

Effect of Mathematical Models on Experimental Data for the Gas and Liquids

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Abstract: The new analysis of the influence the method of calculating macro-parameters to experimental data is made for the mixture a rarefied gas and gas with internal degrees of freedom. The delay process is counted, which is important in describing of the discrete space and in describing the relaxation of the complicated molecules. The analysis of the recording the Lagrangian function for the collective interaction of the particles is made with counting of changing position of the inertia center. This equation should have a modified Liouville equation and the Boltzmann equation. General consideration of all effects gives us cumbersome system of equations. New another definition of temperature is obtained for molecules with vibration and rotation degree of freedom and for mixture. This is making another value for pressure of the mixture a rarefied gas and gas with internal degrees of freedom. Probably, exactly, these values are measured in all experiments. The simplest interaction of two homogeneous flows is studied which move in the same direction at different speeds.

Key words: Angular momentum, conservation laws, non-symmetrical stress tensor, Boltzmann equations, Chapman-Enskog method, conjugate problem the Navie-Stokes.

1. Introduction

The paper analyzes the provisions of the underlying mathematical models of continuous mechanics and the kinetic theory. A feature of the kinetic theory is that the focus is on processes inside elemental volume. For continuous media the streams across the border are the main processes. As a result in classical continuous mechanics is ignored volume processes, in the kinetic theory are ignored streams across borders (part).

Classical formulations lead to the loss of influence of the angular momentum, the self-diffusion and thermal diffusion. 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. At present for continuous mechanics formulation of equilibrium force conditions are used.

These give us symmetric pressure tensor and disturbance of continuous medium that require from us to perform some addition conditions. L.D. Landau, C de Groot, P. Mazur, I. Deyrmati, I. Prigogine, L.I.Sedov, A.A. Ishlinskii, D.D. Ivlev et al. point at the role of angular momentum. It is the most developed area in the momentum theory of elasticity (R. D. Mindlin, V. A. Palmov, A. G. Gorshkov, E. I. Starovoitov, A. V. Yarovoy, V. Levin, S. E. Kanaun, E. L. Aero, etc.). Any movement of an elementary volume of liquid at the moment can be considered as a result of the following motion: quasi solid motion that is moving on selecting pole, rotating motion around this pole and deformation moving medium.

This theorem was proved by H. Gelmholtz. L. Prandtl formulated conception of hardplastic body as the theory of ideal plasticity. Usually we do not take into account twist velocity. The angular momentum is

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responsible for the twist velocity. Thus, in the classical Newton mechanics we have four conservation laws: masses, linear momentum, energy, angular momentum.

In continuous mechanics we use only three first laws. The process of changing for the elementary volume the position of inertia axis leads to a change in angular momentum, changing the force acting on the volume. Each of the effects is considered separately. Angular momentum gives emergence of additional forces. It 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 mode 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]. The disadvantages of the classical kinetic theory apply the inability to describe the effects of self-diffusion and thermal diffusion.

Determining the average speed does not allow to calculate the effects, bound with gradients of physical parameters. Gradients of physical values do an additional flow through the boundary elementary volume. Distribution function is changing in process of collisions and leads to changing the phase velocity that is doing another observing velocity.

This velocity gives self-diffusion and thermal diffusion. In this work we give another definition of temperature for molecules with vibration and rotation and for mixture of molecules. It determines another value for pressure and temperature than in classic case [2]. These are new effects that connect with nonlinearity of definition the pressure and temperature. In this work the influence of the angular momentum

and the delay are investigated for: the interaction of many particles, kinetic theory, the structural of molecules. Particular attention is paid to delay the process, which is important for discrete tasks.

