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Effect of a Solid Wall on the Formation of a Porous Layer Structure

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Abstract—The formation of a near-wall layer in a bulk material has been studied by computer-aided modeling. Numerical calculation results have been compared with the experimental data.

Keywords: porosity, packing of particles, near-wall layer, adhesion coefficient
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INTRODUCTION

Liquid or gas filtration depends directly on the porosity of a filtration bed. The structure of a porous material is usually modeled by the packing of particles. The works [1, 2] were devoted to the packing of spherical particles and performed using the method of discrete elements. In contrast to continuous medium methods, this method takes into account phenomena at the level of individual pores and particles [3, 4]. The approaches and results of the above works were used in the studies [5–8] to solve the problems of particle sedimentation, liquid filtration on bulk filters, and bulk material flows. The experimental studies [9] have revealed an oscillatory character of the bulk bed porosity near the solid wall of a container, into which spherical particles were dispersed.

This work is devoted to the numerical modeling of the formation of a near-wall layer in a bulk filter. The mathematical model we used was the statistical model of the formation of the filtration bed [7].

FORMULATION OF THE PROBLEM

The formation of a bulk material bed is modeled by the random packing of spherical particles. To accomplish this, particles with arbitrary selected coordinates at the top face of a unit cube pass towards its bottom. The initial coordinates of a particle are determined by a random number generator. The particle is affected by the gravity force $\mathbf{F}_g$ and the adhesion force $\mathbf{F}_{ad}$ upon its contact with another particle. The forces of elastic interaction and friction between the particles are not taken into account. The force of resistance to the motion of a particle in a medium is also neglected. The gravity force is determined as

$$\mathbf{F}_g = mg, \quad (1)$$

where g is the acceleration due to gravity.

The adhesion force is written in the form [10]

$$\mathbf{F}_{ad} = \frac{A}{6H_0^2} r^* n, \quad (2)$$

where A is the Hamaker constant, H_0 is the distance between the surfaces of interacting particles (intermolecular distance), $r^* = \frac{2r_1r_2}{r_1 + r_2}$ is the reduced radius of colliding particles, and $\mathbf{n}$ is the unit vector.

The adhesion force is oriented from the center of a static particle to the center of a sedimenting particle. The particle can adhere to a previously settled particle upon collision. The forces that act on a particle are schematized in Fig. 1. The equilibrium (adhesion) condition is written in the form of a critical value for the angle α as follows:

$$\cos(\alpha) \le K, \quad (3)$$

where K is the adhesion coefficient representing the ratio of the force retaining a mobile particle on a static particle to the force trying to shear it away. In this formulation, the adhesion force is the retention force and the gravity force is the shear force.

The adhesion coefficient K varies from 0 to 1. In practice, the adhesion coefficient is usually determined experimentally.

If the particle has not adhered to an earlier settled particle, it continues to move along a tangent to the static particle surface at a velocity determined as $\mathbf{v}' = \mathbf{v} - \mathbf{n}(\mathbf{vn})$, where $\mathbf{v}'$ is the particle velocity after collision, $\mathbf{v}$ is the particle velocity before collision, and $\mathbf{n}$ is a unit vector passing from the center of a static particle to the center of a moving particle.

The stop condition for a particle is the attainment of contact with the bottom cube face or a stable position with three support points. The particle cannot change its position after being stopped.

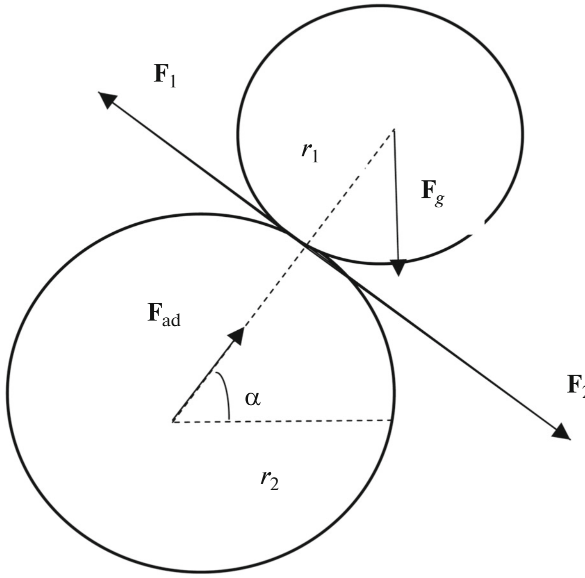

Fig. 1. Scheme of acting forces.

