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THE STRUCTURE-PHENOMENOLOGICAL STUDY OF TWO-PHASE LIQUID SYSTEMS

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Abstract The structure-phenomenological theory of stress state in arbitrary gradient flows of dilute suspensions of ellipsoidal particles with the Newtonian carrier fluid is constructed. The use of the dynamical method of Landau in the structural part of the theory allows us to obtain general rheological equation of such suspensions before the examination of rotational dynamics of suspended particle in gradient flows of the suspension carrier fluid. As an illustration, the dilute suspension of Brownian ellipsoidal particles is studied. Dynamics of suspended particles in such a suspension is defined not only by hydrodynamical forces but also by rotational Brownian motion. The obtained rheological equation of such a suspension is used to study its rheological behaviour in a simple shear flow. As a result, it is proved that such a suspension behaves as an elasticoviscous fluid presenting the effect of Weissenberg and pseudoplastic dependence of suspension effective viscosity on the rate of shear.

1. INTRODUCTION

Advances in mathematical modelling of the flow of liquid media depend to a large extent on the correct choice of their models. Such a choice essentially depends on the structure of a real liquid medium and on its properties.

This paper describes the procedure of application of structure phenomenological approach proposed for the first time in [1, 2] to study two-phase liquid systems. To this aim, we derive the constitutive equations for stress in dilute suspensions of rigid axially symmetric elongated particles with a Newtonian carrier fluid.

As a model of suspensions, we use a structure continuum with two internal microparameters, namely the orientation vector and vector of the relative angular velocity of suspended particles. According to [1, 2], the constitutive rheological equation for stress which arise in gradient flows of suspensions is postulated phenomenologically. Its phenomenological rheological constants are found theoretically using the results obtained within the framework of structural studies of suspensions by application of the Einstein energy method [3] or Landau dynamic method [4].

The fundamentals of the structure-phenomenological approach are presented in Sec.1 of this paper to the study of the dilute suspension of uniaxial dumbbells. The choice of such a very schematic hydrodynamic model of suspended particles makes possible to describe concisely and adequately the procedure of application of the structure-phenomenological approach with the use of energy method of Einstein [3] to its structural part.

In Section 2 combining the results derived phenomenologically with the results obtained in the structural part of study by the use of dynamical method of Landau [4] gives the possibility to construct for the first time the general rheological equation for dilute suspension of ellipsoidal particles before the examination of the rotational dynamics of suspended particles in gradient flows of suspensions.

The structure-phenomenological method proposed in [1, 2] was approbated by its repeated use to derive rheological equations for dilute suspensions of axisymmetric model particles of any models used in the structural rheology of suspensions, angular position of which can be described uniquely by a single unit vector [5]. In this paper, the approbation of this method is illustrated by identical coincidence of rheological equation for dilute suspension of Brownian ellipsoidal particles obtained in Section 3 with corresponding rheological equation obtained in [6] by another method.

2. FUNDAMENTALS OF STRUCTURE PHENOMENOLOGICAL STUDY OF DILUTE SUSPENSIONS

Dilute suspensions of axisymmetric undeformable particles are considered in the paper to describe the structure-phenomenological method to study two-phase liquid systems. It is assumed that: 1) the suspended particles are rigid, and have the same form and dimensions; 2) the characteristic dimension d of suspended particles is much less than the characteristic length $\bar{l}$ of the suspension macroflow region but it is much longer than the characteristic dimension l of molecules of the Newtonian carrier fluid of the suspension, i.e.

$$l << d << \bar{l}; \tag{1}$$

3) no-slip condition holds on the surface of suspended particles; 4) the motion of the carrier fluid with respect to the suspended particles is slow; 5) the volume concentration of suspended particles is small; suspension is diluted; 6) suspended particles possess zero buoyancy.

In the structural part the interaction of suspended particles with an arbitrary gradient flow of the Newtonian carrier fluid is considered. The concepts of the Einstein energy method employed in the first structural rheological study of dilute suspension of beads [3] and results obtained by Kuhn & Kuhn [7] in their structural rheological studies of dilute suspension of uniaxial dumbbells are used. The hypothesis $l << d$ and property 3 allow us to consider such an interaction as a hydrodynamic one. For the sake of simplicity, in this section the uniaxial dumbbell with undeformable axis of length L is used as a hydrodynamic model of suspended particles. It is assumed that the dumbbell axis exhibit no hydrodynamic resistance, and dumbbell pointlike centers of hydrodynamic interaction, which are placed at the ends of the axis, interact with the carrier fluid as a spherical particles (beads) of radius $\overline{a}$. This means that, if the ends of the dumbbell axis are flown around by the Newtonian carrier fluid with velocities $U_i^{(k)} (k = 1, 2)$, these ends are subject to forces $\xi U_i^{(k)} (k = 1, 2)$ exerted by the carrier fluid, where $\xi = 6\pi\mu\overline{a}$.

It is assumed that the suspension is diluted to such an extent that the direct interaction between suspended particles, and the hydrodynamic interaction between them through the carrier fluid, may be neglected.

The above-mentioned assumptions lead to the resultant vector F_i and moment $M_i^{(hf)}$ of the hydrodynamic forces acting on the dumbbell as

$$F_i = -2\xi v_{0i}, \tag{2}$$

$$M_i^{(hf)} = (1/2)\xi L^2 \varepsilon_{ijk} n_j (d_{ks} n_s - N_k), \tag{3}$$

where (3), $d_{ks} = (1/2)(v_{k,s} + v_{s,k})$, $N_k = \dot{n}_k - \omega_{km} n_m$, $\omega_{km} = (1/2)(v_{k,m} - v_{m,k})$.

