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MODELING THE BUILDING MATERIALS: APPLICATIONS OF PARTICLE DYNAMICS

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ABSTRACT

Background: *In material science, the selection of the appropriate modeling method is usually performed on the basis of spatial scale. The particle dynamics, if properly combined with essential concepts of specific scale, overlaps a lot of spatial scales. Yet, for many dispersions in construction material science, the pair and external forces can be quite complex.* ***Methods:*** *Particle dynamics is combined with specific scalar criteria that allow to describe the kinetics of structure formation of building materials.* ***Results:*** *The representation of dispersion as particle system is formulated and standalone computation software is developed. We have demonstrated that time dependencies of criteria similar to average distance from the surface of each particle to the surfaces of four nearest particles allow to derive substantial data concerning structure formation at micro-scale level.* ***Conclusions:*** *In the present work we have proposed the model, discussed simulation software, and highlighted some modeling results that demonstrate the capabilities of said model and software. It is shown that the developed software can facilitate the insight that reduces time required for the design of novel materials.*

INTRODUCTION

Rapid design of high-performance and cost-effective building materials is not possible without numerical experiments. At present, many methods are available for modeling the structure and formation of materials that are to be used in construction industry. Depending on spatial scale, the important among these methods are:

(I) Exact, density functional, and semiempirical quantum calculations of atomic and molecular structure (lowest level, up to about 1 nm; these methods are often used for modeling polymeric, bituminous and sulfur binders [1]).

(II) Particle dynamics – quantum molecular dynamics (nanoscale level, up to 100 nm; modeling the properties of mineral binders [2]–[6]), classical (Newtonian) particle dynamics (structure forming of building materials at micro- and macrostructure levels, [7], [8]), dissipative particle dynamics (rheology of liquid phases and fresh mixes, [9]), multibody dynamics (micro- and macrostructure of building materials, assessment of mechanical properties, [10]).

(III) Smoothed-particle dynamics (rheology of liquid phases [11] and fresh mixes [12], fracture mechanics of macrostructure and construction units [13]) that, being meshless, is still often considered as finite element method.

(IV) Conventional finite element methods (macrostructure of materials, construction units).

(V) Geometric methods, that (again, depending on scale) are often combined with Monte-Carlo method [14], fracture mechanics [15], physical chemistry [16], percolation theory [14], [17], [18], particle dynamics and binder chemistry [19], [20].

Here, as before [21], we define the microstructure of building material as the spatial level where structure forming is mainly affected by surface effects (free surface energy, surface tension, wetting); the macrostructure is the level where structure forming is primarily affected by gravity and technological actions (pressure, vibration). The spatial boundary between macro- and microstructure depends on viscosity and specific surface energies; it is near to 100 μm.

It becomes obvious from the literature survey that particle dynamics – if it is properly combined with quantum chemistry, chemical physics, physical chemistry, chemistry, rigid body dynamics, etc. – overlaps wide range of scales; this is not surprising as the particle dynamics initially originated within celestial mechanics. Particle dynamics can be considered the best candidate for use as foundation for multiscale modeling that, by separating levels of descriptions and bridging them together within a framework of a single computational approach [22], permits computation of large scale systems while still yielding accurate results. For instance [5], results obtained by quantum molecular dynamics can be used for further assessment of mechanical values.

At the same time, every application of particle dynamics, including computational material science, requires careful selection of force fields and simulation algorithms. Considering the scales of primary interest – micro- and macrostructure – it have be to stated that particle dynamics models for these levels are always of semiempirical nature. Both the type and parameters of force field are usually selected on the base of thermodynamics of wetting, surface energies and rheology of dispersion. Whereas intermolecular pair forces are almost always attractive for long distances and repulsive for short ones, pair forces between particles of fine filler in many cases can assumed to be either always attractive (some lyophobic

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systems) or always repulsive (any lyophilic systems). Moreover, in case of solvation shells around filler and/or viscosity gradient near the surface of aggregates, the pair force can not longer be assumed to be directed along the line between the centers of particles. Thus, despite the fact that there is currently a lot of software suitable for particle dynamics simulations, many existing software is only of limited use in material science.

