1 - \frac{2}{3k})(1 - \frac{1}{k})$. Here $k$ is a power in the potential of intermolecular interaction $U(r) = cr^{-k}$ ($k = 4$ for Maxwell molecules and $k = \infty$ for hard sphere molecules).
Results

**MM and PMM Molecular Model**

Here it is shown that transport characteristics (heat flux and stresses) for the gas flow with two molecular models – Maxwell model (MM) and VHS Maxwell model (PMM) – calculated by DSMC method are close one to another (in this example it is used the definition of Knudsen number by the hard sphere approximation for relation between viscosity and mean free path). Data on Fig.1 show that the difference in the results is not exceed 2%. So further we’ll use only PMM molecular model for soft molecular model ($k=4$).

**Modified Burnett approximation and transport functions for MM case.**

Well-known Burnett approximation for transport characteristics may be modified with the purpose of simplification. Here we are forced to expose once more the results of [7].

\[
q_y^B = Cq_y^F \frac{p_y^N}{p}, \quad C_{MM} = 3.500, \quad C_{HS} = 3.193
\]

\[
p_{xx}^B = A_x \left( \frac{p_{xy}^N}{p} \right)^2 + B_x \left( \frac{q_y^F}{p^{2RT}} \right)^2, \quad p_{yy}^B = A_y \left( \frac{p_{xy}^N}{p} \right)^2 + B_y \left( \frac{q_y^F}{p^{2RT}} \right)^2
\]

\[
A_{xMM} = 1.600, \quad A_{yMM} = -1.200, \quad B_{xMM} = B_{yMM} = 0
\]

\[
A_{xHS} = 1.51, \quad B_{xHS} = 0.04695, \quad A_{yHS} = -1.163, \quad B_{yHS} = -0.0939
\]

\[
q_y^B = 0, \quad p_{xy}^B = 0
\]

\[
p_{xy}^N = -\mu \frac{\partial u_x}{\partial y}, \quad q_y^F = -k \frac{\partial T}{\partial y}.
\]

Let us introduce transport functions for soft potential case (MM). For this purpose we relate transport characteristics to its values in Newton-Fourier approximation or to modified Burnett approximation (if Newton-Fourier values are equal zero). Than in notation, which is close to notation of [8]:

\[
F_{\eta}^{MM}(a^2) = \frac{p_{xy}}{p_{ys}}, \quad F_k^{MM}(a^2) = \frac{q_y}{q_y^F}, \quad \Phi^{MM}(a^2) = \frac{q_x}{q_x^F}, \quad \Pi_x(a^2) = \frac{p_{xx}}{p_{xx}^B}, \quad a = \frac{p_{xy}^N}{p}
\]

On Fig.2 all transport functions are shown. Of course, all transport functions tends to unity if nonequilibrium parameter ($a$) tends to zero. These results are close to the results of [7,8].
Hard Sphere Molecular Model

As it is seen from equation (1) normal stresses for HS molecular model depends not only on shear stress in Newton approximation (velocity gradient), but also on heat flux in Fourier approximation (temperature gradient). The normal stresses are no more constant outside the boundary Knudsen layers (as for MM case). On Fig. 2 (right) it’s shown the results of DSMC calculation for normal stresses. So for the case of hard sphere molecules it’s necessary to take into account (for construction of generalized Newton-Fourier constitutive relations) that all transport characteristics may depend not only on velocity gradient, but also on temperature gradient. Because the influence of temperature gradient on transport functions is weak, let us introduce these functions in following form:

\[ \Phi^{HS}(a, b) = \Phi_0(a^2) + b^2 \Phi_1(a^2), \]
\[ F_{\eta}^{HS}(a, b) = F_{\eta 0}(a^2) + b^2 F_{\eta 1}(a^2), \]
\[ F_{\kappa}^{HS}(a, b) = F_{\kappa 0}(a^2) + b^2 F_{\kappa 1}(a^2), \]

FIGURE 3. Calculated correction for generalized Newton-Fourier constitutive relations for Couette flow with hard sphere molecules. Symbols – DSMC results, curves – approximation of DSMC results, straight line – limit value of \( (10\Pi_{kl}) \) under \( a \to 0 \) equal to \( B_{HS} \) (see Eq. (1)).
Functions $F_{\gamma 0}$, $\Pi_{\gamma 0}$ with subindex 0 may be determined by the values of transport characteristics in flow, where temperature gradient is equal zero ($b=0$). Calculation of transport functions with subindex 0 leads to the same results as for MM case (see Fig.2). The correction of generalized Newton-Fourier constitutive relations, that is transport functions with subindex 1 are shown on Fig.3. The limit of these functions under $a \to 0$ is known now only for $\Pi_{\gamma 1}$ (see Eq. (1)).

