# Effects of dispersion and structure molecules on time relaxation

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**Abstract**

Here in the mechanics the influence of the angular momentum and the delay are investigated. Non-symmetric stress tensor is obtained. The delay process is counted, which is important in describing of the discrete space and for the relaxation of the complicated molecules. The analysis of the recording the Lagrangian function for the collective interaction of the particles are made with changing distance of the inertia center. Another definition of temperature is obtained for molecules with vibration and rotation and for mixture. This is making another value for pressure. The analysis is complemented by new results of computational experiments. The simplest interaction of two homogeneous flows that moving in the same direction at different speeds is investigated.

*Keywords*: angular momentum, conservation laws, nonsymmetrical stress tensor, Boltzmann equations, Chapman-Enskog method, conjugate problem the Navie-Stokes, the molecular dynamics method.

## 1 Introduction

In classical mechanics, the basic laws are the laws of conservation of mass, momentum and energy. The law of conservation of angular momentum is carried out indirectly on the basis of the law of the balance of power. The paper analyzes the provisions of the underlying mathematical models of continuum mechanics and the kinetic theory. We propose to include in the new model two types of effects: nonlocal effects and dispersion, i.e. we examine the impact of non-locality in time and space and the effect of the angular momentum on the processes occurring in the gas and liquid; we give a new interpretation of the conservation law of motion, which does not contain the arbitrary choice of the axis of rotation of the elementary volume. Each of the effects is considered separately. Angular momentum gives emergence of additional forces that can play the role of small perturbations affecting the stability of the structure. The resulting effects may affect in a critical and near a critical modes of aircraft, rockets, various devices, structures, as well as in some of the natural processes. The value of the additional force is determining by the gradient of physical quantities (density, velocity, momentum). The role of the delay observed

in experiments with shock waves in a rarefied gas, in lasers based on polyatomic gases, in chemical reactions. In some experiments with shock waves we can see the influence of the second viscosity [1]. In this work we give another definition of temperature for molecules with vibration and rotation and for mixture of molecules. This is making another value for pressure and temperature than in classic [2]. These new effects connect with nonlinear of definition the pressure and temperature. The influence of the angular momentum and the delay are investigated in the mechanics for: the interaction of many-particles, kinetic theory, the structural of molecules. Attention is drawn to the delay process, which is important in describing the discrete space. The analysis of the recording of the Lagrangian function [3,4] for the collective interaction of the particles with the change of the center of inertia of the moving particles and the effect influence angular momentum are made. Elementary volume can rotate around the axis of inertia or to be involved in the rotational movement. In both cases the flow density varies across the border on the value $\frac{d(\rho u)}{dr}\cdot(r'-r)+\cdots$ by the rotation of the elementary volume [5-9]. For rarefied gas the second term (on space) in integral of collision of the Boltzmann equation is taken into account to calculate the self-diffusion and thermo-diffusion that was foretold by S.V. Vallander. It should be noted that for the kinetic theory (the Boltzmann equation) the law of conservation of angular momentum does not hold. Macroscopic parameters are determined in the equilibrium function of the Chapman-Enskog distribution in which used parameters of the Euler equations. Fromt this implies for the Chapman-Enskog distribution function formally we have values (density, linear moment and energy) with the first-order error. This fact was noted by Hilbert without further use and correction. The Boltzmann equation is invariant with respect to the choice of macro parameters. Therefore, the coincidence of the Navier-Stokes equations and the construction is of formal nature, order of approximation for the parameters in a locally equilibrium distribution function different. The Hilbert paradox was being solved. To solve this problem the iteration procedure was suggested. The new stress tensor is obtained for the molecules with their rotations and oscillations. Summary records of all effects lead to a cumbersome system of equations and therefore require the selection of main effects in a particular situation. Study is continued of the problem of Faulkner-Scan with a constant vortex at the outer edge of the boundary layer and with changing the vortex. The emergence of "banded" structures revealed under certain conditions of flow at the outer edge. We have results that small differ from classic results for the flows without vortex on the upper boundary.

