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The Structures of Heterogeneous Condensed Mixtures

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ABSTRACT

In this article has been proposed an analog model and a new algorithm for random distribution of hard spheres in space (hard disks on the plane), which is applicable to any distribution of particle diameters and volume concentrations up to the maximum possible corresponding to close packing of the particles. The proposed method is called the method of viscous suspension. There has been conducted a simulation of the structure of heterogenous condensed mixtures (HCM) containing one or two monodisperse particles in a wide range of their volume concentrations. We determined the main statistical characteristics describing the internal structure of HCM. It has been shown that the method of viscous suspension allows simulating an appearance of regular structures when the volume concentration of the particles is close to the maximum possible corresponding close packing. It has been demonstrated that the contact particles make in HCM extensive clusters, whose dimensions increase with the increase of volume concentration of the particles.

Keywords : heterogeneous condensed mixtures (HCM), suspension, concentration, particle

INTRODUCTION

The problem of random spatial arrangement of solid spheres (or discs in the plane), with a given diameter distribution is not only applied but also the fundamental significance, as occurs in many areas of science [1-4].

The analytical solution of this problem even in the simplest case is missing, so the primary method of research is computer modeling. However, and in this case there is no common method of placing in space particles with diameters of random given distribution [5,6]. Direct solution of this problem by sorting even for the small number of particles occupies an unacceptable time and very often does not lead to the final result. The main difficulty consists in the fact that the allocation of particles should not overlap.

Currently are known and completely investigated methods of distributing particles in space as a “point process of solid shells”, “Gibbs’ point process”, “Strauss’ model”, “the spatial process of birth and destruction”, etc. [1-3]. However, the application of these methods is very limited because they have the weak convergence for large bulk densities of filled space, close to the maximum, and time consuming for the calculation of one embodiment.

The greatest difficulties arise when particles are placed in space with wide spectrum of sizes. Methods mentioned above frequently lead to that of the size distribution of particles which is different from the distribution of the initial particles.

Suggested in the publication [7] is the method of disposal of particles in space (disks in the plane) that does not depend on distribution of the initial particle size and the bulk density of their placement in space, has good convergence facilitating the investigation of the system with a bulk density filling

THE PHYSICAL MODEL AND COMPUTER IMPLEMENTATION

Digressing from actual system studied, we consider the following model problem [7,8]. Let there be a system of N spherical particles with known radii $r_i\ (i=1,...,N)$ We assume that the particles can move freely, approaching each other within distances shorter than the sum of their radii, and the repulsive force acting between them vanishes for non- overlapping particles. Hence, the system of spherical particles coinciding with the centers of the corresponding spheres. Thus, we shall consider a system consisting of N point particles with repulsive forces acting between them. The forces are assumed to be central and paired. For two point particles i and j corresponding to spheres with radii r_i and r_j, the force is given by the relations [7]:

$$F_{ij}(r)=\frac{x_i-x_j}{|x_i-x_j|}F_j,$$

$$F_{ij}(r)=\begin{cases}F_0\ for & r<r_i+r_j,\\ 0\ for & r\geq r_i+r_j,\end{cases}$$

where x_i is the radius-vector of the ith particle, $r=|x_i-x_j|$ is the distance between the centers of the spheres, and $F_0(r)$ is a certain function which will be defined below [9].

Particle motion in that system can be studied numerically by the molecular-dynamic method [10]. Particles in the system are in continuous random motion. To use that process to arrange the spheres randomly in space, it is necessary to “freeze” the system at a certain moment, i.e., to cease the calculation by fixing the particle coordinates. We shall call that method a molecular-dynamic point process. It can be regarded as a molecular-dynamic version of the Gibbs point process [2,3,11]. That processes are related to one another as the

molecular-dynamic method and the Monte Carlo method in statistical physics [10]. Obviously, in the "frozen" state of the system, overlapping of some spherical particles is possible, and additional, rather complicated procedures, for example, a gaping procedure, are required to obtain a system of nono-overlapping, randomly arranged particles.