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. The influence of this effect cannot be seen in literature. 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 $(d(\rho u))/dr \cdot (r \square - r) + \dots$ 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 which were 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 function of the Chapman-Enskog distribution which used parameters of the Euler equations. From 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 in equilibrium function. 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 is 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 as for mixture gases. Summary records of all effects lead to a

cumbersome system of equations and therefore require the selection of main effects in a particular situation. Investigation was carried out for the problem of Faulkner-Scan with a constant vortex at the outer edge of the boundary layer and with changing the vortex in previous works. 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. The simplest interaction of two homogeneous flows is studied. They move in the same direction at different speeds.

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2. Investigated Method for the Lagrangian Function

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

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

Here the author would like to highlight some of the issues of theoretical mechanics. In the theoretical mechanics the Lagrangian form is considered [10, 11]. Always implicitly assumed that $U(r_1, r_2, \dots)$ —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 it is well, but under

nonequilibrium thermodynamic effects and perturbations lead to an uneven distribution of the physical parameters and the big role of collective effects, which is 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

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

$$\mathbf{a} = \sum_i \frac{m_i \mathbf{r}_i}{m_i}, \text{ for electrical interaction } \mathbf{a} = \sum_i \frac{e_i \mathbf{r}_i}{e_i}.$$

In view of the time we are invited to consider force formula

$$\mathbf{F} = \mathbf{F}_0 + \nabla \left((\mathbf{R} - \mathbf{a}) \times \frac{\partial U}{\partial \mathbf{R}} \right), \quad \mathbf{R} \text{ —the current}$$

radius. This formula is transformed with the permeability derivatives and directions of forces in the formula

$$\mathbf{F} = \mathbf{F}_0 + \nabla \left((\mathbf{R} - \mathbf{a}) \cdot \frac{\partial U}{\partial \mathbf{R}} \right).$$

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 Results for Kinetic Theory

We derive an equation for the N-particle distribution function near the surface, taking into account the

gradient of the particle density. In deriving the modified equation we designations leave the conventional. We

$$\begin{aligned} j \frac{1}{V^s} \frac{\partial F_s}{\partial t} = & - \frac{1}{V^s} \sum_{i=1}^s \frac{\mathbf{p}_i}{m} \frac{\partial F_s}{\partial \mathbf{r}_i} + \frac{1}{2V^s} \sum_{\substack{i,j=1 \\ (j \neq i)}}^s \frac{\partial \Phi(|\mathbf{r}_i - \mathbf{r}_j|)}{\partial \mathbf{r}_i} \frac{\partial F_s}{\partial \mathbf{p}_i} + \\ & + \frac{1}{V^{s+1}} \sum_{i=1}^s \int \sum_{j=s+1}^N \frac{\partial \Phi(|\mathbf{r}_i - \mathbf{r}_j|)}{\partial \mathbf{r}_i} \frac{\partial F_{s+1}(t, \mathbf{r}_1, \dots, \mathbf{r}_s, \mathbf{r}_j, \mathbf{p}_1, \dots, \mathbf{p}_s, \mathbf{p}_j)}{\partial \mathbf{p}_i} d\mathbf{r}_j d\mathbf{p}_j + \\ & + \frac{1}{V^{s+1}} \sum_{s+1}^N \int \frac{\mathbf{p}_j}{m} \frac{\partial F_{s+1}(t, \mathbf{r}_1, \dots, \mathbf{r}_s, \mathbf{r}_j, \mathbf{p}_1, \dots, \mathbf{p}_s, \mathbf{p}_j)}{\partial \mathbf{r}_j} d\mathbf{r}_j d\mathbf{p}_j \\ & + \frac{1}{V^{s+1}} \sum_{i=1}^s \sum_{j=s+1}^N \int \frac{\partial \Phi(|\mathbf{r}_i - \mathbf{r}_j|)}{\partial \mathbf{r}_j} \frac{\partial F_{s+1}(t, \mathbf{r}_1, \dots, \mathbf{r}_s, \mathbf{r}_j, \mathbf{p}_1, \dots, \mathbf{p}_s, \mathbf{p}_j)}{\partial \mathbf{p}_j} d\mathbf{r}_j d\mathbf{p}_j \\ & + \frac{1}{2V^{s+2}} \sum_{\substack{i,j=s+1 \\ (j \neq i)}}^s \frac{\partial \Phi(|\mathbf{r}_i - \mathbf{r}_j|)}{\partial \mathbf{r}_i} \frac{\partial F_{s+2}(t, \mathbf{r}_1, \dots, \mathbf{r}_s, \mathbf{r}_j, \mathbf{p}_1, \dots, \mathbf{p}_s, \mathbf{p}_j)}{\partial \mathbf{p}_j} d\mathbf{r}_i d\mathbf{r}_j d\mathbf{p}_i d\mathbf{p}_j \end{aligned}$$