The inertia forces and their moments are usually neglected in the rheology of suspensions.Because of this, the equations of motion of the uniaxial dumbbell under the action of hydrodynamic forces are

$$F_i = 0, \tag{4}$$

$$M_i^{(hf)} = 0. \tag{5}$$

Then (2) and (4) imply that the translational velocity v_{0i} of a suspended particle with respect to the carrier fluid is equal to zero, i.e. the suspended particles execute only a rotary motion. The equation of the rotary motion of the dumbbell particles

$$d_{ik} n_k - d_{km} n_k n_m n_i - N_i = 0 \tag{6}$$

is obtained by the vector product of (5) by n_i and taking into account (3).

In the framework of this structural part, the rate of mechanical energy dissipation per unit volume of the suspension

$$\Phi = 2\mu d_{km} d_{km} + n_0 (\xi L^2/2)(\langle N_i N_i \rangle - - 2 d_{ij} \langle N_i n_j \rangle + d_{ij} d_{ik} \langle n_j n_k \rangle) \tag{7}$$

is computed too. The first term in (7) is the rate of mechanical energy dissipation per unit volume of the Newtonian carrier fluid of the suspension in the absence of suspended particles, while the second one is the rate of the mechanical energy dissipation on flowing around beads of n_0 model suspended particles contained in the unit volume of the suspension, which is calculated by the formula $n_0 \xi \sum_{k=1}^{2} \langle U_i^{(k)} U_i^{(k)} \rangle$.

Transition from microcharacteristics of a separate suspended particle to macrocharacteristic of suspension in (7) takes place during averaging of the function Φ over elementary volume of the suspension containing a sufficiently large number of suspended particles. In (7), the result of the spatial averaging is presented. The angular brackets $\langle\rangle$ in (7) denote the averaging which yet should be made in the phase space of coordinates of the orientation vector n_i of suspended dumbbell particles with the use of the distribution function F of the angular positions of the vector n_i, which satisfies the equation

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial n_i}(F\dot{n}_i) = 0. \tag{8}$$

In order to construct the rheological equation for stress in the suspension of dumbbell particles within the framework of structure-phenomenological approach, such a suspension should be modeled by a structural continuum. The possibility of such modeling is provided by the hypothesis $d << \bar{l}$. Analysis of the results obtained in this structural part of the present study allows us to choose the orientation vector n_i of suspended dumbbell particles and vector N_i defining their relative angular velocity with respect to the suspension carrier fluid as internal microparameters of the structural continuum modeling the considered dilute suspension. The form of the phenomenological rheological equation for stress T_{ij} in the suspension

$$T_{ij} = t_{ij} + n_0\langle\tau_{ij}(d_{km}; n_l; N_p)\rangle \tag{9}$$

is determined by the structure of the expression for the rate of mechnical energy dissipation per unit volume of the considered suspension defined by (7). The averaging in (9) denoted by the brackets $\langle\rangle$ should be carried out as in (7) in the space of coordinates of the orientation vector n_i of suspended dumbbell particles with the use of the distribution function F, which satisfies (8). The term t_{ij} is the stress arising in gradient flows of the Newtonian carrier fluid of suspension in the absence of suspended particles. The other term in (9) is the stress caused by the presence of n_0 suspended particles per unit volume of the suspension. Taking into account that uniaxial dumbbell is symmetric with respect to the center of the axis L, the function τ_{ij} has not to change its sign while replacement of n_i by $-n_i$. This property defines the final form of arguments of the function τ_{ij}: d_{km}; $n_l n_q$; $N_p n_l$.

The explicit form of the phenomenological function τ_{ij} can be determined by comparing the expression for the rate of mechanical energy dissipation per unit volume of the suspension, provided by formula [8]

$$\Phi = t_{ij}d_{ij} + n_0\langle\tau_{ij}\rangle d_{ij} + n_0\langle N_i\varepsilon_{ijk}n_j M_k^{(hf)}\rangle, \tag{10}$$

with the expression (7), obtained within the framework of the structural approach. It follows that τ_{ij} should be a polynomial of its arguments, linear in

d_{km} and N_p, namely

$$\tau_{ij} = (\mu_0 + \mu_1 d_{km} n_k n_m)\delta_{ij} + \mu_2 n_i n_j + \mu_3 d_{km} n_k n_m n_i n_j$$
$$+\mu_4 d_{ij} + \mu_5 d_{ik} n_k n_j + \mu_6 d_{jk} n_k n_i + \mu_7 n_i N_j + \mu_8 n_j N_i,$$

derived by using results obtained in [9].

Taking into account that $t_{ij} = -p\delta_{ij} + 2\mu d_{ij}$, from (9) it follows that the stress tensor T_{ij} in the dilute suspension of dumbbell particles should be defined by the phenomenological rheological equation

$$T_{ij} = -p\delta_{ij} + 2\mu d_{ij} + n_0(\mu_0 + \mu_1 d_{km}\langle n_k n_m\rangle)\delta_{ij}$$
$$+\mu_2\langle n_i n_j\rangle + \mu_3 d_{km}\langle n_k n_m n_i n_j\rangle + \mu_4 d_{ij} \tag{11}$$
$$+\mu_5 d_{ik}\langle n_k n_j\rangle + \mu_6 d_{jk}\langle n_k n_i\rangle + \mu_7\langle n_i N_j\rangle + \mu_8\langle n_j N_i\rangle,$$

where the unknown phenomenological constants $\mu_i(i = \overline{0,8})$, obtained from term-by-term comparison of (7) and (10), are

$$\mu_o = \mu_1 = ... = \mu_4 = \mu_6 = \mu_7 = 0, \quad \mu_5 = -\mu_8 = \xi L^2/2.$$

with due regard for the formula $\langle \tau_{ji} n_j\rangle - \langle \tau_{ij} n_j\rangle = \langle \varepsilon_{ijk} n_j M_k^{(hf)}\rangle$ [8]. Then, (11) becomes

$$T_{ij} = -p\delta_{ij} + 2\mu d_{ij} + n_0(\xi L^2/2)(d_{ik}\langle n_k n_j\rangle - \langle n_j N_i\rangle). \tag{12}$$

Equations (12), (8) and (6) form the closed set of equations defining the stress state in the dilute suspension of dumbbell particles, the rotary motion of which is determined solely by hydrodynamic forces. When the dynamics of suspended particles is defined in addition by other forces, (6) ought to be changed [10].

