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COMPUTER SIMULATION OF THE STRUCTURE OF DISPERSE SYSTEMS BY THE PARTICLE METHOD

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A computer simulation model of the internal structure of disperse systems, based on the particle method, is suggested. Numerical studies of these structures are carried out with use of the developed model.

In the last few decades, the vigorous development of computer engineering has resulted in the creation of a radically new powerful tool of investigation of physical processes — computational experiment. Under conditions where theoretical methods encounter serious difficulties and practical experiments are either extremely laborious or in principle impossible, computational modeling appears to be the only technique of investigation of the processes considered. At present the creation of computational models has received much recognition and has become a rapidly developing trend in science and technology. The use of modeling, as compared with the traditional laboratory methods, saves money and operating time. In investigations based on computational experiments the representation of a physical phenomenon in the form of the corresponding mathematical model, a computational algorithm, and a computer program plays a decisive role. In computational experiment a mathematical model represents a tested material and at the same time an algorithm of its performance. In [1], it is shown that one of the widely employed methods in constructing mathematical models is modeling with the aid of particles or, more precisely, by the particle method. Also, it is pointed out that the particle method, if properly used, can demonstrate its obvious merits.

Based on the theoretical and experimental material gained [2–9], a simulation model of disperse systems is constructed based on the particle method. In the present work, a model is described that can be used for investigation of the internal structure of disperse systems. Below, we outline the theoretical principles of the particle method that have been employed in constructing the simulation model.

The particle method is common to the class of models in which a discrete description of physical phenomena includes consideration of interacting particles. Any classical system can be described if the positions and the velocities of the particles constituting it and the law of their interaction are known. Each particle has a number of constant (e.g., mass, size) and variable (position, velocity) characteristics.

The variable characteristics change in conformity with the equation of motion. The state of a multiphase system is determined by the attributes of a final ensemble of particles, while evolution of the system is described by the laws of interaction of these particles. The suggested simulation model is based on investigation of the evolution of spherical particles in the three-dimensional space. The evolution process is separated discretely into time intervals. On each of them the motion of a particle is determined with account for its running coordinates and the forces acting on the particle. A value of the interval is chosen from the condition of constancy of the particle velocity on this interval of the evolution time of the system. Here, the maximum displacement of the particle does not exceed the prechosen value. It is assumed that a dispersion medium in the disperse system possesses the Newtonian rheological properties and its state in the model is characterized by the viscosity, the temperature, and the shear rate. The volume content and the size of particles in the system is also taken into account.

In the worked-out simulation model the velocities and the coordinates of particles are determined with allowance for the following propositions. Evolution of the system is considered as a result of the interaction of particles not only with each other but also with the medium. Here, the Brownian motion of particles and the van der Waals interaction of particles with both the medium and with each other are taken into consideration. For taking account of the Brownian motion of particles, in the model the classical Einstein–Smoluchowski formula [10] is used in the model:

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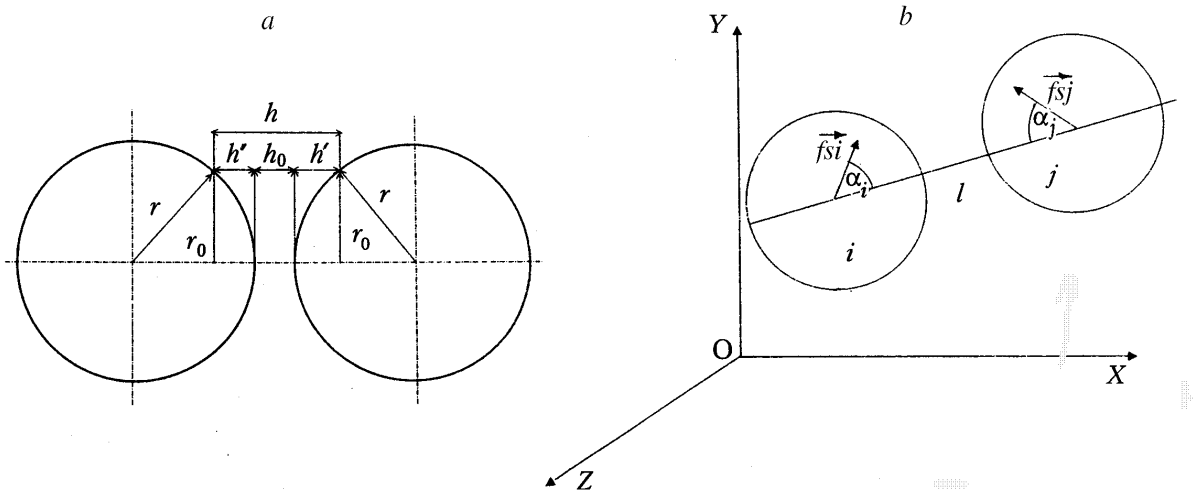