This difficulty will be greater the closer the volume-filling density is to the maximum possible value. To overcome this, we assume that the viscous force acting on a particle is equal to $-\mu v$, where v is the velocity vector of the particle and μ is the proportionality factor (viscosity). Owing to the action of the viscous force, free (non-overlapping) particles stop with time, and for large values of the coefficient μ, the system should rapidly attain a state of equilibrium in which all particles are immovable and do not overlap. This stage is regarded as a random arrangement of solid spherical particles in space. If the system contains even two overlapping particles, they will fly apart under the action of the repulsive force [7].

The dynamics of this system is governed by the system of equations [7]:

$$m_i \frac{d^2 x_i}{dt^2} = \sum_{j \neq i} F_{ij} - \mu v_i,$$

where m_i is the mass of the i th particle and t is the time.

This equation describes the dynamics of a viscous suspension consisting of a system of particles between which repulsive forces are acting.

Generally, this method is not dissimilar in implementation to the molecular-dynamic method. The dynamic equations of the system includes a number of unknown parameters and functions $(\mu_i, m_i,$ and $F_0)$ They are not essential from the view-point of the problem solved (random arrangement of particles in space), but they are very important from the view-point of implementation and convergence of the calculation method.

Because we are interested neither in the final steady-state distribution of the particles in space nor in the process of relaxation of the system to this state, the problem can be significantly simplified [7].

Increasing the viscosity of the system leads to more rapid relaxation of the system to the state of equilibrium. Therefore, in calculations, the value of μ should be large enough in order that the inertia term on the left side of the equation of the system in next form

$$v_i = \frac{1}{\mu} \sum_{j \neq i} F_j .$$

With an appropriate choice of the parameter F_0, we can set $\mu = 1.$

Below, in article [7] was restricted to the case $F_0 = const.$ Assuming that the function F_0 depends on the distance between the particles and their radii (for example, increases with decrease in distance between the particles), we can improve the convergence of the process to the state of equilibrium by assuming faster scatter of overlapping particles. However, as calculations show the gain thus obtained is minimal and it does not justify the complication of the model [9].

Thus, we can write the evolution equation in next form

$$\frac{dx_i}{dt} = \sum_{j \neq i} \frac{x_i - x_j}{|x_i - x_j|} \Delta_{ij} . \quad (1)$$

Equation (1) does not contain parameters describing the viscous medium. The solution of this equation converges to a state in which the right side vanishes for all i. The system can be in this state during long period where external disturbances are absent. This state is an equilibrium state.

The process governed by equation (1) may be used for random arrangement of particles in space. Commonly the proposed method called the viscous-suspension method or, by analogy with other processes of arrangement of solid particles in space [2,3,11], the viscous-suspension point process.

Equation (1) describes the regular dynamics of the system of solid spheres and contains no randomness elements. The random nature of the equilibrium distribution of solid particles is determined by random initial conditions. The initial conditions are specified using a random-number generator, which determines the initial, coordinates of each particle [78]. This is equivalent to the fact that the centers of the region and the system then evolves to the state of equilibrium according our equation. In the point process of arranging solid shells, the size distribution of the particles arranged in space can differ from that of the initial particles since the particles are constantly put in or removed from the system if they overlap with other particles [65,66,73]. "In contrast to this, in the viscous-suspension method, it is possible to perform a system of particles with specified characteristics that are to be randomly arranged in space. It is hoped in this case that if there is at least one of the system in which particles do not overlap, the system will sooner or later attain this state. Unfortunately, a rigorous mathematical proof of this statement is not available. However, the numerous calculations performed for various systems up to volume densities of space filling equal to 0.95 of the maximum possible value for a given system have not revealed any attractors that did not coincide with the equilibrium state of system (1). The implementation of this method is generally similar to that of the molecular-dynamic method in statistical physics but there are some differences" [7].

"First, solution Equation (1) does not require high-order calculation schemes, which are often used in the molecular-dynamic method because of the instability ("scatter") of phase trajectories. It suffices to employ the simple integration scheme $x_i(t + \delta t) = x_i(t) + v_i \delta t,$ where δt is the integration step and v_i are the right sides of equation (1). Without loss of computational stability, the integration step can be large enough, for example, $\delta t = 0.0$. It should be kept in mind, however, that the displacement of overlapping particles in one step is of order δt. This should be taken into account in calculating the coordination number of the system (the number of contacts between particles) and in calculating states similar to close packing. In the first case, this is due to the fact that in the steady state of the system, contacting particles, the choice of a large integration step leads to the potentially attainable packing density becoming lower than the theoretically possible density corresponding to $\delta t = 0.$

The calculation procedure consists of an exhaustive search of all particles of the system in a given step and calculation of new coordinates of the particles. In calculating the right sides of equation (1), for each particle, we perform an exhaustive search for the remaining particles of the system. When the force acting on a particle is determined by simple exhaustion, the calculation time increases in proportion to the square of the number of particles in the system, and even for low-density packing, a calculation of the system takes too much time.