The aim of the present work is to tersely discuss the model and simulation software that can be used for multiscale modeling of building materials, and also to present some modeling results.

MATERIALS AND METHODS

We have already mentioned the model in [5], and further explained it in more detail in [23]. Thus, here it is appropriate only to highlight the key points and to describe the statistical values that are going to be monitored during simulation.
he motion law of particles in dispersion:

$$, \quad i = \overline{1, N} \, , \tag{1}$$

where m_i is the mass of i-th particle, $\mathbf{r}_i = (x_i; y_i; z_i)$ is the position of particle, k_i is the parameter that depends on form of the particle and viscosity of the dispersion medium, u_i is the velocity of the dispersion medium at point $\mathbf{r}_i$, U_i is the scalar force potential at the point $\mathbf{r}_i$, and N is the number of particles.

The potential in right side of (1) can be the sum

$$U_i = U_b(\mathbf{r}_i) + U_g(\mathbf{r}_i) + \sum_{\substack{j=1 \\ j \neq i}}^{N} U_p(r_{ij}), \tag{2}$$

of potential U_b of boundary interaction, gravitational potential U_g, and the pair potential $U_p(r_{ij})$ (here r_{ij} is the distance between surfaces of the particles). Unfortunately, such simple representation does not allow to take into account the extra viscous forces that are caused by crossed solvation shells.

The (1) can be rewritten in equivalent form

$$\begin{cases} \dot{\mathbf{r}}_i = \mathbf{v}_i \\ \dot{\mathbf{v}}_i = \mathbf{g} + \dfrac{1}{m_i}\left(\displaystyle\sum_{\substack{j=1 \\ j \neq i}}^{N} \mathbf{F}_{ij} + \mathbf{F}_{i,b} + \mathbf{F}_{i,e} \right), \end{cases} \tag{3}$$

where

$$\mathbf{F}_{ij} = -\mathbf{F}_{ji} = \frac{\mathbf{r}_{ij}}{r_{ij}} F_{ij}\left(r_{ij} - R_i - R_j\right)$$

is the pair force, F_{ij} is the modulus of this force:

$$F_{ij} = \frac{\partial}{\partial r} U_p(r_{ij}),$$

R_i is the radius of particle,

$$\mathbf{F}_{i,b} = \frac{\mathbf{n}_{i,b}}{n_{i,b}} F_{i,b}\left(n_{i,b} - R_i\right)$$

is the boundary force, $F_{i,b}$ is the modulus of this force:

$$F_{i,b} = \frac{\partial}{\partial n_{i,b}} U_b(n_{i,b}),$$

$\mathbf{n}_{i,b}$ is the vector drawn from the center of the particle to the nearest point of the boundary, m_i is the mass of the particle, $\mathbf{g}$ is the gravitational acceleration,

$$\mathbf{F}_{i,e} = 6\pi\eta R_i\left(\mathbf{u}_i - \mathbf{v}_i\right)$$

is the force of viscous friction, and $\mathbf{v}_i$ is the velocity of the particle.

The latter form allows to introduce arbitrary extra nonconservative force. In particular, the force that are due to solvation shells can assumed to be proportional to the area of the cross section; the direction of such force are along the $\mathbf{v}_i$ that is projected to the plane of the cross section [23].

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There can be three primary types of pair potential. For the lyophilic systems, this potential correspond to repulsion; thus, it can be taken in form

$$U_p(r_{ij}) = U_0 \left(\frac{r_0}{r_{ij}} \right)^k , \qquad (4)$$

where U_0 is the characteristic energy, r_0 is the characteristic distance, k is the empirical parameter (for intermolecular forces, it is conventional to assume $k = 12$).

