Influence dispersion in gas and solid for moving body

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Abstract

The purpose of this work is development of more full mathematical model for continuous mechanics and rarefied gas for great gradients. It is devoted to the influence of consideration an angular momentum variation in an elementary volume. Conjugated conditions at surface without the Knudsen layer are written to count friction and heat flow to the surface by solution the Boltzmann equation without collision integral in thin layer and by solution. We considered different aspect of interaction gas O_2 with solid structure (aluminium-oxide film on aluminium substrate) with different potential. As example for solid the beams under different conditions are investigated.

1.Introduction

Many experimental facts tell us about the importance of an angular momentum variation in an elementary volume and cross flux on it's sides. There are: rolling up of nano-tubes, twisting of the thin jets, rolling up of thin film and etc. Some effects of the influence of the variation the angular momentum in an elementary volume for gas, liquid and solid mechanics was studied in our previous papers. The asymmetric press tensor was obtained. It can be essential for theory of turbulence and the theory of cracks. The degree of asymmetric stress tensor we received from momentum equation (in projections). For a rigid body the equations are used of the phenomenological theory, but changed their interpretation. We elucidate the contribution of cross-effects in the conservation laws of continuum mechanics, including the self-diffusion, thermal diffusion, etc., which indicated S. Wallander. Resolved the paradox of Hilbert in the solution of the Boltzmann equation by the Chapman-Enskog method. Refined model of the boundary conditions for rarefied gas flows and transient flow near the moving surfaces. We establish conditions for the existence of the A.N. Kolmogorov inertial range on the basis of the proposed theory.

Usually the problem of the inertial N. A. Kolmogorov region in boundary layer is analyzed for a linear velocity. This velocity can be only near surface but there the velocity is small; so this region far from surface in big vortex. Our model tell us about logarithm profile for boundary layer for inertial region. Gas-surface interaction plays an essential role in processes connected with atmosphere re-entry vehicles. It is necessary to know aerodynamic characteristics. These conditions are known badly for rarefied gas and for turbulence streams [1-27] To solute the Boltzmann equation is more difficult than Navier-Stokes equations. So better to solute Navier-Stokes equations. Usually for the classical case near the surface the Knudsen layer is considered [23]. This layer has the length of order of free path. M. Lunc, J. Luboncki, V.C.Liu , R.G. Patterson, W. Bule, F.O.Goodman, H.Y.Wachman, R G. Barantsev, Yu. A.Ryzhev, G.V. Dubrovskii and the others investigated the interaction molecules with surface. At present majority experimental and theoretical results were received for dispersion of monovelocity beam of atoms. Another type of works are investigation of nanostructures, but we do not discuss this problem. We discuss the problems that can be appearing to considerate the classic theory of continuous mechanics because of the symmetry of the stress tensor. In general case the equilibrium conditions of forces are the special case of more common conditions of equilibrium for angular momentum. From these an asymmetric tensor followed. The aim of this paper is to give phenomenological method of deriving the modified equations, previously obtained from the kinetic theory. Explain the loss of continuity of the environment in the classical description with large gradients of physical quantities. Some examples are provided. For gas the equation for the angular momentum was received from the modified Boltzmann equation. The modified laws of conservation were received for the particles without structure. The order of the new equations (for the density and for the linear momentum, energy) is more than in classical case. If we deal with continual medium the external boundary condition for boundary layer can be determined as the value of rotor velocity or as of value normal velocity. That is for the vertical velocity. For the longitudinal velocity it is need to put friction. In turbulence layer we need to set a friction too [24,25]. For the rarefied gas the boundary conditions would be included the value gas flow besides the classical boundary conditions. At present the theory of description turbulence does not clear in spite of existence a large number theories. Usually we consider the following theory for turbulence streams: Direct Numericl Simulation, Large Eddy Simulation, Reynols-Averaged Navie-Stokes and some others. In the previous papers we investigated numerically and analytical method the modified Blasius problem, the Falkner-Skan problem, the flow near infinite plate. The formation of new structures were discovered at external boundary. Gas-surface interaction plays an essential role. Conjugated conditions at surface without the Knudsen layer are written to count friction and heat flow to the surface by solution the Boltzmann equation without collision integral in thin layer and by solution the Navie-Stokes equations with addition new terms. We considered different aspect of interaction gas O_2 with solid structure (aluminium-oxide film on aluminium substrate) with different potential. As example for solid the beams under different conditions are

investigated. For great velocity the film of Al_2O_3 partly is blowing. We considered different aspect of interaction gas O_2 with aluminium plate. Computer simulation by molecular dynamic method of nonequilibrium gas and surface molecules interact in little region (12 angstrom) near surface. We investigate the different potential. The distribution function is reconstructed. We considered the long tail of distribution function on process of taking out molecules from surface.