To reduce the calculation time, it is possible to examine only the nearest neighbors of the particle considered. To this end, the entire calculation region was divided into cells whose size was equal to the largest particle size. We took into account only particles in the nearest 27 cells for the spatial problem and only particles in the nearest nine cells for the plane problem. A list of all particles was compiled so that the particles located in the cell considered could be found without additional check. In calculating the displacement of a particle, we checked in each step whether it moved to another cell or not; if it did, the list of particles was corrected [7].

As the boundary conditions in the viscous-suspension method, we use periodicity conditions or bounded by solid proof walls.

As in the molecular-dynamic method, the main restriction is the time of calculation of one variant, which depends on the number of particles in the system and, hence, on the maximum dimensions of the calculation region. In the analysis performed, a region with dimensions 10 x 10 x10 was used for arrangement of spheres in space and a region with dimensions 25 x 25 was used for arrangement of disks in a plane"[68]. The dimensions are given in relative units. The scale is the diameter of the oxidizer particles. We note that for the plane problem, the calculation time is reasonable even for a calculation with dimensions $\approx 200 \times 200$ [8,12].

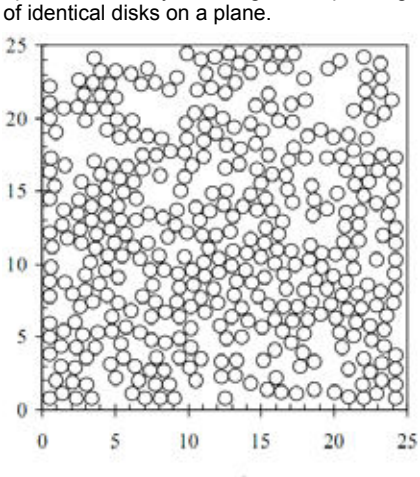
USE OF THE METHOD OF VISCOUS SUSPENSION

Some results of the calculations showing possibilities of the method of viscous suspension.

Since the problem of placement of solid particles is geometrical, we will consider it into the dimensionless form: all dimensions assign to certain geometric scale, as will be usually chosen the diameter of a typical particle. In calculations will be used solid impermeable walls as the boundary conditions.

In the beginning, each calculation was conducted by the random initial placement of particles in the computational domain. This placement is ended as soon it reached a predetermined value of the volume concentration of particles of various types. The calculation terminates when right parts of (1) vanishes.

For description, examine the placement of the plane problem i.e solid disks on the plane. Let us consider system of identical disks of unit diameter. The only variable parameter in determining the condition of the system, is the bulk density of the filling ρ (volumetric concentration of particles), which we shall define as the ratio of the particles to the volume of the same shape. Obviously, $\rho \le \rho_{\max}$, where $\rho_{\max} = \frac{\pi}{2\sqrt{3}}$ maximal possible density of filling corresponding to close packing of identical disks on a plane.