In general case, the pair potential in lyophobic systems has to represent both repulsion and attraction:

$$U_p(r_{ij}) = U_0 \left(\left(\frac{r_0}{r_{ij}} \right)^k - 2 \left(\frac{r_0}{r_{ij}} \right)^l \right) , \qquad (5)$$

where l is the empirical parameter ($l = 6$ for intermolecular interaction).

For dispersions with solvation shells, the pair potential can be taken in form of sum of Mie and Morse terms:

$$U(r_{ij}) = U_0 \left(\left(\frac{r_0}{r_{ij}} \right)^k - 2 \left(\frac{r_0}{r_{ij}} \right)^l + \exp\left(-(r_{ij} - r_0)^2 \right) \right) . \qquad (6)$$

To properly analyze the results, it necessary not only to visualize the particle positions, but also to monitor some statistical parameters during the simulation of the dispersion. We propose to monitor the following parameters:

(I) Average distance from the surface of each particle to the surfaces of four nearest particles (along with standard deviation):

$$R_{4av} = \frac{1}{N} \sum_{i=1}^{N} R_{4i} , \qquad (7)$$

$$R_{4std} = \sqrt{ \frac{1}{N-1} \sum_{i=1}^{N} (R_{4i} - R_{4av})^2 } , \qquad (8)$$

where R_{4i} is the distance from the surface of i-th particle to the surfaces of four nearest particles.

(II) Average number of particles, distances to surfaces of which are less than some predetermined value, e.g. radius of the current particle (along with standard deviation):

$$Nn_{av} = \frac{1}{N} \sum_{i=1}^{N} Nn_i , \qquad (9)$$

$$Nn_{std} = \sqrt{ \frac{1}{N-1} \sum_{i=1}^{N} (Nn_i - Nn_{av})^2 } , \qquad (10)$$

where Nn_i is the number of particles, distances to surfaces of which from i-th particle are less than some predetermined value.

(III) Average number of particles in k-th parallelepiped subdomain of bounding box of all particles (along with standard deviation):

$$Ns_{av} = \frac{1}{N} \sum_{k=1}^{K} Ns_k , \qquad (11)$$

$$Ns_{std} = \sqrt{ \frac{1}{K-1} \sum_{k=1}^{K} (Ns_k - Ns_{av})^2 } , \qquad (12)$$

where Ns_k is the number of particles in k-th parallelepiped subdomain of bounding box of all particles, K is the number of equal subdomains (in most cases it is enough to subdivide the bounding box into $K = 27$ subdomains).

(IV) Average absolute value of velocity of the particles (along with standard deviation):

$$v_{av} = \frac{1}{N} \sum_{i=1}^{N} |\mathbf{v}_i| , \qquad (13)$$

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$$v_{std} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(\left|\mathbf{v}_i\right| - v_{av}\right)^2} \; , \tag{14}$$

where $\mathbf{v}_i$ is the velocity of i-th particle.

The proposed parameters (7)–(14) allow to make decisions about local (7)–(10) and global (11), (12) homogeneity of the dispersion. Parameters (13) and (14) can be used as indicators of stationary state.

RESULTS

Simulation software

The proposed model (including (3)–(6)) along with routines for (7)–(14) is implemented as standalone portable software [24] that is controlled by command files of specific format. At any moment during simulation it is possible to export representation of the system into MaxScript (built-in language of Autodesk 3DS MAX package) program that can be used for visualization.

The boundary of the modeling volume can be almost arbitrary in shape (though, if it is not a box, than parameters (11) and (12) are useless) due to its constructive solid geometry (CSG) representation; currently, planes, cylinders and spheres can be used in CSG tree. The fragments that define the CSG trees are embedded in the command file. Within the domain defined by any CSG tree, particles can be distributed either on equidistant basis or in according with some 1D, 2D, and 3D probability distribution (currently, uniform and normal distributions are implemented for any number of dimensions). In latter case, the trial-end-error approach is used to preserve minimum particle-to-particle separation distance. The examples of initial distributions are presented in [Fig. 1].