3. GENERAL RHEOLOGICAL EQUATION FOR DILUTE SUSPENSIONOF ELLIPSOIDAL PARTICLES

The rheological equation (11) is phenomenological. It can be generalized as

$$T_{ij} = (a_0 + a_1 d_{km}\langle n_k n_m\rangle)\delta_{ij} + a_2\langle n_i n_j\rangle + a_3 d_{km}\langle n_k n_m n_i n_j\rangle + a_4 d_{ij} \tag{13}$$
$$+a_5 d_{ik}\langle n_k n_j\rangle + a_6 d_{jk}\langle n_k n_i\rangle + a_7\langle n_i N_j\rangle + a_8\langle n_j N_i\rangle,$$

where a's are new phenomenological rheological coefficients.

The equation (13) can be used instead of (11) to obtain (12). Phenomenological coefficients a's are found similar to the coefficients μ's in (11).

In [5] it was proved that (13) is notable by the fact that it is a phenomenological rheological equation for dilute suspensions of axisymmetric model particles of any models used in the structural rheology of suspensions, angular position of which can be described uniquely with a single unit vector n_i. In this section (13) is used to obtain the general rheological equation for dilute suspension of axisymmetric ellipsoidal particles with axis of symmetry $2a$ and equatorial diameter $2b (a > b)$. Due to the use of the Landau dynamic method [4], instead of the Einstein energy method [3] in the structural part of present theory, the phenomenological coefficients a's in (13) are determined theoretically before the examination of the rotational dynamics of suspended ellipsoidal particles in gradient flows of suspension.

According to [2], first we find the stress tensor σ_{ij} in the carrier fluid of suspension on the surface of the sphere S surrounding an ellipsoidal suspended particle, the center of which coincides with the center of particle and radius R considerably exceeds its dimensions. The use of the Jeffery results [11], who found disturbances of flow of the Newtonian carrier fluid induced by an ellipsoid suspended in it, allows us to determine the stress σ_{ij} on the surface of the sphere S in moving coordinate system $Ox_1x_2x_3$ with axes Ox_1, Ox_2, Ox_3 coinciding with principal axes of ellipsoidal particle

$$
\begin{aligned}
\sigma_{ij} &= -p\delta_{ij} + 2\mu d_{ij} + \\
&\quad +10\mu\left(\frac{5}{R^2}\Phi\delta_{ij} + \frac{4x_ix_j}{R^7} - \frac{x_i}{R^5}\frac{\partial\Phi}{\partial x_j} - \frac{x_j}{R^5}\frac{\partial\Phi}{\partial x_i}\right), \\
\Phi &= A_{km}x_kx_m, \\
A_{11} &= \frac{d_{11}}{6\beta_0''}, \quad A_{12} = \frac{\alpha_0 d_{12} + b^2\beta_0'(\omega_{12}+\omega_3)}{2\beta_0' B}, \\
A_{13} &= \frac{\alpha_0 d_{13} + b^2\beta_0'(\omega_{13}-\omega_2)}{2\beta_0' B}, \\
A_{21} &= \frac{\beta_0 d_{21} + a^2\beta_0'(\omega_{21}-\omega_3)}{2\beta_0' B}, \\
A_{22} &= \frac{d_{22}}{4b^2\alpha_0'} + \frac{d_{11}(\beta_0''-\alpha_0'')}{12b^2\beta_0''\alpha_0'}, \quad A_{23} = \frac{d_{23}}{4b^2\alpha_0'}, \\
A_{31} &= \frac{\beta_0 d_{31} + a^2\beta_0'(\omega_{31}+\omega_2)}{2\beta_0' B}, \quad A_{32} = \frac{d_{32}}{4b^2\alpha_0'}, \\
A_{33} &= \frac{d_{33}}{4b^2\alpha_0'} + \frac{d_{11}(\beta_0''-\alpha_0'')}{12b^2\beta_0''\alpha_0'}, \\
B &= a^2\alpha_0 + b^2\beta_0.
\end{aligned}
$$

In accordance with the structural theory used by Landau [4] while studying dilute suspensions, we take as a tensor defining the stress state in the suspension being considered here the tensor σ_{ij}, which is averaged over the volume of sphere S surrounding the suspended particle. Passing from integration over the volume of sphere to integration over its surface, we find the necessary stress tensor in the dilute suspension of ellipsoidal particles

$$\langle\sigma_{11}\rangle_{vol} = -p + \left(2\mu + \frac{4\mu V}{3ab^2\beta_0''}\right) d_{11}, \langle\sigma_{22}\rangle_{vol} = -p + \left(2\mu + \frac{2\mu V}{ab^4\alpha_0'}\right) d_{22}$$