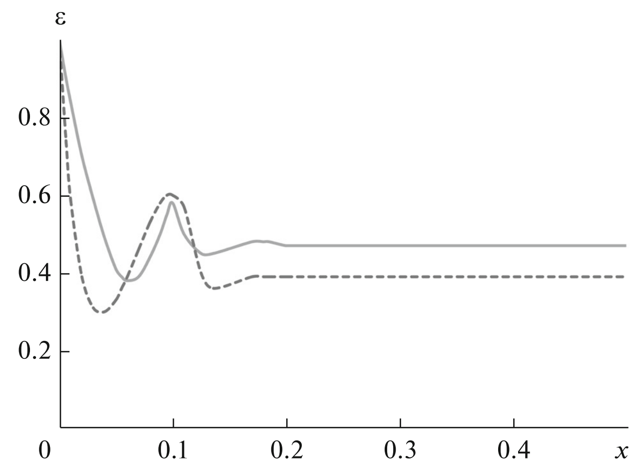

Fig. 2. Porosity distribution along the container: calculation of a porous bed formed of a monodisperse ensemble of particles (solid), experimental bulk bed porosities [9] (dashed).

For each set of moving particles, the system of mass center motion equations is written as follows:

$$\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{F}_i}{m_i}, \quad \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \tag{4}$$

where m_i is the mass of the particle, t is the time, $\mathbf{x}_i$ is the mass of the center coordinate, v_i is the velocity vector of the particle, and $\mathbf{F}_i$ is the resulting force acting on a particle.

It is assumed that the particle i at a certain time moment has N_i points of contact with other particles and/or the computational region boundaries, and the resulting force $\mathbf{F}_i$ is determined as follows:

$$\mathbf{F}_i = m_i\mathbf{g} + \sum_{j=1}^{N_i} \mathbf{F}_{\text{ad}}(r_i r_j). \tag{5}$$

A more detailed mathematical formulation of the problem in terms of the method of discrete elements is given in [8].

The formulated problem is solved via the numerical integration of equation set (4) with allowance for Eqs. (1)–(3) and (5) and the boundary and initial conditions [8]. The numerical implementation of the problem is performed using the CKIF-Cyberia multiprocessor cluster with the MPICH code parallelization library [11].

RESULTS AND DISCUSSION

Figure 2 depicts the results of calculating the porous bed formed of a monodisperse ensemble of particles along the x axis of the container are shown as solid lines. The dimensionless particle radius was taken equal to 0.05 (nondimensionalization was performed with respect to the container size), and the force of adhesion between particles and a particle and the container wall was neglected, i.e., the adhesion coefficient was taken equal to zero. The porosity at the container wall is unity, as a sphere contacts the wall surface at a point. The porosity is observed to further fluctuate. The porosity is minimal (0.38) at a distance of 1.5 particle radii from the container wall and maximal (0.55) at a distance of two radii, and fluctuations occur up to five particle radii. The period of fluctuations is equal to the particle diameter, and their amplitude descends to attain a porosity of 0.42. The dashed line in Fig. 2 shows the porosities of the experimental bulk bed [9]. The comparison of calculated and experimental results demonstrates their qualitative agreement.

The results of calculating the porosity of a monodisperse packing along the x axis of the container at different adhesion coefficients are plotted in Fig. 3. As the adhesion coefficient increases, the probability of adhesion between particles grows, and the bulk bed become looser, i.e., the average porosity over the entire container volume increases. The adhesion force imparts a dissipative character to the oscillatory porosity change process, so the amplitude of fluctuations descends more quickly than in the absence of adhesion.

The volume filled with a mixture of coarse and fine balls will have a lower porosity than the same volume filled with coarse or fine balls alone (this statement is true when the adhesion force is small). In a mixture, fine balls fill the space between coarse balls. The porosity of the mixture depends on the ratio between particle and fraction sizes [8].

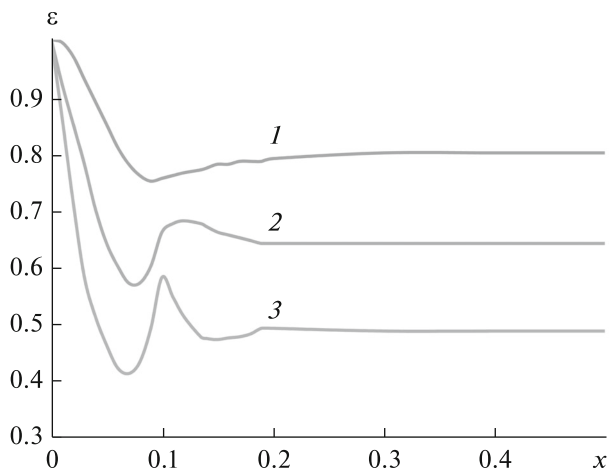

Fig. 3. Porosity distribution at a different adhesion coefficient K of (*1*) 1, (*2*) 0.2, and (*3*) 0.6.