Fig. 1: Examples of initial particle distributions, left to right: simple cubic lattice of particles inside spherical boundary; 1D-normal, 2D-uniform distribution of particles inside cylinder; 3D-uniform distribution of particles inside complex CSG object.

Solution of (3) is performed by embedded Runge-Kutta method of order 4.5. Obviously, this method is not tailored specifically for particle dynamics, but – for real world dispersions – requirements for stability and consistent way to control the time step are often the primary arguments that determine the choice of integration algorithm. For now, we are considering the improvement of integration scheme as further work. Real-time visualization is also implemented in solver, though quality of the produced images are still far from typographic. Such visualization is only suitable for monitoring of the solution process.

The simulation software [24] is distributed under BSD license, but currently available only in source form. For some extra details, the paper [21] can also be referred.

Example of simulation

As an illustration we have performed comparative analysis of four lyophobic systems. The (5) was used as pair potential. Conventional values of 12 and 6 are used as k and l, respectively. The orders of magnitude for characteristic energy U_0 and characteristic distance r_0 were estimated earlier [25][26,27] during analysis of surface effects in the microstructure of disperse filled polymer matrix composites of different type and volume fraction v_f of the fine filler. The parameters of the systems are summarized in [Table 1]. All particles were uniformly distributed inside the sphere; diameters of particles were equal to 10 um.

Table 1: Parameters of the lyophobic systems

Number of system	v_f	U_0, J	r_0, nm
1	0.1	10^{-23}	100

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2	0.1	10^{-23}	1000
3	0.1	10^{-26}	1000
4	0.01	10^{-23}	1000

Time dependencies for local homogeneity parameters (7) and (8) are presented in [Fig. 2-5]. Final configurations of particles are presented in [Fig. 6].
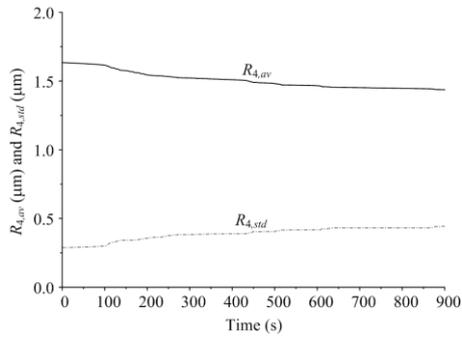
Fig. 2: Time dependencies for (7) and (8), system #1.
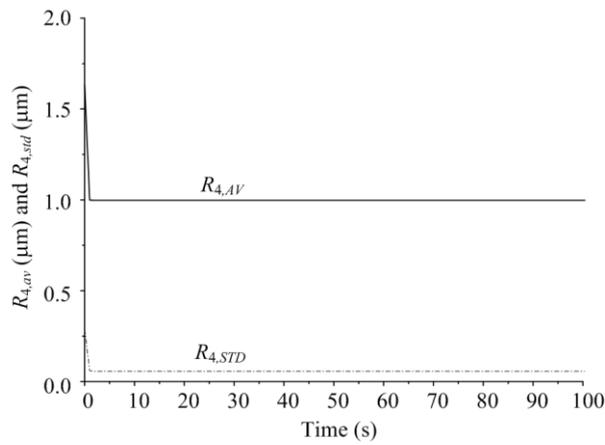
Fig. 3: Time dependencies for (7) and (8), system #2.
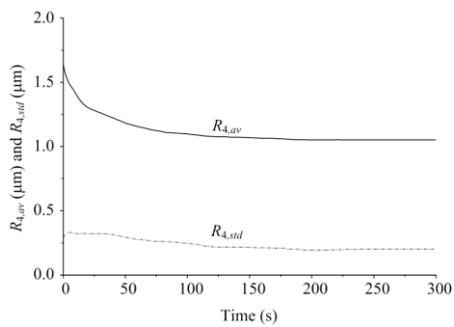
Fig. 4: Time dependencies for (7) and (8), system #3.
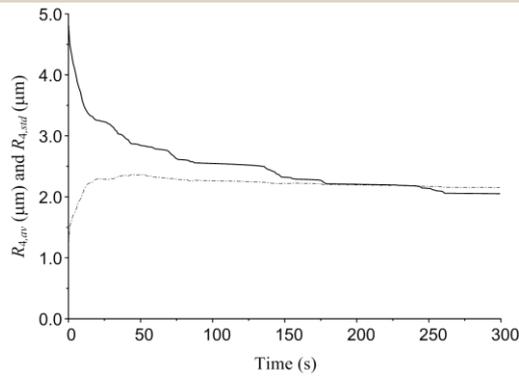
Fig. 5: Time dependencies for (7) and (8), system #4.