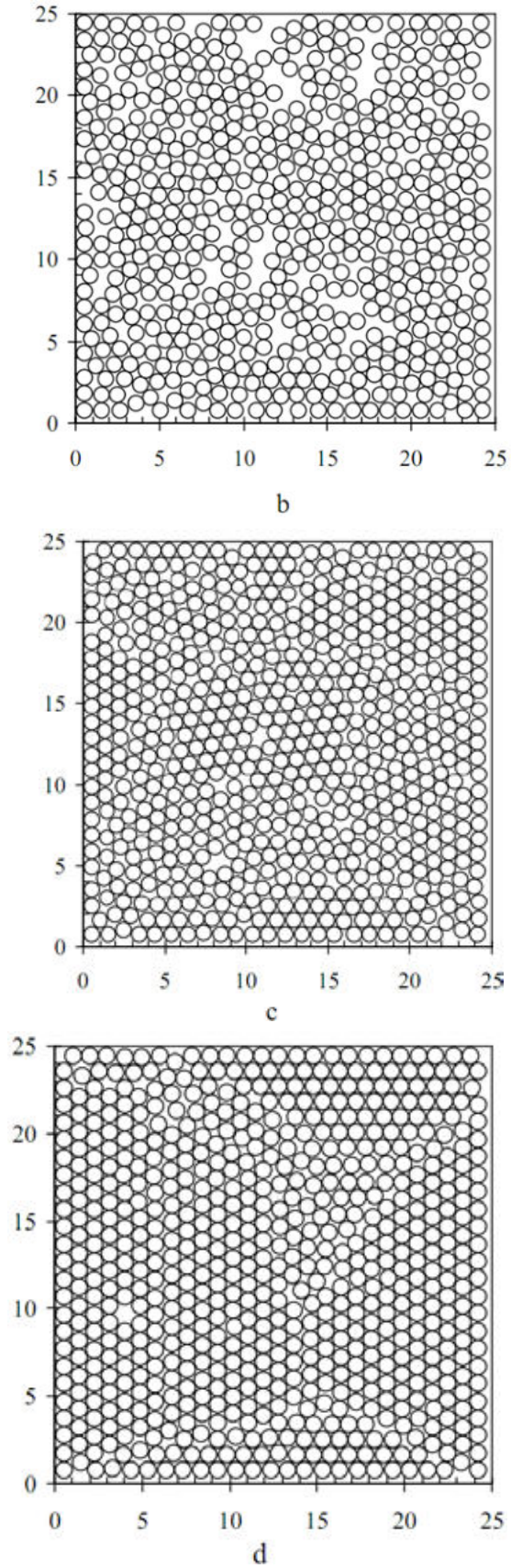


Figure 1: Placement of solid disks on the plane by means of method of a viscous suspension for different volumetric densities of filling**:** a – 0.5; b – 0.7; c – 0.8; d – 0.84

Sources: [13,14**]**

Fig. 1 (a-d) present options for random allocation of solid disks inside the square region with different volume concentrations of particles [13,14]. It is believed that the space of between the particles filled with a continuous binder, which provides strength system with any volume concentrations of particles.

Fig. 1 shows the way an ordered arrangement of particles occurs while their volume density increases in the region under consideration. For $\rho < 0.5$, any regular patterns of particles are not observed. The particles are randomly distributed in a volume. For $\rho = 0.5$, a quite large number of clusters of contact particles is observed. Here the particles form a hexagonal ordered structure characteristic for close packing.

Further increase of the volume density ρ results in increased number of particles integrated in ordered structures close hexagonal ones.

If $\rho = 0.8$ the obtained structure resembles disparate elements of crystalline grid surrounded by regions with amorphous structure. For $\rho = 0.8$4 the system consists of separate regions of closely packed particles separated by thin transition zones. However, being dense like this, the system has small areas with amorphous structure.

Thus, it is obvious that the appearance of a regular structure in the system of hard spheres is not connected with a specific mechanism of particle interaction, but is a purely geometric property of the system.

The pair correlation function $g(r)$ which is defined as

$$g(r) = \frac{dN(r, dr)}{4\pi r^2 n dr} \quad (2)$$

is one of the most important characteristics of the system of particles for the plain problem where $dN(r, dr)$ is a number of particles in a spherical (circular) layer $[r, r + dr]$ averaged over all the particles selected as the center of the spherical (circular) layer; n is an average number of particles per unit of volume.

The pair correlation function is one of the most general characteristics of the hard particle system irrespective from application (see e.g. [8,12,14]). For periodic structures correlations do not decay at infinity and have a periodic nature. If the pair correlation function with increasing distance r tends to unity, the particles are randomly distributed. My calculations of the pair correlation function confirm this fact.

Since the actual calculation volume is limited, the minimum distance to the volume bounds was calculated for each particle, and the contribution of each particle in $dN(r, dr)$ was determined for each r smaller than this distance. This makes it possible to avoid distortion of function $g(r)$ due to boarder effects. When calculating $dN(r, dr)$ and the correlation function it was taken that $dr = 0.1$.

