Numerical simulation of filtration of mine water from coal slurry particles

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Abstract. The discrete element method is applied to model a technology for clarification of industrial waste water containing fine-dispersed solid impurities. The process is analyzed at the level of discrete particles and pores. The effect of filter porosity on the volume fraction of particles has been shown. The degree of clarification of mine water was also calculated depending on the coal slurry particle size, taking into account the adhesion force.

1. Introduction
Clarification of liquid containing fine particles of solid impurities is usually carried out by filtration of the liquid through a layer of porous material, an example of which is a bulk layer. There has been a considerable progress in solving the problems of fluid flow in a medium based on the continuum mechanics assumptions [1; 2]. However, the issues directly related to the formation of the bulk layer structure and the deposition of impurity particles in the channels of the porous medium have been beyond the scope of research. Answering these questions, relying only on the methods of continuum mechanics, seems to be problematic as the process is occurring at the level of discrete particles.

The structure of a bulk layer is modeled as a packing of spherical particles, which is numerically simulated using a discrete element method. The theoretical basis of the discrete element method is presented in [3; 4]. This method allows one to explore media composed of discrete particles. In [5; 6] the discrete element method was applied to modeling the processes of formation of filtration and sedimentation layers of a bulk material. The process of liquid clarification from solid impurities is analogous to the formation of sediments.

This study is devoted to numerical simulation of fluid clarification to remove suspended solid particles using the discrete element method. As a mathematical model, we apply the model of formation of a porous layer of a bulk material [6].

2. Problem formulation
A cube with an edge of unit length is filled with a monodisperse ensemble of sand particles with a radius of \( R \). This results in the formation of a filtration layer with the porosity of \( \varepsilon_0 = 0.42 \). The volume between the particles, equal to \( (1-\varepsilon_0) \), is filled with water. Then impurity particles with a radius of \( r = \text{const} \) are subsequently let into the cube through its top face with randomly selected coordinates towards the bottom of the container. It is assumed that a particle experiences the force of
gravity, $F_g$, the force of resistance to motion through the medium, $F_{st}$, and, if contacted with other particles, the adhesion force, $F_{ad}$. The elastic interaction and friction forces are not taken into account.

The number of particles in the filtration layer is defined as equal to $N_g$, while that of impurity particles is $N_f$. An impurity particle with a radius of $r_i$ may interact with both impurity particles and those of the filtration material. The resulting force for the particle $r_i$ can be expressed as

$$F_i = F_{g,i} + F_{st,i} + \sum_{j=1}^{N_f} \left[ F_{ad}(r_i, r_j) \right] + \sum_{j=1}^{N_g} \left[ F_{ad}(r_i, R_j) \right].$$  \hspace{1cm} (1)

For each impurity particle, $r_i$, the set of motion equations for its center of mass has a form of

$$\begin{align*}
\frac{dv_i}{dt} &= \frac{F_i}{m_i}, \\
\frac{dx_i}{dt} &= v_i, \quad i = 1..N_f,
\end{align*}$$  \hspace{1cm} (2)

where $m_i$ is the particle mass, $t$ is the time, $F_i$ is the resulting force acting on the particle, $x_i$ is the spatial coordinate of the particle center, and $v_i$ is the particle velocity vector.

The force of gravity is written as

$$F_{g,i} = m_i g,$$  \hspace{1cm} (3)

where $g$ is the acceleration due to gravity.

A significant computing load is related to the calculation of a continuous interparticle medium that limits the number of particles involved in the simulation, so we use a simplified description of such a medium.

The force of resistance to the particle motion through the medium is calculated by the Stokes law:

$$F_{st,i} = -6\pi \mu \nu r_i v_i,$$  \hspace{1cm} (4)

where $\mu$ is the dynamic viscosity of the fluid.

The adhesion force (in the case of electrically neutral fluid between the particles) is determined by the expression [7]:

$$F_{ad} = \left[ \frac{A}{6H_0} \right] e = K_{ad} * r^* \hat{e},$$  \hspace{1cm} (5)

where $A$ is the Hamaker constant, $H_0$ is the distance between the surfaces of interacting particles (the intermolecular distance), $r^* = \frac{2\nu r_j}{r_i + r_j}$ is the equivalent radius of colliding particles, $e$ is the unit vector directed from a motionless particle $r_j$ to a depositing one $r_i$, $K_{ad}$ is the adhesion coefficient.