Usually we suggest that for $|\mathbf{r}_j| \rightarrow \infty$, $\frac{\partial F_n}{\partial \mathbf{r}_j} \rightarrow 0$, $|\mathbf{p}_j| \rightarrow \infty$, $\frac{\partial F_n}{\partial \mathbf{p}_j} \rightarrow 0$.

There are: t —time, r —coordinate, p —momentum, ρ —density, Φ —potential of molecules interaction. The last three terms are equal to zero at indicated conditions. For nonequilibrium case spatial derivatives do not equal to null. It does not equal to null in case, as example for interaction blowing gas from the surface with nonequilibrium gas of flow near the body. For the enumerated cases particles are not pairwise permutable and we do not have sum. Besides the flows of molecules have to include as the boundary conditions.

$$\begin{aligned} & \int \sum_{i=s+1}^s \frac{\partial \Phi_{ij}}{\partial \mathbf{r}_i} \frac{\partial F_{s+1}(t, \mathbf{r}_1, \dots, \mathbf{r}_s, \mathbf{r}_j, \mathbf{p}_1, \dots, \mathbf{p}_s, \mathbf{p}_j)}{\partial \mathbf{p}_i} d\mathbf{r}_j d\mathbf{p}_j \\ & \approx N \int \frac{\partial \Phi_{is+1}}{\partial \mathbf{r}_i} \frac{\partial F_{s+1}}{\partial \mathbf{p}_i} d\mathbf{r}_{s+1} d\mathbf{p}_{s+1} \end{aligned}$$

As a result of the change of angular momentum for the given points in time we have in the following way.

The new Boltzmann equation is

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{c}_i \left[\frac{\partial f}{\partial \mathbf{r}_i} \right] + \mathbf{c}_i \left[\mathbf{r}_{ij} \frac{\partial f}{\partial \mathbf{r}_i} \right] - \frac{\mathbf{F}}{m} \frac{\partial f}{\partial \mathbf{c}_i} = I.$$

Here I—collision integral.

We can suggest the new formulation of some macrovalues (temperature, stress tensor, flow heat): in

calculate the change in angular momentum at any point. The new N. N. Bogolubov equation is

classic theory [11-15]

$$\frac{3}{2} k T = \frac{1}{n} \sum_k \int \frac{m_k c^{k2}}{2} f_k d\boldsymbol{\xi}_k, \quad (n = \sum_{k=1}^N n^k),$$

here k —number of components, T —temperature, $c^k = \boldsymbol{\xi}_k - u$, one's velocity of molecules, $\boldsymbol{\xi}_k$ velocity of molecules. Another definition is

$$\frac{3}{2} k T = \frac{\int \left(\sum_k \frac{n_k}{n} m_k \right) \left(\sum_k \frac{n_k}{n} c_k \right)^2 f d\boldsymbol{\xi}}{2}$$

Then we have one term is traditional and another is as the second viscosity. For stress tensor we can have

$$P_{ij} = \int \left(\sum_k \frac{n_k}{n} m_k c_k \right)_i \left(\sum_k \frac{n_k}{n} m_k c_k \right)_j f d\boldsymbol{\xi}$$