## 2 The Lagrangian function

Here I would like to highlight some of the issues of theoretical mechanics. In the theoretical mechanics the Lagrangian form is considered [3,4]

$$L=\sum_i \frac{m_a v_i^2}{2}-U(r_1,r_2,\ldots).$$

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assumed that $U(r_1, r_2, \ldots)$ — the full potential of the interaction of all particles, but in practice it is usually known interaction potentials of the two particles, and we use their sum. At equilibrium, or at small strains, but under nonequilibrium thermodynamic effects and perturbations lead to an uneven distribution of the physical parameters and the role of collective effects, that determined by the growing influence of the angular momentum. In addition, when these strains change position of the center of mass of elementary volume, that sign.

$$\frac{dL}{dt}=\sum_i \left[\frac{\partial L}{\partial q_i}\dot{q}_i+\frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i\right]+\sum_i \left[\frac{\partial L}{\partial (q_i-a)}\big(\dot{q}_i-\dot{a}\big)+\frac{\partial L}{\partial (\dot{q}_i-\dot{a})}\big(\ddot{q}_i-\ddot{a}\big)\right],$$

$$a=\sum_i \frac{m_i r_i}{m_i}, \quad \text{for electrical interaction} \quad a=\sum_i \frac{e_i r_i}{e_i}.$$

In view of the time we are invited to consider force formula
$F = F_0 + \nabla\big((R-a)\times\frac{\partial U}{\partial R}\big)$, $R$ — the current radius. This formula is transformed with the permutability derivatives and directions of forces in the formula

$$F = F_0 + \nabla\big((R-a)\cdot\frac{\partial U}{\partial R}\big).$$

Usually, however, such as the Hamiltonian system of two interacting molecules after separation of the center of mass is represented as the sum of the Hamiltonians of isolated molecules $H_0 = H_A + H_B$ operator and their electrostatic interaction [10]
$H = H_0 + V$

$$V=-\sum_{a=1}^{n_A}\sum_{j=1}^{N_B}\frac{Z_a}{r_{aj}}-\sum_{b=1}^{n_B}\sum_{j=1}^{N_B}\frac{Z_b}{r_{bj}}+\sum_{i=1}^{N_A}\sum_{j=1}^{N_B}\frac{1}{r_{ij}}+\sum_{a=1}^{n_A}\sum_{b=1}^{n_B}\frac{Z_a Z_b}{R_{ab}},$$

where the indices $A$, $B$ numbered core indices $i$, $j$ — the electrons of molecules $A$, $B$, respectively, the atomic units.

# 3 The kinetic theory

We can suggest the new formulation of some macrovalues (temperature, stress tensor, flow heat): in classic theory [11-15]

$$\frac{3}{2}kT=\frac{1}{n}\sum_k \int \frac{m_k (c^k)^2}{2} f_k \, d\xi_k, \quad \big(n=\sum_{k=1}^{N} n^k\big),$$

here $k$ — number of components, $T$ — temperature, $c^k{=}\xi_k{-}u$ (velocity of "$k$" components), "$q$" — heat flow, $f$ — distribution function, one's velocity of molecules, $\xi_k$ velocity of molecules. Another definition is

$$\frac{3}{2}kT=\frac{\int \big(\sum_k \frac{n_k}{n} m_k\big)\big(\sum_k \frac{n_k}{n} c^k\big)^2}{2} f \, d\xi.$$

Then we have one term is traditional and another is as the second viscosity. For stress tensor we can have $P_{ij}=\int \left(\sum_k \frac{n_k}{n} m_k c^k\right)_i \left(\sum_k \frac{n_k}{n} m_k c^k\right)_j f d\xi$.
For the flow of the heat

$$q=\frac{\int \left(\sum_k \frac{n_k}{n} c^k\right) \left(\sum_k \frac{n_k}{n} m_k\right) \left(\sum_k \frac{n_k}{n} c^k\right)^2}{2} f d\xi.$$

What we take in experiment?
$f_\nu^{(0)}=n^\nu \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m}{2kT}(c^\nu)^2\right)$ or for exclusive temperature
$f_\nu^{(0)}=n^\nu \left(\frac{m}{2\pi kT^\nu}\right)^{3/2} \exp\left(-\frac{m}{2kT^\nu}(c^\nu)^2\right)$.