2. Continuous mechanics

The modified equations were received from the kinetic theory. The issue arose when writing the law of conservation of density. Try to get it out of the equation is principles of fenomenological. The equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} + \frac{\partial}{\partial x_i}\left(x_i \frac{\partial \rho u_i}{\partial x_i} \right) = 0.$$

The figure 1 shows that the linear velocity $v = \omega \times (r \wedge' -r)$ is the velocity with respect to M for kvazi-solid movement around axis without div ϱu. The point M may itself be involved in the rotation. For an elementary volume $v = \omega \times (r \wedge' -r)$ formula means a rotation around the axis of

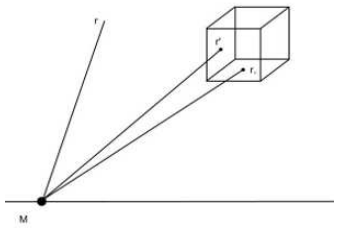

Fig.1

the velocity at centre of inertia but axis of moving of elementary volume can be lie outside it. So we have for twisting an elementary volume

$$\int_{(s)} (\nabla \rho \boldsymbol{u}(\boldsymbol{r}' - \boldsymbol{r_c}))_n ds = \int_{(s)} div(\nabla \rho \boldsymbol{u})(\boldsymbol{r}' - \boldsymbol{r_c}) dv$$

Our results can be summarized as follows for all continuous mechanics : in phenomenon theory we have four equilibrium equations but if we choose equilibrium of force the three equilibrium equations and symmetric tensor are received; so our interpretation bases on traditional theory. The degree of asymmetric stress tensor we can received from momentum equation (in projections nonsymmetric tensor τ is indicated) .

$$x\left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z\left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \tau_{zx} - \tau_{xz} = 0$$

$$x\left(\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) - y\left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} \right) + \tau_{yx} - \tau_{xy} = 0$$

$$y\left(\frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \right) - z\left(\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{zy}}{\partial z} \right) + \tau_{zy} - \tau_{yz} = 0$$

For elasticity theory equations did not change but were proposed another interpretation and added the angular momentum equation to the classic equations. Now for consideration of angular momentum the theory of brothers E.,Cossssrat, F. Cosserat and their modifications are used. Their theory contains additional constant with dimension of length that determined from experiments. The main task of our work is closer definition of model for continuous mechanics. Early we suggested to include angular momentum in the Boltzmann equation, Navie-Stokes equations and in the theory of elasticity. Now we do accent at examples. If we write equations for stress values of elasticity theory we have six unknown quantities and three equations in classical case. In our case we add the equation for angular momentum but we have nine unknown quantities. As a result we have old situation. We suppose that only possible solution we can receive using the classical supposition. Consequently we need to add equations to write the geometrical and physical property.

3. Examples. Beams.

Now consider four educational problems for long beam. The first is beam under longitudinal force. Suggested that $\sigma_x = \sigma_y = \tau_{xy} = 0$,

$\sigma_z = \sigma_0 = \frac{N}{\epsilon} = \text{const}; \quad \tau_{yz} = \tau_{zx} = 0.$

There are three angular momentums are equal to zero. So new way the problem do not new results. The second is clean curve.

$\sigma_z = ax + by, \quad \tau_{zy} = \tau_{zx} = 0.$

$N = 0, \quad M_x = M_z = 0.$

There are angular momentums are equal to zero. Consequently the laws of forces are fulfill as in this case all three laws of force's balance must be equal to zero. For problem about transverse beam gives same results as for the second case. But for problem about twisting of the primate beam we have another solution $\tau_{xy} = f(z)$ besides classic solution ($\sigma_x = \sigma_y = \sigma_z = \tau_{xy} = 0$). This result we have as two angular momentums are equal to zero.