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At the level of microstructure, the primary factors of influence are surface forces. It was stated [18] that such forces can lead to the forming of clusters, which influence significantly both on rheological properties of mixes and on the operational properties of the building materials.

As it follows from [Fig. 2], during the structure forming in system #1, the average R_{4av} slowly decreases. This can point to the fact that there can be cluster formation. However, such clusters are comprised from relatively small fraction of filler's particles [Fig. 6(a)]. Because of this, local homogeneity of the system #1 decreases over time ([Fig. 2], R_{4std}).

For system #2 the characteristic distance r_0 becomes the same order of magnitude as the size of the particles. In this case the rate of structure forming increases dramatically. During several seconds the entire system moves to the nearest local minima of potential energy. And, since the R_{4av} becomes almost exactly equal to characteristic distance r_0 [Fig. 3], this minima can even be considered as global. Most particles become parts of one percolation cluster [Fig. 6b]; this is also reflected by fast increase of local homogeneity ([Fig. 3], sharp decline of R_{4std}).

The characteristic distance r_0 is the primary factor that controls the cluster forming. For the system #3, value of characteristic energy is lowered by three orders of magnitude. Nevertheless, there are no principal changes in the peculiarities of cluster formation [Fig. 6c]: the R_{4std} is still decreases over time [Fig. 4]. The only difference is in that the rate of cluster forming is also slowed down by three orders of magnitude.
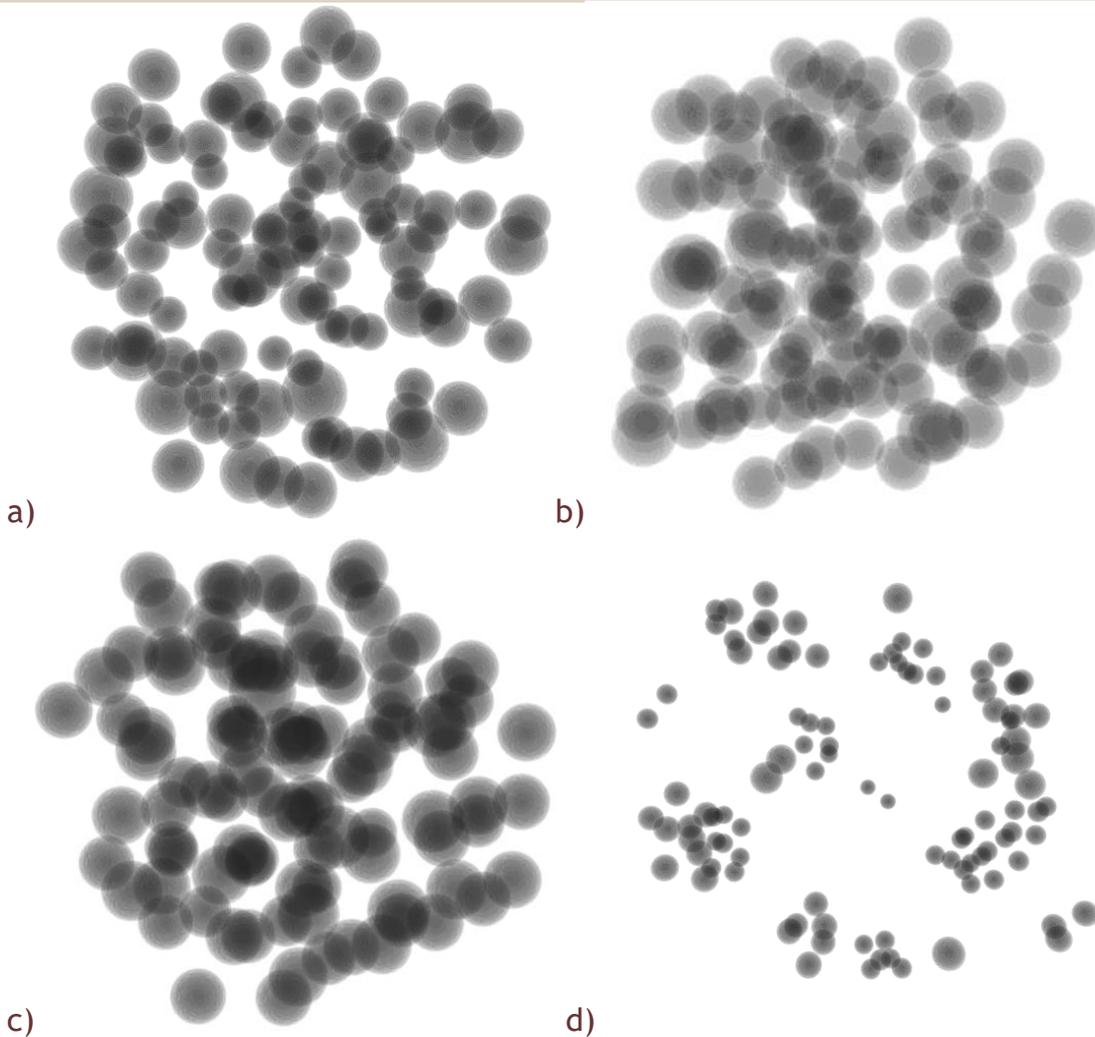
Fig. 6: Final configuration of particles, for systems: a – #1, b – #2, c – #3, d – #4.