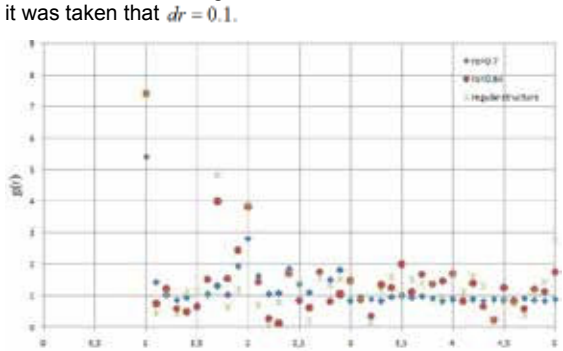


Figure 2: The pair correlation function of the hard sphere system Sources: authors

Fig. 2 shows pair correlation functions of a system of similar spheres with a unit diameter for several packing densities in a rectangular area. At low packing densities $\rho \le 0.7$ the correlation function decays quickly and at a distance of about 3-4 particle diameters it is close to unity. When density increases to 3-4 particle diameters it is close to unity. When packing density increases the correlation length increases as well and the correlation function decays more slowly. At high packing densities $\rho > 0.84$ the correlation function almost never decays, which fact demonstrates appearance of a regular structure with an infinite correlation length. To compare with, Fig. 1.2 shows a theoretical pair correlation function (X-symbols) for a close packing of similar discs in a plane, obtained with the same radial intermittency. It is obvious that even with $\rho > 0.84$ the pair correlation function repeats all the characteristic features of a correlation function for close packing.

When the volume density of space filling particles increases, the time required for calculating one option (the time for relaxation of a system to a desired state) increases as well. Analysis has shown that the calculation time has a strong nonlinear dependence on ρ.

As packing density increases, the free volume of space within which particles may move to reach an equilibrium condition decreases. The closer the system to close packing, the less free space remains and the system requires more time to reach an equilibrium condition.

Let's introduce the parameter $\zeta = \rho_{\max} - \rho$, which will be called the particle mobility. This parameter characterizes the possibility of particles moving without being crossed. The higher mobility ζ, the further the system of particles from close packing and the less average time it requires to reach an equilibrium condition. Although similarity of the geometric system and thermodynamics under consideration are to a large extent relative , we introduce the notion of "geometric temperature" of a solid particle system, which is naturally defined as monotonic function of mobility $T = f(\rho_{\max} - \rho)$ where $f(\zeta \le 0) = 0.$

Under zero "geometric temperature" particle mobility in the system is zero, and the system will never be able to come to equilibrium. With the increase of "the temperature" the mobility of the particles increases, which allows them to reach the equilibrium condition quicker. Thus, as in thermodynamics, increase of "the temperature" accelerates the process of establishing an equilibrium condition.

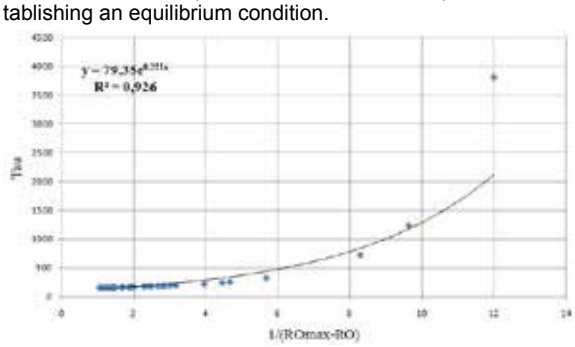


Figure 3: Nondimensional time for relaxation of the hard sphere system to an equilibrium condition depending on the volume concentration
Sources: authors

Fig. 3 represents the dependence of the relaxation time τ from the equilibrium condition of the parameter $1(\rho_{\max} - \rho)$ for the hard sphere described by equations (1) and (2). Timing was done in steps. A step was a cycle of calculation of movements of all the particles during time δt.

Dependence of the relaxation time of the system from "the temperature" can be approximately represented as the Arrhenius dependence well known from the kinetic theory

$\tau = A\exp\left(\frac{B}{T}\right)$, where A and B are some parameters independent from the type of computer and weakly dependent on the calculation algorithm and its computer implementation. If particles have low mobility, the dependence of temperature from mobility may be represented as the power function $T = (\rho_{\max} - \rho)^n$, where $n > 1$.