For full temperature we can't conclude the right probability. The highest probability - transitions with a change in the quantum number by one $a_{\nu\mu}^{\nu+1,\mu}=a_\nu^{\nu+1}$. Deactivation process is
$a_\nu^{\nu-1}=a_{\nu-1}^\nu \exp\left(\frac{\Delta E^\nu}{kT}\right)$. In my opinion $a_\nu^{\nu-1}=a_{\nu-1}^\nu \exp\left(\frac{\Delta E^\nu}{kT^{\nu-1}}\right)$. For the internal energy remains the old equation, but with modified temperature value.

# 4 Interaction of two homogeneous flows

The simplest interaction is two homogeneous flows that moving in the same direction at different speeds. The classical formulation proposed in [16] (Fig. 1).

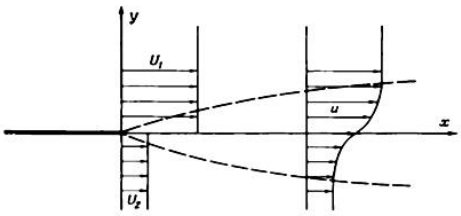


Figure 1: The overall picture of the interaction of two streams

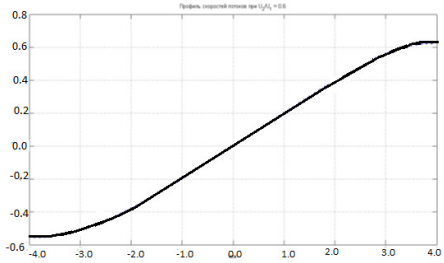


Figure 2: Stream interaction painting, $\frac{U_2}{U_1}$=0.6

The problem is on the singularity. Two singularities dictate (the boundary conditions are set at infinity) a non-standard method of solution. Approximation boundary conditions at zero, and then the iterative process to satisfy the boundary conditions.

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$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=U_e\frac{\partial U_e}{\partial x}+\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial y}\left(\mu y\frac{\partial^2 u}{\partial y^2}\right),\quad \frac{\partial u}{\partial x}+\frac{\partial \nu}{\partial y}=0,$$

$u$, $v$ — velocity on $x$, $y$.
Once we have the dimensionless equations

$$-1/2\eta\Phi\frac{d\Phi}{d\eta}+V\frac{d\Phi}{d\eta}=\mu\frac{d^2\Phi}{d\eta^2}+\frac{d}{d\eta}\left(\mu\eta\frac{d^2\Phi}{d\eta^2}\right),$$

$$-1/2\eta\frac{d\Phi}{d\eta}+\frac{dV}{d\eta}=0.$$

In this way

$$\mu\frac{d}{d\eta}\left(\eta\frac{d^3\psi}{d\eta^3}\right)+\mu\frac{d^3\psi}{d\eta^3}+2\Psi\frac{d^2\psi}{d\eta^2}=0.$$

Here $\Psi^*=\sqrt{\mu/U_1}\,\Psi,\quad y_1=1/2\sqrt{\mu/U_1}\,\eta$.
Then we have $2\eta\Psi^{''''}+2\Psi^{'''}+\Psi\Psi^{''}=0$.
With boundary conditions

$$\Psi(0)=0,\Psi^{'}(0)=1-a,\Psi^{''}(0+)=\Psi^{''}(0-),\Psi(-\infty)=a.$$

The analytical solution has been found. Numerical results are presented in Fig. 2.

# 5 Conclusion

We propose the modified equations of continuum and Boltzmann equation in early works taking into account dispersion and delay, as well as the position of the center of inertia of the elementary volume. The possibility to describe discrete medium in the framework of continuum mechanics. Set the role of dispersion and delays in physical and chemical relaxation processes. The effect of angular momentum and, as a consequence, the nonsymmetrical of the stress tensor in the elementary volume was received. A model of the collective effects in the Lagrangian function was build. The results of the numerical solution of the modified problem of interaction of two parallel streams moving in the same direction are given.

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