$$+\frac{2\mu V(\beta_0'' - \alpha_0'')}{3ab^4\beta_0''\alpha_0'}, \langle\sigma_{33}\rangle_{vol} = -p + \left(2\mu + \frac{2\mu V}{ab^4\alpha_0'}\right) d_{33} + \frac{2\mu V(\beta_0'' - \alpha_0'')}{3ab^4\beta_0''\alpha_0'}, \langle\sigma_{12}\rangle_{vol}$$

$$= \left(2\mu + \frac{4\mu\alpha_0 V}{ab^2\beta_0' B}\right) d_{12} + \frac{4\mu V b^2(\omega_{12} + \omega_3)}{ab^2 B}, \langle\sigma_{21}\rangle_{vol} = \left(2\mu + \frac{4\mu\beta_0 V}{ab^2\beta_0' B}\right) d_{21}$$

$$+\frac{4\mu V a^2(\omega_{21} - \omega_3)}{ab^2 B}, \langle\sigma_{13}\rangle_{vol} = \left(2\mu + \frac{4\mu\alpha_0 V}{ab^2\beta_0' B}\right) d_{13} + \frac{4\mu V b^2(\omega_{13} - \omega_2)}{ab^2 B}, \langle\sigma_{31}\rangle_{vol}$$

$$= \left(2\mu + \frac{4\mu\beta_0 V}{ab^2\beta_0' B}\right) d_{31} + \frac{4\mu V a^2(\omega_{31} + \omega_2)}{ab^2 B}, \langle\sigma_{23}\rangle_{vol} = \left(2\mu + \frac{2\mu V}{ab^4\alpha_0'}\right) d_{23}, \langle\sigma_{32}\rangle_{vol}$$

$$= \left(2\mu + \frac{2\mu V}{ab^4\alpha_0'}\right) d_{32}. \tag{14}$$

The coefficients $a_i (i = \overline{0, 8})$ given by (13) are found now by comparing the components T_{ij} of the stress tensor in the suspension, which is postulated phenomenologically, with the corresponding components $\langle\sigma_{ij}\rangle_{vol}$ obtained in the structural part of the theory. To this aim, it is necessary to pass, first, in (13) to the moving coordinate system $Ox_1x_2x_3$ connected with ellipsoidal suspended particle. In such a transition $n_1 = 1$, $n_2 = 0$, $n_3 = 0$, $\dot{n}_1 = 0$, $\dot{n}_2 = \omega_3$, $\dot{n}_3 = -\omega_2$, and the components of the stress tensor T_{ij} defined by (13) become

$$\begin{aligned}
T_{11} &= a_0 + a_1 d_{11} + a_2 + (a_3 + a_4 + a_5 + a_6) d_{11}, \\
T_{22} &= a_0 + a_1 d_{11} + a_4 d_{22}, \\
T_{33} &= a_0 + a_1 d_{11} + a_4 d_{33}, \\
T_{12} &= (a_4 + a_6) d_{12} + a_7(\omega_3 + \omega_{12}), \\
T_{21} &= (a_4 + a_5) d_{21} + a_8(\omega_3 - \omega_{21}), \\
T_{13} &= (a_4 + a_6) d_{13} + a_7(-\omega_2 + \omega_{13}), \\
T_{31} &= (a_4 + a_5) d_{31} + a_8(-\omega_2 - \omega_{31}), \\
T_{23} &= a_4 d_{23}, \quad T_{32} = a_4 d_{32}.
\end{aligned} \tag{15}$$

The comparison of (14) and (15) yields

$$\begin{aligned}
a_0 &= -p, \quad a_1 = \frac{2\mu V(\beta_0'' - \alpha_0'')}{3ab^4\beta_0''\alpha_0'}, \\
a_2 &= 0, \quad a_3 = \frac{2\mu V}{ab^2}\left[\frac{\alpha_0'' + \beta_0''}{b^2\beta_0''\alpha_0'} - \frac{2(\alpha_0 + \beta_0)}{\beta_0'(a^2\alpha_0 + b^2\beta_0)}\right], \\
a_4 &= 2\mu\left(1 + \frac{V}{ab^4\alpha_0'}\right), \\
a_5 &= \frac{4\mu V}{ab^2}\left(\frac{\beta_0}{\beta_0'(a^2\alpha_0 + b^2\beta_0)} - \frac{1}{2b^2\alpha_0'}\right), \\
a_6 &= \frac{4\mu V}{ab^2}\left(\frac{\alpha_0}{\beta_0'(a^2\alpha_0 + b^2\beta_0)} - \frac{1}{2b^2\alpha_0'}\right), \\
a_7 &= \frac{4b^2\mu V}{ab^2(a^2\alpha_0 + b^2\beta_0)}, \quad a_8 = -\frac{4a^2\mu V}{ab^2(a^2\alpha_0 + b^2\beta_0)}.
\end{aligned} \tag{16}$$

The use of the results in [11] allows us to compute the values of the functions $\alpha_0, \beta_0, \alpha_0', \beta_0', \alpha_0'', \beta_0''$ and to obtain

$$\begin{aligned}
ab^2\alpha_0 &= 2 - 2A, \quad ab^2\beta_0 = A, \\
ab^4\alpha_0' &= \frac{2p_0 - 3A}{4(p_0^2 - 1)}, \quad ab^4\beta_0' = \frac{3A - 2}{p_0^2 - 1}, \\
ab^2\alpha_0'' &= \frac{(4p_0^2 - 1)A - 2p_0^2}{4(p_0^2 - 1)}, \\
ab^2\beta_0'' &= \frac{2p_0^2 - (2p_0^2 + 1)A}{p_0^2 - 1},
\end{aligned} \tag{17}$$

where $p_0 = a/b$ and

$$A = \frac{p_0^2}{p_0^2 - 1} - \frac{p_0 \ln(p_0 + \sqrt{p_0^2 - 1})}{(p_0^2 - 1)^{3/2}}$$

for $p_0 > 1$.