Fig. 3 shows the function $\tau = 79.35e^{0.321x}$ as a firm line. The function adequately describes this experimental dependence in the area of low mobility of particles $(\rho_{\max} - \rho) \le 0.25$ and conforms to the results obtained by S.A. Rashkovsky (Moscow Institute of Heat Technology, Russia Federation) [6].

Thus, it should be recognized that it is impossible to achieve an equilibrium condition by the method of viscous suspension within a definite time when particles are closely packed. This result seems to be fundamental rather than only a property of the method of viscous suspension [7].

This allows us to make the following statement: whatever the algorithm of particle distribution in space, infinite time is required to achieve equilibrium condition when particles are closely packed.

The analysis of Fig. 1 (a-d) demonstrates that the contact particles make clusters, and the average number of particles in a cluster grows while the volume density increases.

After the particles were distributed in the system (i.e. after an equilibrium condition was reached) clusters were identified. The algorithm of cluster identification in an equilibrium condition of the system is obvious and is based on the following definition of the cluster: a particle is assigned to a cluster, if it adjoins at least one particle belonging to this cluster. Implementation of the algorithm selecting "isolated clusters" is quite a simple process which consists in creating a list of the particles and keeping a running list of clusters. The particles included in the list are analyzed sequentially. Each particle of this list must be checked for being joined with a particle which is a member of any cluster. If it is joined with that particle, it is removed from the list of particles and placed in the corresponding cluster on the list of clusters. In other case it is added to the list of clusters, but as a new cluster, etc.

The concept "contact particles" requires some explanation. The persistence of the analytical model connected with the final length of step δt results, strictly speaking, in the absence of contact particles in the final equilibrium condition, in the average clearance between the surfaces of the particles being $\delta t / 2$. Therefore, it is further considered that in an equilibrium condition particles contact if the clearance between them does not exceed $k_e \delta t$, i.e. if condition $|x_i - x_j| < r_i + r_j + k_e \delta t$ is fulfilled. Here k_e is a certain parameter which was taken to be $k_e = 1.2 - 1.5$.

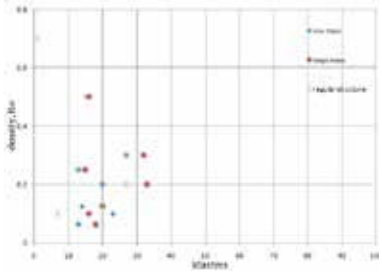


Figure 4: Distribution of clusters according to «the mass» in the hard sphere system for different volume concentrations

Sources: authors

The clusters are characterized by the number of particles contained in them (the mode number of the cluster or the dimensionless mass of the cluster - the cluster mass rated as the mass of one particle). As calculations of hard sphere systems show (Fig. 4) at low packing densities $\rho \le 0.3$ the bulk of the system accounts for clusters containing no more than 10-30 particles. However, when $\rho \ge 0.6$, more than 70 % of mass of the system is concentrated in one large cluster that provides cohesiveness of the system.

There is a logical question: how the size of the largest cluster in the system changes with the increase of the packing density, and which packing densities provide bound structure extending from one end of the system to the other. The critical packing density which provides cohesiveness of the system is called the percolation limit [16-18].

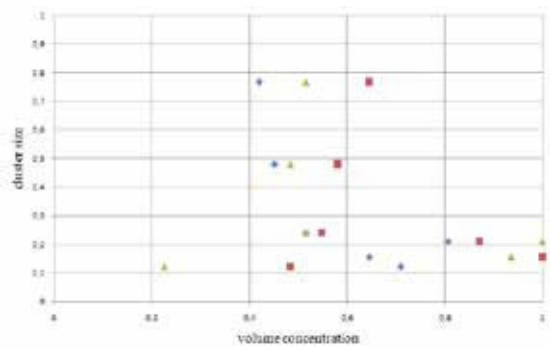


Figure 5: Dependence of the maximum size of the largest cluster of the hard sphere system on the volume concentration of spheres
Sources: authors

Fig. 5 shows the maximum size of the largest cluster of the hard sphere system related to the size of the system depending on the packing density.