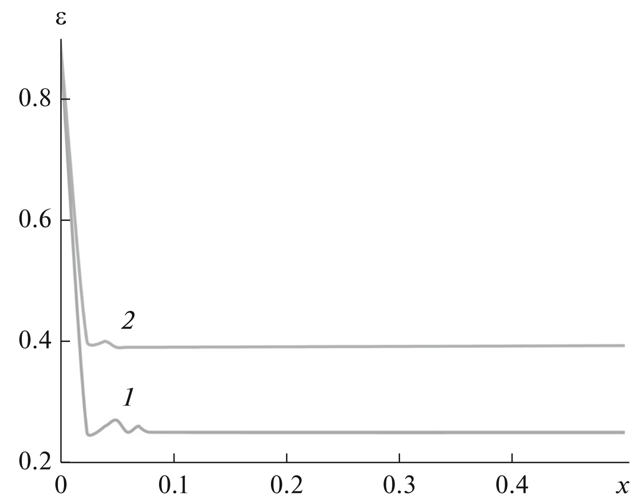

Fig. 4. Calculated bed porosity distribution for a bidisperse packing at (*1*) $r_1/r_2 = 10$, $K = 0$ and (*2*) $r_1/r_2 = 10$, $K = 0.3$.

The results of modeling a a near-wall layer for a bidisperse packing are shown in Fig. 4. The content of fine particles is 24 vol %, which corresponds to the most dense packing [8]. Curve *1* corresponds to the calculation at $r_1/r_2 = 10$ and $K = 0$. The fluctuations in porosity near the container wall are determined by the size of a fine particle; then, the presence of coarser particles begins to affect the character of fluctuations. As the distance from the wall grows, the fluctuation amplitude decreases and the porosity stabilizes at a value of 0.25. Curve *2* corresponds to the calculation at $r_1/r_2 = 10$ and $K = 0.3$ (close to natural materials, such as sand and coal). As the distance from the wall grows, the porosity stabilizes at a value of 0.38.

Under real conditions, bulk filters are formed of particles of nearly the same size. A porous bed of sand particles and a polydisperse ensemble of admixture particles is formed during the purification of water from solid admixture particles, e.g., on a sand bed. The effect of a solid wall on the formation of a near-wall layer in a four-fraction mixture was estimated by calculation. The ratio of particle sizes was taken equal to $r_1/r_2 = 10$, $r_1/r_3 = 20$, and $r_1/r_4 = 30$ (r_1 is the sand particle radius). The volumetric fraction content was the same, and the adhesion coefficient was $K = 0.3$. The calculation results show that the porosity abruptly descends from 1 at the container wall to 0.23. The oscillatory character of the porosity is hardly observed (on the considered scale of particle size). This is explained by the presence of particles, which differ considerably from each other in size and the dissipative action of the adhesion force.

The picture of container filling with particles is symmetric, so the results of calculating the porosity along the x axis (to only $x = 0.5$) are given in Figs. 2–4.

CONCLUSIONS

Using a wide size spectrum of particles in bulk filters reduces the width of the near-wall layer, the density of the bulk bed and the parameters of the near-wall layer can be controlled by selecting the sizes of particles and the percent ratio of fractions. When designing filtration equipment, it should be taken into account that the filtration rate is maximal along the solid wall. To equate the liquid flow rate over the cross section of the container, it is necessary to reduce the thickness of the near-wall layer. To accomplish this, it is reasonable to use finely disperse material to lad bulk filters near the walls.

NOTATION

- A Hamaker constant, J;
- $\mathbf{F}_i$ resulting force that act on a particle;
- $\mathbf{F}_{ad}$ adhesion force;
- H distance between the surfaces of interacting particles, m;
- K_{ad} adhesion coefficient;
- r^* effective radius of two particles (reduced to the computational region size);
- $\mathbf{v}_i$ particle velocity vector;
- $\mathbf{x}_i$ mass center coordinate;
- ε filter porosity.

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