Equations (16) and (17) show that rheological constants $a_1, a_3, a_4, \ldots$ in (13) depend only on the dynamic viscosity coefficient μ of the suspension carrier fluid, volume concentration V of suspended particles and on the axial ratio p_0 of ellipsoid of revolution modelling the axisymmetrical suspended particles of the real suspension.

The rheological equation defined by (13) with coefficients given by (16) and (17) is the general rheological equation for dilute suspension of ellipsoidal particles with Newtonian carrier fluid. This equation needs to be complemented by constitutive equation for the internal microparameters n_i and N_i in order to obtain the rheological equation of dilute suspensions of ellipsoidal particles in any special case.

In our framework of the structure-phenomenological approach, the constitutive equation for n_i and N_i of the structural continuum modelling the real dilute suspension is obtained from the equation of rotary dynamics of suspended ellipsoidal particles in gradient flows of the suspension carrier fluid.

4. RHEOLOGICAL EQUATION FOR DILUTE SUSPENSION OF BROWNIAN ELLIPSOIDAL PARTICLES

As an illustration of use of (13) with coefficients a's defined by (16) and (17) as the general rheological equation for dilute suspensions of ellipsoidal particles, we obtain here the rheological equation for dilute suspension of Brownian ellipsoidal particles. Dynamics of such suspended particles is defined not only by hydrodynamic forces, which arise in gradient flows of the suspension carrier fluid, but it is also defined by the rotational Brownian motion. According to [12], the effective radius $r = \sqrt[3]{ab^2}$ of such particles satisfies the condition $10^{-8}m < r < 10^{-6}m$ if the suspension carrier fluid is water.

The constitutive equation for n_i and N_i of the structural continuum which models the dilute suspension of Brownian ellipsoidal particles is obtained as a result of the vector multiplication by the vector n_i of the equation of rotary motion of suspended ellipsoidal particles in gradient flows of the suspension carrier fluid, which take the form $M_i^{(hf)} + M_i^{(Bf)} = 0$, irrespective of the moment of inertia of suspended particles as it usually takes place in the rheology of suspensions. Taking into account that $M_i^{(Bf)} = -kT\varepsilon_{ilm} n_l \frac{\partial \ln F}{\partial n_m}$, and

$$[M_i^{(hf)} \times n_i] = W(\lambda(d_{ik}n_k - d_{km}n_k n_m n_i) - N_i), \tag{18}$$

we obtain [2] the constitutive equation

$$N_i = \lambda(d_{ik}n_k - d_{km}n_k n_m n_i) + D_r \left(n_i n_k \frac{\partial \ln F}{\partial n_k} - \frac{\partial \ln F}{\partial n_i} \right) \tag{19}$$

for the internal microparameters n_i and N_i. In (18) and (19), $\lambda = (p_0^2 - 1)/(p_0^2 + 1)$; $D_r = kT/W$ and

$$W = 4\nu\mu \frac{p_0^4 - 1}{p_0^2 \left[\dfrac{2p_0^2 - 1}{2p_0^2\sqrt{p_0^2 - 1}} \ln \dfrac{p_0 + \sqrt{p_0^2 - 1}}{p_0 + \sqrt{p_0^2 - 1}} - 1 \right]},$$

if $p_0 > 1$ [13]; here, $\nu = 4\pi ab^2/3$.

The substitution of N_i, defined by (19), into (13) and taking into account (16) yields the rheological equation of the dilute suspension of Brownian ellipsoidal suspended particles

$$T_{ij} = -p\delta_{ij} + 2\mu(1 + \frac{V}{ab^4\alpha_0'})d_{ij} + +12\mu D_r \frac{V}{ab^2}\frac{a^2-b^2}{a^2\alpha_0 + b^2\beta_0}(\langle n_i n_j\rangle - \frac{1}{3}\delta_{ij}) +$$

$$+2\mu\frac{V}{ab^2}\left[\frac{\alpha_0''}{b^2\alpha_0'\beta_0''} + \frac{1}{b^2\alpha_0'} - \frac{4}{\beta_0'(a^2+b^2)}\right] d_{km}\langle n_k n_m n_i n_j\rangle +$$

$$+2\mu\frac{V}{ab^2}\left[\frac{2}{\beta_0'(a^2+b^2)} - \frac{1}{b^2\alpha_0'}\right](d_{jk}\langle n_k n_i\rangle + d_{ik}\langle n_k n_j\rangle). \qquad (20)$$

The distribution function F of angular positions of ellipsoidal suspended particles, used in (20) for averaging, is defined by the equation

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial n_i}((\omega_{ik}n_k + \lambda(d_{ik}n_k - d_{km}n_k n_m n_i))F) =$$

$$= D_r(\Delta F - 2n_k\frac{\partial F}{\partial n_k} + n_k n_m \frac{\partial^2 F}{\partial n_k \partial n_m}) \qquad (21)$$

obtained from (8) by taking into account (19).

Equation (20) coincides with the rheological equation for the dilute suspension of the Brownian ellipsoidal particles obtained in [6] by another method. This fact confirms the validity of our structure-phenomenological theory of the stress state in the dilute suspensions of ellipsoidal particles presented here. Such a coincidence confirms in particular the status of the equation (13) with coefficients given by (16) and (17) as a general rheological equation for the dilute suspension of ellipsoidal particles with the Newtonian carrier fluid.