Fig. 1. Schemes of the interaction of two spherical particles for calculation of the van der Waals forces (a) and the supporting force (b).

$$v = \frac{1}{\sqrt{\tau}} \sqrt{\frac{RT}{N_A} \frac{1}{3\pi K_f r}} \ .$$

The suggested model also allows for the processes of formation of particle agglomerates and their spatial structures, which, in essence, is the basic feature for the phenomenon of structure formation. Here, the stability of spatial structures is determined by the van der Waals forces acting between particles. As is known, these forces are electromagnetic, they act between any two neutral atoms or molecules at a distance slightly larger than their sizes. The presence of the attracting forces between the neutral atoms leads naturally to the appearance of similar forces between any two macroscopic bodies whose surfaces are at very small distances from each other. Thus, the known Lifshits theory [11] describes the van der Waals interaction between two infinite plane-parallel bodies. We will extend this theory to spherical particles that can be considered as the components of disperse systems. For this purpose, let us consider two spherical particles that are at a distance h_0 from each other. From Fig. 1a it is seen that

$$h = 2h' + h_0 , \quad \text{while} \quad h' = r - \sqrt{r^2 - r_0^2} ,$$

then

$$h = 2\left(r - \sqrt{r^2 - r_0^2}\right) + h_0 . \tag{1}$$

The force of interaction of the two spheres is equal to the sum of forces acting over all radii of the section or

$$F = \int_0^r F_{r_0} 2\pi r dr_0 . \tag{2}$$

Substituting the Lifshits equation [11] for calculating the van der Waals forces between the two infinite plane-parallel bodies into relation (2) and replacing the distance between the bodies by the quantity h, according to (1), we arrive at an equation for calculation of the van der Waals forces between spherical particles:

$$F = \int_0^r \frac{3\,'cr_0 dr_0}{16\pi^2 \left[2\left(r - \sqrt{r^2 - r_0^2}\right) + h_0\right]^4 \sqrt{\varepsilon_{30}}} \int_0^\infty \left\{ \frac{(s_{10} - p)\,(s_{20} - p)}{(s_{10} + p)\,(s_{20} + p)} + \frac{(s_{10} - p\varepsilon_{10}/\varepsilon_{30})\,(s_{20} - p\varepsilon_{20}/\varepsilon_{30})}{(s_{10} + p\varepsilon_{10}/\varepsilon_{30})\,(s_{20} + p\varepsilon_{20}/\varepsilon_{30})} \right\} \frac{dp}{p^2} ,$$

where $s_{10} = \sqrt{(\varepsilon_{10}/\varepsilon_{30}) - 1 + p^2}$; $s_{20} = \sqrt{(\varepsilon_{20}/\varepsilon_{30}) - 1 + p^2}$.

To exclude the penetration of particles into each other and to provide a description of the simultaneous displacement of particles in the case of their contact, a supporting force has been introduced in the model. This force is determined as follows. Any two interacting particles, for instance, *i* and *j*, are considered (Fig. 1b). For each contacting particle a total projection of the forces acting on particles is calculated, namely, the van der Waals forces and the hydrodynamic forces occurring in a shear flow due to the gradient velocity of the flow, and also the forces caused by hydrodynamic interaction of the particles. We will denote these projections for the particle *i* by *fsxi*, *fsyi*, and *fszi* and for the particle *j* by *fsxj*, *fsyj*, and *fszj* respectively. Then for *i* and *j* we have

$$|fsi| = \sqrt{fsxi^2 + fsyi^2 + fszi^2} \quad \text{and} \quad |fsj| = \sqrt{fsxj^2 + fsyj^2 + fszj^2}\,.$$

Next, we draw a line *l* through the centers of the particles *i* and *j* and find the projection of **fsi** and **fsj** onto *l*:

$$fs_{li} = |fsi| \cos\alpha_i\,, \quad fs_{lj} = |fsj| \cos\alpha_j\,.$$

Now we denote by *d* the following quantity:

$$d = \sqrt{(xj - xi)^2 + (yj - yi)^2 + (zj - zi)^2}\,,$$

then

$$\cos\alpha_i = \frac{fsxi\,(xj - xi) + fsyi\,(yj - yi) + fszi\,(zj - zi)}{d\,|fsi|}\,, \quad \cos\alpha_j = \frac{fsxj\,(xi - xj) + fsyj\,(yi - yj) + fszj\,(zi - zj)}{d\,|fsj|}\,.$$