It is obvious that if density is equal to $\rho \approx 0.4 - 0.6$ for the systems of spheres with the same diameter, the sizes of the largest cluster are close to the sizes of the whole system. Thus, these packing densities in the system provide a cluster extending to the entire system and ensuring its coherence.

If packing densities $\rho < 0.4$ the probability of building of a cluster, covering the entire system is close to zero. If packing densities $\rho > 0.6$ there are significant fluctuations in the sizes of clusters. At the same time the system can be formed of small clusters having dimensions substantially smaller than the system, and of large clusters, covering the entire system. The fluctuations decrease with increasing size of the system, and we can assert that for a system of infinite volume there will be a threshold density in the range of $\rho \approx 0.4 - 0.6$, above which the system with a probability of 0.9 forms a bound cluster spreading over the entire system. Packing densities above 0.6 provide only some isolated clusters whose dimensions are much smaller than the system. Thus, the packing density $\rho = 0.6$ can be considered the percolation limit for systems of spheres with the same diameter.

In the chemical stereology the concept of coordination number [19], defined as the number of contacts with near-neighbors is fundamental. Let's consider how the coordination number in the hard sphere system changes with the increase in the density of filling the space.

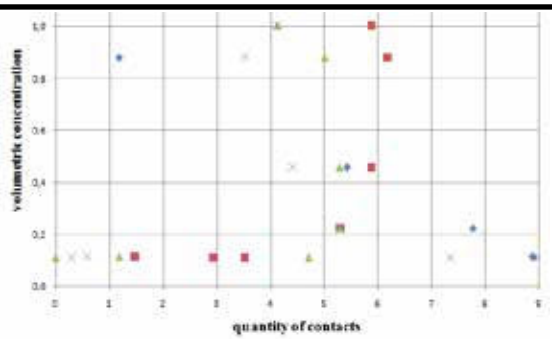


Figure 6: Distribution of number of particle contacts in the hard sphere system for different volume concentrations
Sources: authors

Fig. 6 shows the function of distribution of the number of contacts in systems with different volume densities. It is clear that when packing density increases, the number of contact particles grows. At low packing densities $\rho < 0.4$ prevail particles contacting with 1 or 2 particles or not contacting with any other particle. And at high packing densities $\rho \geq 0.8$ the system is dominated by particles contacting simultaneously with four or more particles. It should be noted that up to $\rho = 0.8$ any particles contacting simultaneously with six other particles, as it should be in close packing, are absent in the system.

POLYDISPERSE PARTICLE SYSTEM
The method of viscous suspension [6] equally well applicable to both monodisperse systems and for systems with random distribution of particles according to their size.

Illustratively let's consider some of the results of simulation of bidisperse hard sphere systems. It should be noted that bidisperse hard sphere systems can be considered as two-dimensional models HCM or as "cuts" of real HCM. They allow to vividly demonstrate how particles are distributed in real systems. For three-dimensional systems such demonstration is difficult.

It is believed that the system contains hard spheres of two different diameters. We will continue to use the dimensionless variables: all linear dimensions shall be attributed to the large diameter of the particles. Thus, large particle diameter is equal to unity, and the diameter of fine particles is equal to the predetermined value $d < 1$.

Let us introduce volume concentrations of large particles v_1 and of small particles v_d. And the packing density shall be represented as $\rho = v_1 + v_d$.

In publication [6] represent the structures of bidisperse systems for $d = 0.5$ and $v_1 = 0.5$, obtained in a simulation experiment by the method of viscous suspension. The analysis of results shows that large particles are grouped in compact units with fine particles on edges. Fine particles make linear extended structures, the length of which can reach dozens of particles. This is typical for relatively large diameters d of fine particles.

The picture slightly changes when fine particles diminish in sizes. The analysis of [6] shows that in this case fine particles make compact units located between several neighboring large particles. However, in this case as well the clusters of contact fine particles elongate in one direction. We can say that they form bits of "threads", arranged between the large particles. The above figures clearly show that on micro-level particles are unevenly distributed within the specified region. This primarily applies to fine particles. Large particles are more evenly distributed. The more concentrated large particles are (when concentration of fine particles is fixed) or fine particles (when concentration of large particles is fixed), the more unevenly fine particles are distributed in the specified volume and the larger clusters they make.