5. RHEOLOGICAL BEHAVIOUR OF DILUTE SUSPENSION OF BROWNIAN ELLIPSOIDAL PARTICLES

The use of the constitutive equations (20) and (21) shows that the dilute suspension of Brownian ellipsoidal particles behave as an elasticoviscous fluid in the simple shearing flow

$$v_x = 0, \qquad v_y = Kx, \qquad v_z = 0 \qquad (K = const) \qquad (22)$$

presenting the effect of Weissenberg and pseudoplastic dependence of the suspension effective viscosity on the rate of shear K.

The computation of the components T_{xy}, T_{xx}, T_{yy}, T_{zz} of the tensor T_{ij} by means of (20) allows us to obtain the expressions of the effective viscosity of the suspensions $\mu_a = T_{xy}/K$ and the differences of normal stresses $\sigma_1 = T_{yy} - T_{zz}, \quad \sigma_2 = T_{xx} - T_{zz}$ in the simple shear flow (22) of the suspension,

$$\mu_a = \mu\left(1 + \frac{V}{ab^4\alpha_0'}\right) + 6\mu\frac{D_r}{K}\frac{V}{ab^2}\frac{a^2-b^2}{a^2\alpha_0+b^2\beta_0}\langle\sin 2\phi\sin^2\theta\rangle + \mu\frac{V}{ab^2}(\frac{\alpha_0''}{b^2\alpha_0'\beta_0''} + \frac{1}{b^2\alpha_0'}$$

$$-\frac{4}{\beta_0'(a^2+b^2)})\langle\sin^2 2\phi\sin^4\theta\rangle + 2\mu\frac{V}{ab^2}\left(\frac{2}{\beta_0'(a^2+b^2)} - \frac{1}{b^2\alpha_0'}-\right)\langle\sin^2\theta\rangle; \quad (23)$$

$$\sigma_1 = 12\mu\frac{D_r}{K}\frac{V}{ab^2}\frac{a^2-b^2}{a^2\alpha_0+b^2\beta_0}\left[\langle\sin^2\phi\sin^2\theta\rangle - \langle\cos^2\theta\rangle\right]$$

$$+\mu\frac{V}{ab^2}[\left(\frac{\alpha_0''}{b^2\alpha_0'\beta_0''} + \frac{1}{b^2\alpha_0'} - \frac{4}{\beta_0'(a^2+b^2)}\right)\times(2\langle\cos\phi\sin^3\phi\sin^4\theta\rangle - \langle\sin 2\phi\sin^2\theta\cos^2\theta\rangle)$$

$$+\left(\frac{2}{\beta_0'(a^2+b^2)} - \frac{1}{b^2\alpha_0'}\right)\langle\sin 2\phi\sin^2\theta\rangle]; \quad (24)$$

$$\sigma_2 = 12\mu\frac{D_r}{K}\frac{V}{ab^2}\frac{a^2-b^2}{a^2\alpha_0+b^2\beta_0}\left[\langle\cos^2\phi\sin^2\theta\rangle - \langle\cos^2\theta\rangle\right]$$

$$+\mu\frac{V}{ab^2}[(\frac{\alpha_0''}{b^2\alpha_0'\beta_0''} + \frac{1}{b^2\alpha_0'} - \frac{4}{\beta_0'(a^2+b^2)}) \times (2\langle\sin\phi\cos^3\phi\sin^4\theta\rangle$$

$$\langle\sin 2\phi\sin^2\theta\cos^2\theta\rangle) + (\frac{2}{\beta_0'(a^2+b^2)} - \frac{1}{b^2\alpha_0'})\langle\sin 2\phi\sin^2\theta\rangle]. \quad (25)$$

In Eqs. (23)-(25), ϕ and θ are the angles of the spherical coordinate system, in which $n_x = \cos\phi\sin\theta$, $n_y = \sin\phi\sin\theta$, $n_z = \cos\theta$.

The computations of averaged values in (23)-(25) require the knowledge of the distribution function of axes of suspended ellipsoidal particles over all possible angular positions ϕ and θ. This function is found by solving (21), which in the steady case, that is at $\partial F/\partial t = 0$, in spherical coordinate system (ϕ, θ), takes the form

$$\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F}{\partial\theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2 F}{\partial\phi^2} = \sigma[\frac{1}{2}(1+\lambda\cos 2\phi)\frac{\partial F}{\partial\phi} + \frac{\lambda}{4}\sin 2\phi\sin 2\theta\sin\theta\frac{\partial F}{\partial\theta} -$$

$$\frac{1}{2}\lambda\sin 2\phi(3\sin^3\theta - 2\sin\theta + 2)F] \quad (26)$$

for the simple shear flow (22) of suspension. In (26), we have $\sigma = K/D_r$.

The solution of (26) is obtained in the form of the double series

$$F(\phi,\theta)=\sum_{j=0}^{\infty}\lambda^{j}\left[\frac{1}{2}\sum_{n=0}^{j}a_{n0,j}P_{2n}(\cos\theta)+\right.$$
$$\left.+\sum_{n=1}^{j}\sum_{m=1}^{n}\left(a_{nm,j}\cos 2m\phi+b_{nm,j}\sin 2m\phi\right)P_{2n}^{2n}(\cos\theta)\right].$$

For coefficients $a_{n0,j}, a_{nm,j}, b_{nm,j}$ we have obtained recurrence relations, which allow us to find the distribution function F with any degree of accuracy.

The computations of the averaged values in (23)-(25) according to formula

$$\langle a(\phi,\theta)\rangle=\int_{0}^{2\pi}d\phi\int_{0}^{\pi}a(\phi,\theta)F(\phi,\theta)d\theta$$

allow us to obtain numerical values of the effective viscosity μ_a and differences of normal stresses σ_1 and σ_2 for the aqueous dilute suspension of the ellipsoidal Brownian particles with effective radius $r=10^{-7}m$ that are shown in figs.1, 2.