And, finally, the essential feature of system #4 is the significantly lower volume rate of the filler. For this system, initial values of average distances between particles become considerably large as compared to ones for previous two systems. This, to some extent, can be viewed as the decrease of characteristic distance r_0: as for the first system, the local homogeneity decreases if compared with the initial value ([Fig. 5], R_{4std}). There are, albeit, distinctions. The cluster forming process can be divided into stages (the boundary is near to 150 s, [Fig. 5]. During the first stage numerous isolated clusters are formed from particles that were initially near to each other. Forming of such clusters is reflected by substantial decrease of R_{4av}; but it must be noted that even to the end moment the R_{4av} is twice as large as characteristic distance r_0. During the second stage the R_{4av} slowly decreases, whereas R_{4std} remains practically constant. No percolation cluster is formed in the system #4; there are only isolated clusters [Fig. 6(d)].

CONCLUSION

Till present, no theoretical description of building material allows to derive a model for certain prediction of key operational properties.

Yet, the advantage of the particle dynamics is its both micro- and macroscale considerations, which allow to apply different levels of resolution, from microstructure up to coarse-grained macrostructure. It is shown in the present work that particle dynamics is the promising approach for simulating the microstructure of building materials, in particular – disperse filled polymer matrix composites. The performed simulations are useful for understanding the peculiarities of cluster forming in dispersions and facilitate the insight that can significantly reduce time required for the design of novel high-performance building materials.

The directions of further efforts will be extensive verification of simulation software, parallelization, code cleanup and implementation of the advanced visualization features.

CONFLICT OF INTEREST

The authors declare no competing interests in relation to the work.

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