If $fs_{li} > 0$, the projection of the supporting force for the particle *i* onto the axes *x*, *y*, and *z* is

$$foxi = fsxi - kf \cdot fs_{lix}\,, \quad foyi = fsyi - kf \cdot fs_{liy}\,, \quad fozi = fszi - kf \cdot fs_{liz}\,, \tag{3}$$

where *kf* is the coefficient of amplification determined from the condition of stability of evolutionary development of the investigated system and

$$fs_{lix} = (((-fs_{li} + fs_{lj})/2 + fs_{li})\,(xj - xi))/d\,, \quad fs_{liy} = (((-fs_{li} + fs_{lj})/2 + fs_{li})\,(yj - yi))/d\,,$$

$$fs_{liz} = (((-fs_{li} + fs_{lj})/2 + fs_{li})\,(zj - zi))/d\,.$$

If $fs_{li} < 0$, the projection of the supporting force onto the axes *x*, *y*, and *z* for the particle *i* is

$$foxi = fsxi\,, \quad foyi = fsyi\,, \quad fozi = fszi\,.$$

If $fs_{lj} > 0$, the projection of the supporting force onto the axes *x*, *y*, and *z* for the particle *j* is

$$foxj = fsxj - kf \cdot fs_{ljx}\,, \quad foyj = fsyj - kf \cdot fs_{ljy}\,, \quad fozj = fszj - kf \cdot fs_{ljz}\,, \tag{4}$$

where

$$fs_{ljx} = (((-fs_{lj} + fs_{li})/2 + fs_{lj})\,(xi - xj))/d\,; \quad fs_{ljy} = (((-fs_{lj} + fs_{li})/2 + fs_{lj})\,(yi - yj))/d\,;$$