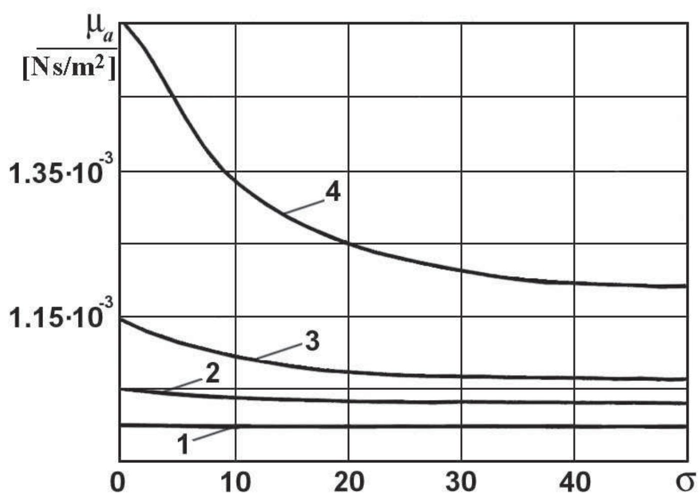

Fig. 1. Dependence of μ_a on $\sigma=K/D_r$ for the dilute suspension ($V=0.01$) in water $\mu=0.001\,\mathrm{N\,s/m^2}$ of ellipsoidal particles with effective radius $r=10^{-7}$ m; curves 2-4 corresponds to values $p_0=4,10,25$; curve 1 corresponds to the viscosity of the suspension carrier fluid in the absence of suspended particles.

The obtained results indicate that the dilute suspension of the Brownian ellipsoidal particles behaves similarly to visco-elastic fluids. So, it reveals the dependence of μ_a on the shear rate K (fig.1), which is characteristic to viscous non-Newtonian pseudoplastic fluids. The expression (23) of μ_a coincides with the expression for the effective viscosity of considered dilute suspension of Brownian ellipsoids obtained in [14] within the frames of structural theory with the use of Einstein energy method. As a result, numerical values of μ_a obtained above are in complete agreement with numerical values of characteristic viscosity $(\mu_a - \mu)/(\mu V)$ of the considered suspension which were calculated in [15] by method of averaging, similar to above mentioned one, and later were confirmed experimentally in [16].

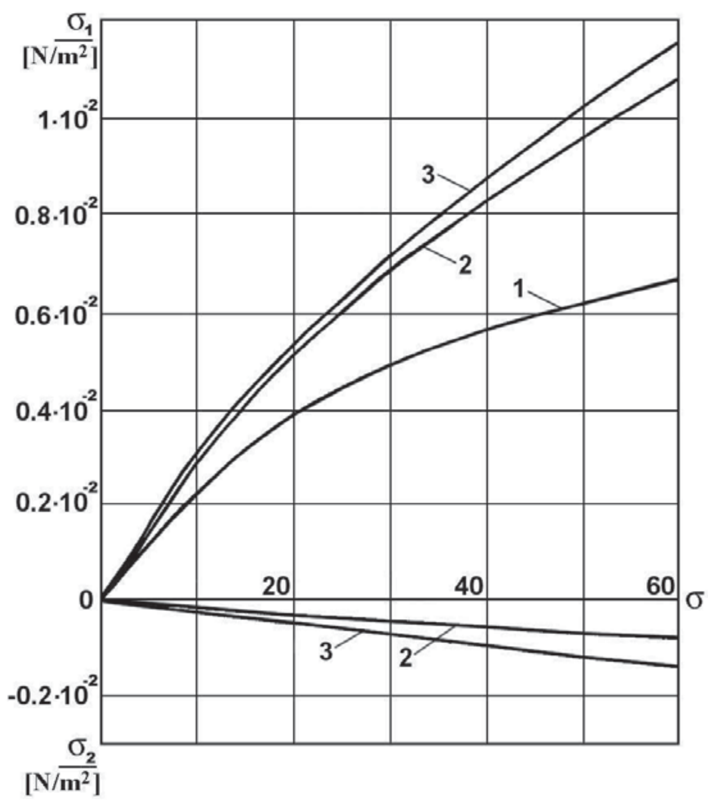

Fig. 2. Dependence of $\sigma_1 = T_{yy} - T_{zz}$ and $\sigma_2 = T_{xx} - T_{zz}$ on $\sigma = K/D_r$ for the dilute suspension ($V = 0.01$) in water $\mu = 0.001\,\mathrm{N\,s/m^2}$ of ellipsoidal particles with effective radius $r = 10^{-7}m$ at temperature $T = 300^o, {}^oK$; curves 1, 2, 3 correspond to values $p_0 = 4, 10, 25$.

The considered suspension reveals the Weissenberg effect in the shearing flow (22), namely the presence of nonzero differences of the normal stresses σ_1 and σ_2, which depend on the shear rate K (fig.2). The presence of the Weissenberg effect in dilute suspensions detected here theoretically still requires an experimental verification.

6. CONCLUSIONS

The advantage of the structure-phenomenological method to study dilute suspensions consists in the capability to combine the continual modeling of the suspension with the possibility to connect the macrorheological characteristics of the suspensions with parameters describing their microstructural and physical properties.

Further investigations show that this method is particularly efficient to obtain rheological equations for dilute suspensions of undeformable particles with non-Newtonian isotropic and anisotropic carrier fluids.