THE STRUCTURE OF HETEROGENEOUS CONDENSED MIXTURES
As suggested by S.A. Rashkovsky, method of viscous suspension [7] may be applied to simulation of a structure having broad class of composite materials which are filled with solid particles having almost spherical form. The author has made a mathematical simulation of metal containing and metal-free HCM structures by the method of viscous suspension.

In general, the system is characterized by volume concentrations of components equal to the ratio of the total volume of particles of a given type to the volume of the entire system. Let us introduce volume concentration of oxidizer particles v_{AP} and aluminum particles v_{IP}. An example of the simulation is shown in Fig. 7.

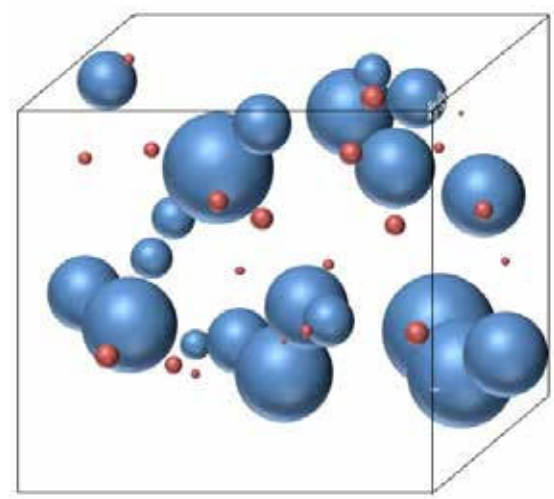


Figure 7: The three-dimensional structure of a metal containing HCM: large particles are polychloracetate (PCA); small particles are Al $(d = 0.25; v_1 = 0.5; v_d = 0.11)$

Sources: authors

The present study considered HCM where the mass content of aluminum ranged between 10 and 20% $(v_{Al} = 0.07...0.14)$ and the mass content of the oxidizing agent ranged between 40 and 70% $(v_{AP} = 0.38...0.66)$. The rest mass of HCM was the share of biding substances.

Further we used a simple formula

$$\gamma = (1 - v_{AP} - v_{Al})\gamma_B + v_{AP}\gamma_{AP} + v_{Al}\gamma_{Al}, \quad (3)$$

where $\gamma_B = 900 \frac{kg}{m^3}; \gamma_{AP} = 1950 \frac{kg}{m^3}; \gamma_{Al} = 2700 \frac{kg}{m^3}$ to assess density of HCM.

We also chose solid and impenetratable walls as a boundary condition to make computations.

At the beginning of each computation we conducted random initial placement of particles in the computational domain. This placement ended as soon as the desired volume concentrations of units were reached. Computation ended when

the right-hand sides of all the equations (2) vanished.

As we mentioned, the method of viscous suspension has no limitations as to the particle distribution according to their size and well converges up to volume concentrations close to the close packing [18]. There is a limitation as for the number of particles involved in the calculation connected with the computer's performance and time limits.

Calculations by the method of viscous suspension were carried out for a wide class of HCM containing several types of dispersed components, each having its own function in the distribution according to size. However, a system with particles of the same diameter already has all the properties inherent in real HCM. What's more? Such a simplification allows distracting from the complex analysis connected with the distribution of particle sizes.

CONCLUSIONS

There has been proposed an analog model and a new algorithm for random distribution of hard spheres in space (hard disks on the plane), which is applicable to any distribution of particle diameters and volume concentrations up to the maximum possible corresponding to close packing of the particles. The proposed method is called the method of viscous suspension.

There has been conducted a simulation of the structure of heterogeneous condensed mixtures containing one or two monodisperse particles in a wide range of their volume concentrations. We determined the main statistical characteristics describing the internal structure of HCM. It has been shown that the method of viscous suspension allows simulating an appearance of regular structures when the volume concentration of the particles is close to the maximum possible corresponding close packing.

It has been demonstrated that the contact particles make in HCM extensive clusters, whose dimensions increase with the increase of volume concentration of the particles.

We have studied the structure of clusters of contact particles. It has been demonstrated that the average coordination number of clusters containing the same number of particles can only take discrete values, which are determined by the presence cyclic elements in the structure.

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