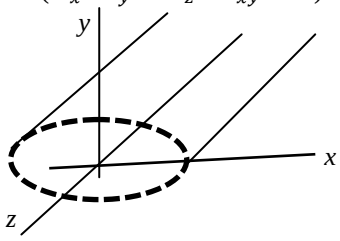

Fig. 2

Consider the Lame and Kirsha problems. In the first problem loading on the sides is steady. So momentum can be only in corner. For the same loading on all sides angular momentum does not work, but for different loading momentum work and added strength will be activity. The result is raising ore go down. For the second problem besides the corner's effects we have momentum near the axis z. So at cross of the circle and axis y we have added forces that have the direction of the stress on side. So new way a problem do not new results. The second is clean curve.

$\sigma_z = ax + by, \quad \tau_{zy} = \tau_{zx} = 0.$

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There are angular momentums are equal to zero. Consequently the laws of forces are fulfill as in this case all three laws of force's balance must be equal to zero. For problem about transverse beam gives same results as for the second case. But for problem about twisting of the primate beam we have another solution $\tau_{xy} = f(z)$ besides classic solution ($\sigma_x = \sigma_y = \sigma_z = \tau_{xy} = 0$). This result we have as two angular momentums are equal to zero.

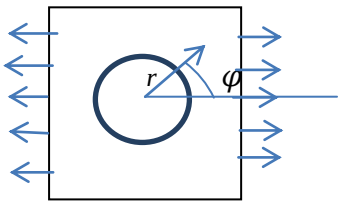

Fig. 3

Consider protozoa another tasks about beam. Closer definition of equilibrium will be obtained if angular momentum would take into attention.

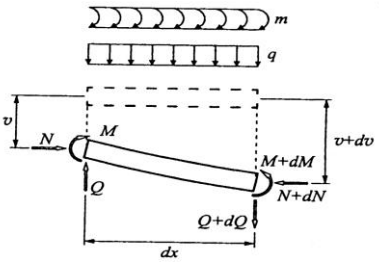

Fig.4 Elementary area of beam

$$dM - Qdx - mdx - Ndv = 0,$$

$$dQ + qdx = 0, \qquad Q'+q = 0.$$

$$M'-Q-m-Nv'=0, \qquad -M''=q-m'-(Nv')'.$$

Now

$$-M'' = q - m' - ((Nv)')'.$$

For this problem the solution for general case and without *N'* (for *N=Const*) is the same. Consequently we can choose the beam of variable cross-section. For beam on elastic foundation results distinguish. For another problem the solutions can be different too.

In case of transmission pressure at beam by intermediate designs of external force *P* (fig. 5) passes through hard lever of length a which can twist around hinge.

$H = \frac{P}{\cos\alpha}$. Here *H*-normal force in hard hinge.

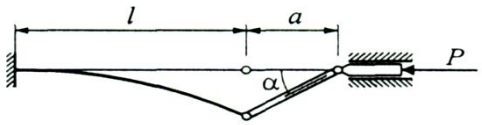

Fig .5

At the end of elastic beam transfers force is *Q=H sin α. As tg α = υ (l)/a* at l we have in classic case

$$Q = H\sin\alpha = N\mathrm{tg}\alpha$$

$$EIv'''(l) + N\left[v'(l) + \frac{v(l)}{a}\right] = 0$$

Now

$$EIv'''(l) + (Nv)' + \frac{P}{\cos\alpha}\frac{v(l)}{Q} = 0$$

So we have at end of length

$$v(0) = 0 \Rightarrow C_1 + C_4 = 0$$

$$v'(0) = 0 \Rightarrow C_2 + kC_3 = 0$$

$$M(l) = 0 \Rightarrow v''(l) = 0 \Rightarrow C_3\sin\nu + C_4\cos\nu = 0 \cdot$$

$$v'''(l) + k^2v'(l) + k^2v(l)/a = 0 \Rightarrow C_1 + C_2(l+a) + C_3\sin\nu + C_4\cos\nu = 0 \cdot$$