For the flow of the heat

$$\mathbf{q} = \int \left(\sum_k \frac{n_k}{n} c_k \right) \left(\sum_k \frac{n_k}{n} m_k \right) \left(\sum_k \frac{n_k}{n} c_k \right)^2 / 2 f d\boldsymbol{\xi}$$

What we take in experiment?

$$f_v^{(0)} = n^v \left(\frac{m}{2\pi k T} \right)^{3/2} \exp \left(-\frac{m}{2kT} c^v \right)$$

or for exclusive temperature

$$f_v^{(0)} = n^v \left(\frac{m}{2\pi k T^v} \right)^{3/2} \exp \left(-\frac{m}{2kT^v} c^v \right).$$

For full temperature we cannot conclude the right probability.

The highest probability—transitions with a change in the quantum number by one

$a_{v\mu}^{v+1,\mu} = a_v^{v+1}$. Deactivation process is

$$a_v^{v-1} = a_{v-1}^v \exp\left(\frac{\Delta E^v}{kT}\right). \text{ In my opinion } a_v^{v-1} = a_{v-1}^v \exp\left(\frac{\Delta E^v}{kT^{v-1}}\right).$$

For the internal energy remains the old equation, but with modified temperature value.

4. Results of Interaction of Two Homogeneous Flows

The simplest interaction is that two homogeneous flows move in the same direction at different speeds. The classical formulation proposed in Ref. [16]. Fig. 1 explains the problem.

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. The problem was solved by student of fourth-year A. G. Garaev. The problem is on the singularity. Two singularities dictate (the boundary conditions are set at infinity) a non-standard method of solution.

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

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0.$$

This task does not keep the parameters with dimensions length or time. So this task is self-similar. Once we have the dimensionless equations

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

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

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 $\psi^* = \sqrt{\mu/U_1} \psi, y_1 = 1/2\sqrt{\mu/U_1} \eta$.

Then we have

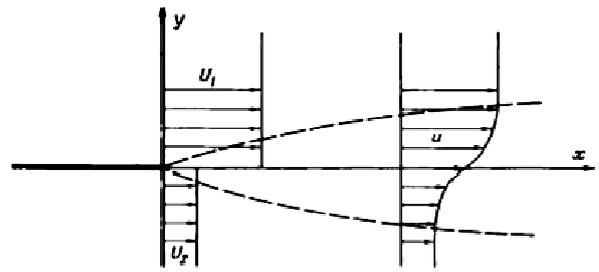


Fig. 1 The overall picture of the interaction of two streams.

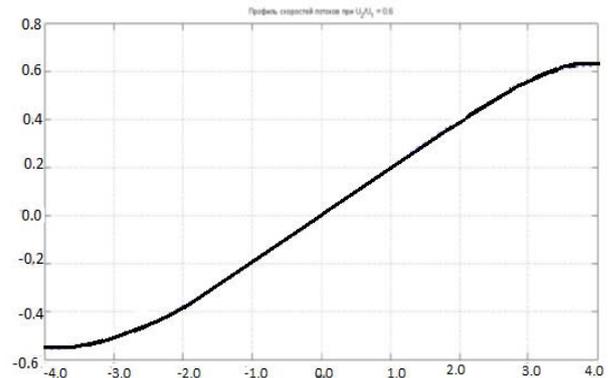


Fig. 2 Stream interaction painting, $\frac{U_2}{U_1} = 0.6$.

$$2\eta\psi'''' + 2\psi'''' + \psi\psi'' = 0$$

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. for $x = 10.0.0$. If comparison solutions for Falkner-Scan and this we see that without perturbations on boundary solutions little different from classic solutions.

5. Conclusions

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 built. The results of the numerical solution of the modified problem of interaction of two parallel streams moving in the same direction are given. The main conclusions are: influence of angular momentum can be great under big gradients physical parameters and gives nonsymmetrical of the stress tensor; delay plays role for discrete medium; it is necessary to take into attention the moving of inertia centre.

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