**STRONG SHOCK WAVE**

In [9] there were shown, that the approach, applied in Couette flow description, may be developed for flow in strong shock wave. There was shown, that there is the second order polynomial dependence of heat flux on gas velocity. The coefficients of this polynomial weak depend on molecular potential. But for determination of generalized Newton-Fourier constitutive relations for shock wave flow it was additionally used the dependence of velocity gradient on velocity itself. For this purpose there was introduced normalized velocity $V = (u_1 - u)/(u_2 - u_1)$, where $u_1$ – velocity in undisturbed flow, $u_2$ – velocity behind shock wave. Then, if coordinate normalized by $\lambda_1$, the velocity gradient, calculated by DSMC method, may be approximated by third order polynomial on $V$:

$$V' = V(1-V)a(1+bV)$$ (4)

This approximation was shown for hard sphere molecules in [9]. On Fig.4 it’s shown this approximation for two other molecular model. It’s seen, that parameters of these approximation essentially depend on molecular model. For example, for these molecular models coefficient $a$ decreases with Mach number opposite to the case of hard sphere molecular model, when it increases (see [9]). Thus this is example of flow, in which the molecular model influence is strong, opposite to Couette flow, when this influence is weak.

**SPHERICAL EXPANSION INTO VACUUM**

The translational nonequilibrium in this flow (measured by relation of normal stress, valued Newton approximation, to pressure) is high. This relation tends to infinity with the distance from the source. Moreover, true normal stress tends to $2p$. Here we investigate the applicability of above used approach to this problem. Lower the generalization of Newton-Fourier constitutive relations are formulated for expansion flow under two molecular models.

The problem statement is usual: monatomic gas expands into vacuum from spherical source with some boundary conditions. Here Maxwell molecular distribution function was used with and without mean gas velocity (the cases of

Mach number in distribution function $M_r=0$ and $M_r=1$ were considered. Knudsen number calculated by source parameters tends to zero, that is thickness of boundary Knudsen layer also tends to zero, and nonequilibrium flow exists at long distance from source. The results of DSMC solutions for MM and HS molecular model are shown on Fig.5. From these results it’s been seen that generalization of Newton-Fourier constitutive relations exist for expansion flow. Besides, the constitutive relation for stress weakly depends on molecular model and relation for heat flux strongly depends on molecular model. Of course, if the nonequilibrium parameters in some zone, close to source, tend to zero ($p_{rr}^N/p \to 0$), then Newton and Fourier relations become true for this zone of expansion flow also.

Note, that the generalization of Newton relation for Maxwell molecular model is close to well-known hypersonic approximation of Hamel-Willis.

ON GENERAL FORM OF CONSTITUTIVE RELATIONS

In accordance to results of above parts, especially to results for Couette flow, we’ve adopted the hypothesis that stress tensor and heat flux vector in arbitrary nonequilibrium flow outside the Knudsen boundary layer depend only on symmetric ($u^s$) and antisymmetric ($u^a$) parts of gradient velocity tensor and on temperature gradient. This may be so only if normal solution of Boltzmann equation degenerates. Hereafter we use notations:

$$
\begin{align*}
  u^s_{ij} &= \frac{1}{2}(u_{i,j} + u_{j,i}), & u^a_{ij} &= \frac{1}{2}(u_{i,j} - u_{j,i}), & t_{ij} &= T_{,i}T_{,j}, & u_{i,j} &= \frac{\partial u_i}{\partial x_j}, & T_{,i} &= \frac{\partial T}{\partial x_i}
\end{align*}
$$

(5)

Consideration of generalized Newton-Fourier constitutive relations based on generalization of Hamilton theorem. This theorem is so: arbitrary tensor function of second rank $F$ upon symmetric tensor of second rank $A$ may be described as

$$
F = f_0 E + f_1 A + f_2 A^2
$$

(6)

Here $E$ – unit tensor, $(A^2)_{ij} = A_{ik}A_{kj}$. Functions $f_i$ depend only on three invariants of $A$. These invariants may be determined as traces of $A, A^2, A^3$ or arbitrary functions on these traces.

The simple consideration of power of tensor $t$ shows that $t^k = (Tr t)^{k-1} t$. Besides it may be shown that tensor $t$ has only one invariant, $Tr t$, (or absolute value of temperature gradient). Therefore, arbitrary function of second rank of tensor $t$ has the form

$$
F_t(t) = f_{10} E + f_{11} t
$$

(7)

Here $f_{10}$ - scalar functions on $t$-invariant.
Similarly straightforward calculation shows, that odd power of $u^a$ proportional to $u^a$, and even power of $u^a$ proportional to $(u^a)^2$. Thus arbitrary function of $u^a$ of second rank may be described as

$$F_{ab}(u^a) = f_{a0} E + f_{a1} u^a + f_{a2} (u^a)^2$$  \hspace{1cm} (8)

Here $f_{ab}$ - arbitrary functions on unique $u^a$-invariant $\text{Tr}((u^a)^2)$ (or $\text{rot } u$).