Now

$$EIv'''(l) + (Nv)' + \frac{P}{\cos\alpha}\frac{v(l)}{Q} = 0$$

4. INFLUENCE DISPERSION NEAR THE SURFACE

The problem for moving gas near the surface has some singularities. To solute the Boltzmann equation is more difficult than Navier-Stokes equations. So better to solute Navier-Stokes equations. We can build the boundary conditions by using the Chapman-Enskog distribution function with macroparameters from the solution of the Navier-Stokes equations at distance some radius interaction from body. In our case the equation for two-part distribution function near the surface is

$$\frac{\partial f_2}{\partial t} + \sum_{i=1}^{2}\left\{\xi_i\cdot\left[\frac{\partial f_2}{\partial x_i}\right] + \xi_i\cdot\frac{\partial}{\partial x_i}\left[x_j\frac{\partial f_2}{\partial x_j}\right] - \frac{X_i}{m}\frac{\partial f_2}{\partial \xi_i}\right\} + \mathbf{X}_{12}\cdot\frac{\partial f_2}{\partial \xi_1} + \mathbf{X}_{21}\cdot\frac{\partial f_2}{\partial \xi_2} + X_{22}\frac{\partial f_2}{\partial \xi_2} = 0\,.$$

Integrating in ξ we obtain the equation for one-particle distribution function with interaction force gas molecule with surface molecules. Suggested algorithm is easily than classical. For $\xi 2$ = 0 in solid body (without movement of the surface molecules) we have trajectory problem. The usual of computer simulation by molecular dynamic method is used.

To simulate the interaction gas with the crystal surface method has been applied molecular dynamics (MD), based on the solution of the Newton's equations [38]. In the first stage of modeling is the initial distribution of particles in space (spatial configuration of the crystal structure and the gas phase) and initial distribution of particle velocities corresponding to the mechanical and thermal motion of the system in the initial state. The generation of initial conditions occurs at the macro and micro levels. At the macroscopic level, wondered the geometric dimensions of the area in which calculations were carried out (L_x, L_y, L_z) and the macroscopic velocity. The macroscopic velocity means directional velocity of the gas stream. Packing particles structure (fcc lattice of the crystal surface) and the velocity distribution of the thermal motion of gas particles and the crystal structure considered at the microscopic level. The thermal velocity distribution at the initial time is generated according to the Maxwell distribution

$$f(v) = \frac{4}{\sqrt{\pi}}\left(\frac{m}{4kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}},$$

where m is mass of atom, k is Boltzmann constant and T gas temperature. The rate of gas particles at the initial moment of time is made up of directed macroscopic velocity and thermal velocity. The second stage computes the values of the coordinates and velocities of particles (describing the evolution of the system over time), which were carried out using the MD equations of motion integration algorithms with predetermined conditions based on the scheme Varlet [38]. The time step was chosen to be 5 *fs*, which is comparable with the period of molecular vibrations of the lattice. The trajectories of the particles were calculated in a macroscopic ensemble under the thermodynamic conditions: constant number of particles, constant volume and constant temperature. The constancy of temperature in the system provides an introduction Noze-Hoover thermostat [39]. The number of gas particles was chosen to be 25, which corresponds to the pressure 1 *atm* in the computational volume 10^6 *ang.* at 290 *K*. The number of particles in the structure of the computational domain is chosen equal to 10000. In this paper, the interaction between particles of type structure-structure described by a Morse potential [40]

$$U(r_{ij}) = D_0\left[e^{-2\alpha(r-r_0)} - 2e^{-2\alpha(r-r_0)}\right]$$

Where r_0 is the equilibrium internuclear separation and D_0 The well depth, is the dissociation energy of the molecule,α is an adjustable shape parameter. For aluminium-oxide film (Fig.6) were used CTIP+MEAM which described in [41]. For particles such as gas-gas and gas-structure described by Lennard-Johnes Potential

$$U(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

Where ε is well depth ε is affective atom diametr. The potential parameters for the structure of the gas-particles were calculated using the formula [38]

$$\sigma_{gs} = \frac{\sigma_s + \sigma_s}{2}$$

And

$$\varepsilon_{gs} = \sqrt{\varepsilon_g + \varepsilon_s}$$

The radius of the particle interaction is chosen to be 2.5 of the lattice constant of the crystal structure. Due to the limited computing resources the distribution function of gas particles is divided into a region of the velocities. For each region MD calculation was processed and distribution function was reconstructed (Fig.7). Some particles due to the directional velocity received energy that enough to penetrate into the crystal structure (Fig. 8).