$$fs_{ljz} = (((-fs_{lj} + fs_{li})/2 + fs_{lj})\,(zi - zj))/d\,.$$

For the case $fs_{lj} < 0$

$$foxj = fsxj\,, \quad foyj = fsyj\,, \quad fozj = fszj\,.$$

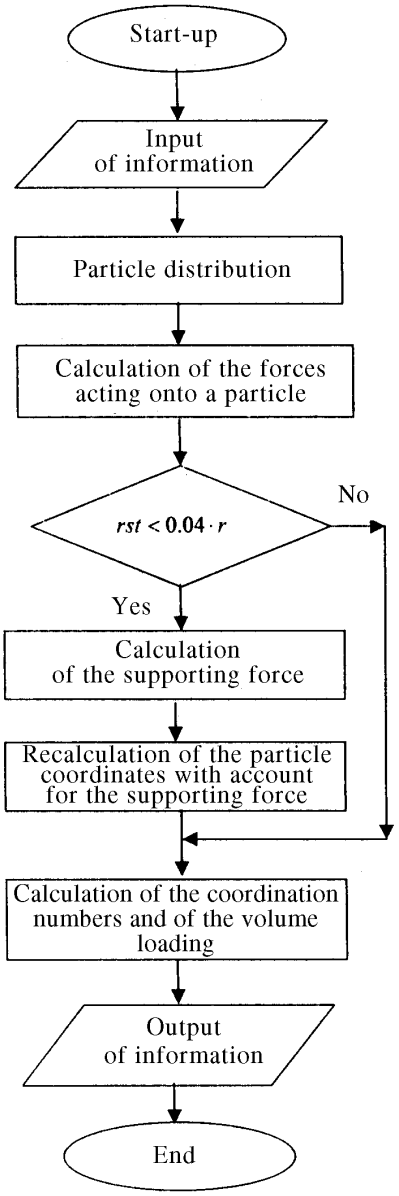


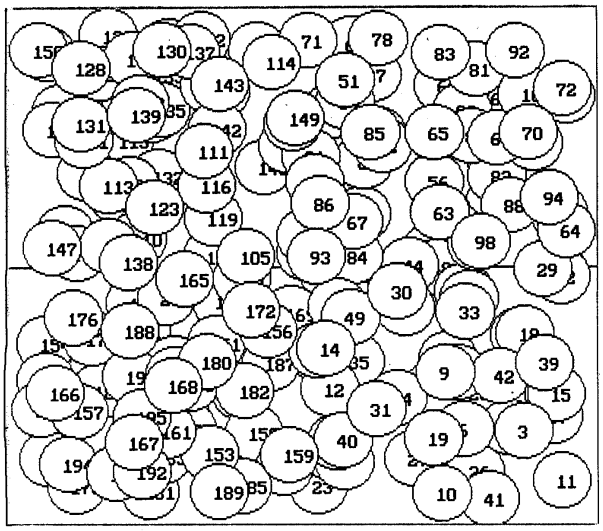
Fig. 2. Algorithm of the computational program.

The differences of the forces calculated by expressions (3) and (4) for each of the considered interacting particles determine their further displacement in space.

Based on the above theoretical representations, a computational program for investigation of the structure of disperse systems has been worked out. An algorithm of the program is given in Fig. 2. The program is realized in TurboPascal, in the known programming language, which reflects the method of structural programming and is implemented on all modern personal computers for scientific calculations.

The input data required for the computer program to work are the number and size of the particles, the degree of volume loading, the temperature, the viscosity of the medium, the shear rate of the system, and the time step. After input of the information, according to the algorithm of the program, the initial distribution of particles in the three-dimensional space occurs with the aid of a random-number generator using the normal distribution law. The cell size is determined in relation to the prescribed degree of volume loading

$$V = \frac{4}{3}\pi r^3 n / V_0 .$$



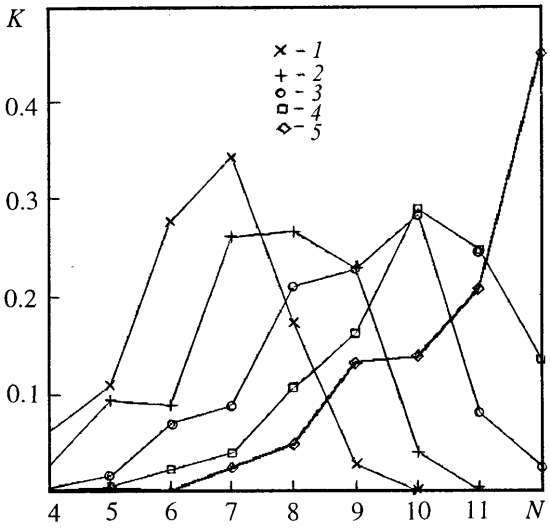


Fig. 3. Example of the particle distribution in the counting cell.

Fig. 4. Distributions of the coordination numbers for different degrees of volume loading of the powder: 1) 0.56; 2) 0.58; 3) 0.60; 4) 0.62; 5) 0.64.

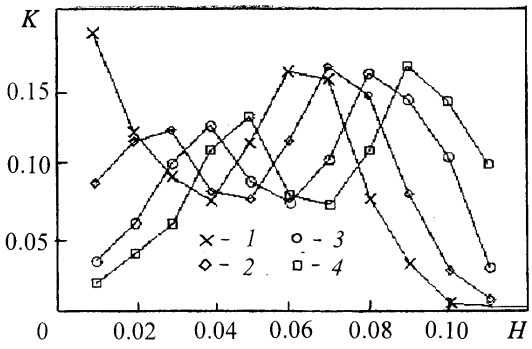
Next, according to the routine of the program, the basic cyclic algorithm of calculation of the resultant forces acting onto each of the particles is executed. The next step is calculation of the velocities and the trajectory of motion of particles, i.e., the position of particles in space at each instant of time. After making all the calculations and determining the new coordinates of the particles the next image of layout of the particles in space and the distribution of the coordination numbers are displayed on the computer's screen. Figure 3 illustrates an example of the particle distribution. At any moment of time it is possible to stop execution of the program, to make entries of the current data and calculated results in a file, and to insert and change the input parameters.

The worked-out simulation model of the internal structure of disperse systems based on the particle method has found wide application in scientific research studies. With its use computational experiments on investigation of these systems have been carried out [4–9]. Numerical computations were made on a computer of the Pentium type. The number of particles in computation was taken within the range 200–350. Its increase in the model entails an increase in the computation time.

As an object for a numerical study of the disperse systems by the method of computer simulation, we chose aluminum powder. This is dictated by the fact that the particles of aluminum are spherical. As a result of the computations carried out, we obtained different degrees of volume loading under the action of the compressing force. From the data on distribution of the coordination numbers for different degrees of volume loading of the powder represented in Fig. 4, it follows that a limiting volume loading of the powder equal to 64% corresponds to the state where more than 40% of the particles have a coordination number equal to 12.