Combining (7), (8) and (6), applied for $u^t$, we may show that arbitrary tensor function of second rank on $u^t, u^a, t$ is the polynomial of second power on $u^t, u^a$, and linear function on $t$. Coefficients of these polynomials are arbitrary functions on self and joint invariant of $u^t, u^a, t$. The complete set of invariants of these tensors consists of three $u^t$-invariants, one $u^a$-invariant, two joint $u^t$-invariants, one $t$ invariant and two joint $t \Leftrightarrow u^t$ invariant (or any functions on this set).

So, general form of stress tensor under our hypothesis may be only polynomial of considered kind. Similarly, the general form of heat flux vector may is product of temperature gradient and arbitrary tensor functions on $u^t, u^a$. Scalar coefficients of this polynomial tensor function are arbitrary functions on the same set of invariants. These functions are transport functions (generalization of transport coefficients in normal series solution of Boltzmann equation) and may be determined only by the solution of Boltzmann equation for various gas flow problems.

The general forms of stress tensor and heat flux vector is extremely complicated one. Now there is no mathematical theory that may give the opportunity for decreasing this complexity. Moreover, there are only three onedimensional problems in which special forms of constitutive relations are determined. It’s evident, that we must introduce some more suppositions, simplifying complex general form.

As an example let us elaborated this path for heat flux in plane flow and let us apply the result to hypersonic flow past plane plate at zero angle of attack. The flow between shock wave and plate surface is in essential shear flow. So we tried to restrict ourself only by Couette flow data for construction of constitutive relation of simplest form. Our suppositions: 1) let us restrict the power of polynomials on $u^t, u^a$ by the linear form; 2) in linear form we preserve only terms, included in Burnett approximation. In this case heat flux vector $q$ is determined by this form

$$q = (Q_0 E + Q_1 u^t + Q_2 u^a)(\text{grad } T)$$ \hspace{1cm} (9)

$Q_i$ are functions of invariants; 3) as invariants we consider

$$I_1 = I_1(u^t) = \text{Tr } u^t = u_{11} + u_{22}$$

$$I_2 = I_2(u^t) - I_1^2 = \text{Tr}((u^t)^2) - I_1^2 = \frac{1}{2}(u_{12} + u_{21})^2 - 2u_{11}u_{22}$$

$$I_3 = I_1(u^a) + I_2 = 2(u_{12}u_{21} + u_{11}u_{22})$$

$$I_4 = \text{Tr } t = T_1^2 + T_2^2$$

$$I_5 = \text{Tr}(u^a t) - I_1 I_4 = (u_{12} + u_{21})T_1T_2 - u_{11}T_2^2 - u_{22}T_1^2$$

The number of invariants is less than the number of independent components of velocity and temperature gradients. For Couette flow problem this set of invariants transforms to

$$I_1^C = I_3^C = I_5^C = 0, \quad I_2^C = \frac{1}{2}u_{12}^2, \quad I_4^C = T_2^2 \quad, \quad x = x_1, \quad y = x_2.$$  

4) Heat flux (9) must coincide with known heat flux in Couette problem. Then $Q_0 \propto F_k(I_2), \quad Q_1 = 4/3Q_2 \propto \Phi(I_2)$.

Because $x$ component of heat flux more interesting value, we, for example, write out this relation:

$$q_1 = -kT_1F_k(I) + \frac{7}{p} \frac{\Phi(I)}{4} \left[ u_{11}T_1 + \frac{1}{2}(u_{12} + u_{21})T_2 \right] + \frac{3}{7} \frac{1}{2}(u_{12} - u_{21})T_2, \hspace{1cm} (10)$$

Functions $F_k, \Phi$ are shown on Fig.2. On Fig.6 it is shown application of Eq. (10) to the determination of longitudinal heat flux ($q_x = q_1$) for flow past flat plate. If we consider this result not as final one, but only as first attempt to construct generalization of Newton-Fourier constitutive relations for two-dimensional flows, than this crude approximation may be adopted as good one.
FIGURE 6. Longitudinal heat flux profile for flow past flat plate at zero angle of attack at the distance from the leading edge correspondent to $Re_x = 4200$. $S_x = 21$, $t_w = 0.2$. 1 – DSMC result, 2 – Fourier relation, 3 – full Burnett relation, 4 – relation of Eq. (10). Approximation 2-4 calculated by the velocity and temperature fields, computed by the DSMC method.

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REFERENCES