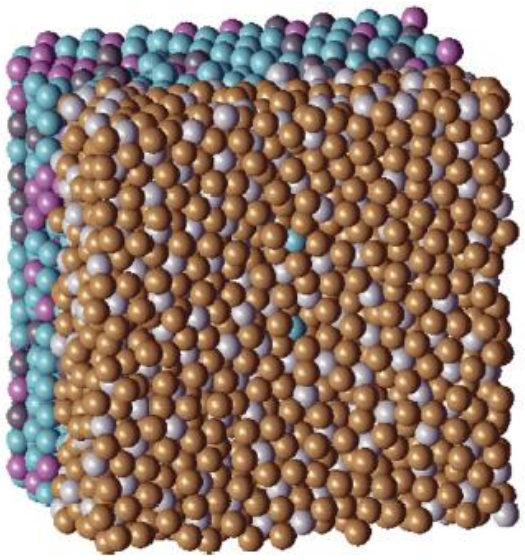

Figure.7 Aluminium-oxide film on aluminium substrate

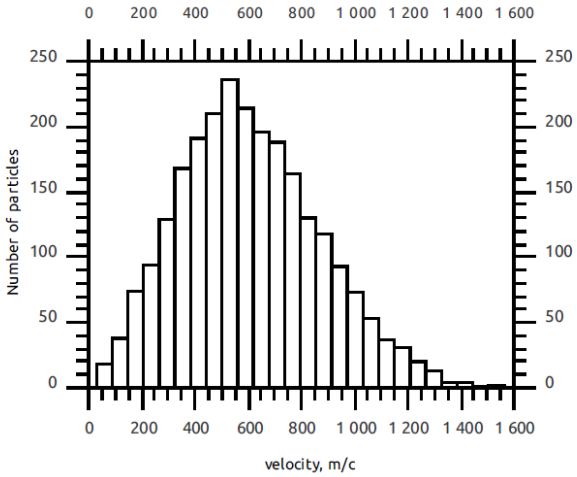

Figure.7 Gase distribution function

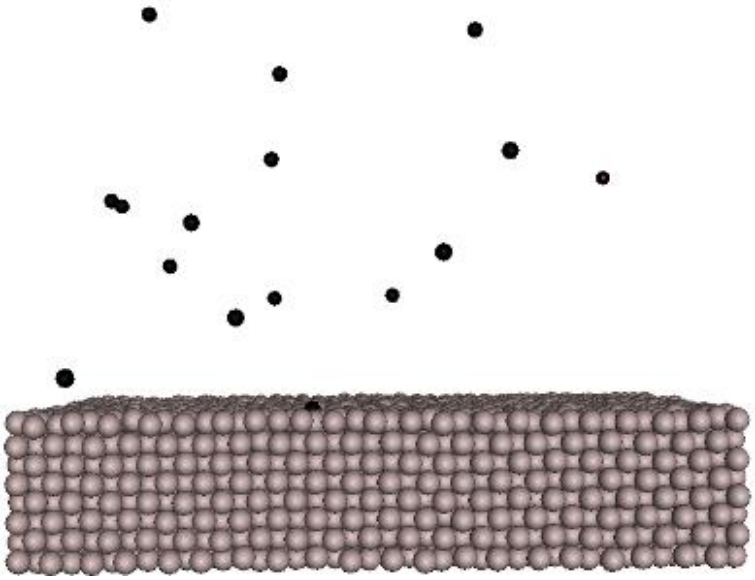

Figure.8 Penetration atom into crystal structure

5. Conclusion

We discuss the problems that can be appearing to consider the angular momentum variation in an elementary volume near the surface and influence the cross flows through the sides of an elementary volume for great gradients of the physical values. The main attention gave to concrete examples. The beams under the different conditions are investigated. We considered different aspect of interaction gas O_2 with aluminium plate with film of Al_2O_3. The molecular dynamic method is used.

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