The computer simulation model also provides the possibility of investigating the nature of contacts between particles in a disperse system. Computational experiments on investigation of the distance between "contacting" particles were carried out. Figure 5 represents distributions of the number of pair contacts as a function of the distance between particles $\left(H = \frac{rst}{2} r\right)$ for different degrees of volume loading. As is seen from the figure, for all volume loadings the dependence of the distribution of the pair contacts of particles on the distance between them has two maxima. A decrease in the volume loading of the system leads to displacement of the maxima toward the larger distance between particles.

Based on the data reported, we can conclude that the actual contacts in the suggested simulation model are realized at a particle–particle distance that is less than 0.02 diam. of a particle. The nature of contacts in disperse systems is considered in detail in [2, 4]. The first maximum corresponds to actual contacts between the particles. Only these contacts are responsible for the general structure of the powder and its mechanical properties under small strains.



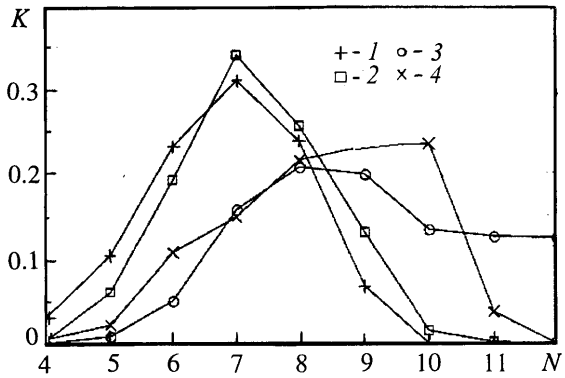


Fig. 5. Distribution of the pair contacts of particles as a function of the distance between them for different volume loadings of the system: 1) 0.64; 2) 0.62; 3) 0.60; 4) 0.56.

Fig. 6. Comparison of the calculated and experimental [2] data: 1, 2) calculations and experiment for a volume loading of 0.56; 3), 4) the same, for 0.63.

The second maximum corresponds to the nearby particles; the presence of such a type of their arrangement in space provides different properties of powders, for instance, compaction of powders under compression conditions [6].

The results of the numerical study of the internal structure of disperse systems are in fair agreement with the experimental literature data (see Fig. 6). The figure represents distributions of the number of pair contacts versus their coordination numbers for different degrees of volume loading. From these data it follows that reduction of the volume loading of the system decreases the mean coordination number of particles and narrows the particle distribution with respect to the coordination numbers. These data also indicate that the suggested simulation model adequately reflects the structure of disperse systems [4].

Thus, numerical studies of the internal structure of disperse systems have been carried with the use of the simulation model based on the particle method. The model makes it possible to describe the processes in investigated systems and to predict the influence of various parameters on their behavior.

NOTATION

v, mean velocity of the particle for an interval of time (a change in the coordinates for an interval of time); τ, time interval; R, universal gas constant; T, absolute temperature; N_A, Avogadro number; K_f, viscosity coefficient of the fluid; r, particle radius; h_0, distance between particles; r_0, radius of the section; F, interaction force of two spheres; F_{r0}, force acting over the section radius; $\hbar$, Planck constant; c, velocity of light; p, variable of integration; ε_{10}, ε_{20}, relative dielectric constants of the particles; ε_{30}, relative dielectric constant of the medium; n, quantity of particles in the model; **fsi** and **fsj**, resultant vectors of the forces for the particles i and j (i = 1, 2, ..., n, j = 1, 2, ..., n); *fsxi*, *fsyi*, *fszi*, projections of the resultant vectors of the forces for the particle i; *fsxj*, *fsyj*, *fszj*, projections of the resultant vector of the forces for the particle j; l, line connecting the centers of the particles i and j; α_i, angle formed by the line l and the resultant vector of the forces for the particle i; α_j, angle formed by the line l and the resultant vector of the forces for the particle j; *foxi*, *foyi*, and *fozi*, projections of the supporting force of the particle i onto the coordination axes; *foxj*, *foyj*, and *fozj*, projections of the supporting force of the particle j onto the coordination axes; V, volume of the counting cell; V_0, initial degree of volume loading of the system; *rst*, distance between the particles; N, coordination number; K, relative share of the pair contacts; H, relative distance between the particles.

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