7. NOMENCLATURE

a_0, a_2 are phenomenological constants in (13), [N/m^2];

$a_1, a_i(i = \overline{3,8})$ are phenomenological constants in (13), [N s/m^2];

$\overline{a}$ is the radius of the dumbbell beads, [m];

$2a$, $2b$ are the axis of revolution and equatorial diameter of ellipsoid of revolution modeling suspended particles, [m];

d is the characteristic dimension of suspended particles, [m];

d_{ij} is the deformation rate tensor, [s^{-1}];

D_r is the coefficient of the rotational Brownian diffusion of suspended particles in the carrier fluid, [s^{-1}];

F is the distribution function of the angular positions of the orientation vector n_i of suspended ellipsoidal particles, dimensionless;

F_i is the resultant vector of the hydrodynamic forces acting on a dumbbell particle [N];

$k = 1.38 \cdot 10^{-23}$J/K is the Boltzmann constant;

K is the rate of shear, [s^{-1}];

l is the characteristic dimension of molecules of the suspension carrier fluid, [m];

$\bar{l}$ is the characteristic dimension of suspension macroflow region, [m];

L is the axis of the suspended dumbbell particles, [m];

$M_i^{(hf)}$, $M_i^{(Bf)}$ are angular momenta of hydrodynamic forces and forces of rotary Brownian motion acting on suspended ellipsoidal particle, [N m];

n_0 is the number of suspended particles per unit volume of the suspension, [m^{-3}];

n_i is the unit vector defining orientation of axisymmetric suspended particles modeled among them by dumbbells and ellipsoids of revolution, dimensionless;

N_i is the vector defining relative angular velocity of suspended particles with respect to the suspension carrier fluid, [s^{-1}];

p is the pressure, [$\mathrm{N/m^2}$];

p_0 is the axial ratio of ellipsoid of revolution modeling the axisymmetrical suspended particles, dimensionless;

P_{2n} are the Legendre polynomials;

P_{2n}^{2m} are the Legendre associated functions.

r is the effective radius of suspended ellipsoidal particles, [m];

R is the radius of the sphere S surrounding an ellipsoidal suspended particle, [m];

S is the sphere surrounding an ellipsoidal suspended particle used to define the stress in the suspension;

t is the time, [s];

T is the absolute temperature, [K];

t_{ij} is the stress tensor in the Newtonian carrier fluid of the suspension in the absence of suspended particles, [$\mathrm{N/m^2}$];

T_{ij} is the stress tensor in the dilute suspension of ellipsoidal particles modeled by a structure continuum, [$\mathrm{N/m^2}$];

$T_{xy}, T_{xx}, T_{yy}, T_{zz}$ are the components of the tensor T_{ij}, [$\mathrm{N/m^2}$];

u_i is the unit vector defining the orientation of suspended particles, directed along the axis L in the case of dumbbell particles and along the axis $2a$ in the case of ellipsoidal particles, [m/s];

$U_i^{(k)}(k = 1, 2)$ are the velocities of the flow around ends of a dumbbell particle by the suspension carrier fluid, [m/s];

v_{0i} is the translational velocity of the dumbbell center with respect to the carrier fluid, [m/s];

v_i is the velocity vector, [m/s];

v_x, v_y, v_z are the components of the velocity vector v_i, [m/s];

$v_{i,k}$ is the velocity gradient tensor, [s^{-1}];

V is the volume concentration of suspended particles, dimensionless;

W is the rotational friction coefficient of ellipsoidal suspended particles in the Newtonian carrier fluid, [N m s];

x_1, x_2, x_3 are coordinates in the moving coordinate system $Ox_1x_2x_3$, axes of which are coinciding with principal axes of ellipsoidal particle, [m];

$\langle\rangle$ denotes the averaging in the phase space of coordinates of orientation vector n_i;

$\langle\rangle_{vol}$ denotes the averaging over the volume placed inside the sphere S;

$\alpha_0, \beta_0, \alpha_0'', \beta_0''$ are the functions determined in (11), [m^{-3}];

α_0', β_0' are the functions determined in (11), [m^{-5}];

δ_{ij} is the Kronecker delta, dimensionless;

Δ is the Laplacian;

ε_{ikm} is the Levi-Civita tensor, dimensionless;

λ is the parameter depending on the geometric characteristics of ellipsoidal particles, dimensionless;

μ is the dynamic viscosity coefficient of the carrier fluid, [N s/m^2];

μ_a is the effective viscosity of the suspension, [N s/m^2];

μ_0, μ_2 are phenomenological constants in (11), [N m];

$\mu_1, \mu_i(i = \overline{3, 8})$ are phenomenological constants in (11), [N m s];

ν is the volume of ellipsoidal suspended particle, [m^3];

ξ is the translational drag coefficient of the dumbbell beads in the Newtonian carrier fluid, [N s/m];

σ is the dimensionless shear rate;

σ_{ij} is the stress tensor in the suspension carrier fluid on the surface of the sphere S surrounding an ellipsoidal suspended particle, [N/m^2];

σ_1, σ_2 are the differences of normal stresses in the simple shearing flow, [N/m^2];

ϕ, θ are the angles of the spherical coordinate system, [rad];

Φ is the rate of mechanical energy dissipation per unit volume of the suspension, [N/(s m^2)] ;

ω_{ik} is the velocity vortex tensor, [s^{-1}];

ω_2, ω_3 are the components of angular velocity of ellipsoidal particle, [s^{-1}].

Subscripts and superscripts

i, k in $v_{i,k}$ denote the derivation of the velocity vector v_i in the direction of coordinate axis k;

hf in $M_i^{(hf)}$ signify hydrodynamic forces;

Bf in $M_i^{(Bf)}$ signify Brownian forces;

the dot over n_i denotes the local time derivation;

vol in $\langle\rangle_{vol}$ signifies volume;

a in μ_a signifies apparent;

r in D_r signifies rotary.

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