3. Boundary and initial conditions

Since the problem is solved in terms of discrete elements, the boundaries of the container are represented by the partial surfaces of pseudoparticles with radii of $r = r_b$ \hspace{1cm} (where $r_b$ is constant and its value is determined so that within the cube concerned the deviation of the sphere surface from the plane is negligible, for example, $r_b = \infty$) and coordinates of $x_{bi}$ $\hspace{1cm}$ (where $i = 1, \ldots, 5$), namely:

1. $\{0.5, 0.5, -r_b\}$ for the bottom boundary;
2. $\{-r_b, 0.5, 0.5\}$ for the left boundary;
3. $\{r_b + 1, 0.5, 0.5\}$ for the right boundary;
4. \((0.5, -r_y+1, 0.5)\) for the front boundary;
5. \((0.5, r_y+1, 0.5)\) for the back boundary.

The boundary conditions are formulated as follows:

\[ x_{bi} = \text{const} \]
\[ |v_{bi}| = 0, \quad i = 1, \ldots 5. \]  

(6)

The initial conditions for the set of particles \(N_r\) are the following:

\[ x_{i,\text{initial}} = \text{random} ; \]
\[ v_{i,\text{initial}} = \text{const} , \]  

(7)

where \(\text{random}\) is an arbitrary real number, from 0 to 1, uniformly distributed. The initial coordinates of the particles, although being random, satisfy the no-intersection condition for any \(i\) and \(j\), namely:

\[ |x_i - x_j| > r_i + r_j . \]

The most complete mathematical formulation of the problem is presented in [6].

4. Numerical simulation

To solve the problem numerically, we integrate the set of equations (2) taking into account expressions (1, 3-5), boundary (6) and initial (7) conditions. When considering the problem of clarifying industrial waste waters from solid particles by means of bulk filters, the following assumption is used. When an impurity particle collides with a previously deposited one or a particle of the filtration material, it will either adhere to one of them or change the vector of its velocity and continue moving along the surface of contact.

A diagram of the forces acting on a particle \(r_i\) while colliding with a particle \(r_j\) (note that \(r_j\) can be both a particle of the filtering material and a previously deposited impurity particle) is shown in Fig. 1.

![Figure 1. Diagram of interaction between particles](image)

The condition for a particle \(r_i\) to stop its motion, i.e. to adhere to one of the particles mentioned above, is determined by the balance between forces holding it on the surface of a particle \(r_j\) and forces tending to continue its motion.

The holding force is \(|F_1| = |F_{\text{ad}}|\), whereas the moving force is \(|F_2| = |F_{g,i} + F_{a,i}|\).

5. Results and discussion

The input parameters were the following: spherical sand particles with a radius of \(R = 5 \times 10^{-4} m\) (in the dimensionless form, \(R = 0.005\), which was derived by dividing the initial radius by the cube width equal to 1); the packing porosity of the sand layer, \(\varepsilon_0 = 0.42\); spherical coal particles with a radius of \(r\)
ranged from \( r = R/10 \) to \( r = R/35 \); the adhesion coefficient, \( K_{\text{ad}} = 110^2 \text{n/m} \); the distance between the surfaces of interacting particles, \( H_0 = 4 \times 10^{-8} \text{m} \); the viscosity of water, \( \mu = 10^{-3} \text{Pa s} \); the density of coal, \( \rho_y = 1.7 \times 10^3 \text{kg/m}^3 \).

Fig. 2 shows the results of calculating the dependence of the porosity in the bidispersed packing (\( R/r = 30 \)) on the volume fraction of fine particles (\( V_r/V \)), where \( V_r \) is the dimensionless volume of fine particles and \( V \) is the volume of the unit cube. Curve 1 corresponds to the calculation in the absence of the adhesion force (\( K_{\text{ad}} = 0 \)), Curve 2 corresponds to the calculation taking into account the adhesion force between impurity particles and sand particles as well as between impurity particles themselves.

![Figure 2. Dependence of porosity on volume fraction of impurity particles](image)

In the absence of adhesive interaction at points \( V_r/V = 0 \) or 1 the porosity of the packing is equal to 0.42, as at these points there is a set of monodisperse particles (either pure sand or impurity particles).

When adhesive interaction is taken into account, at the point \( V_r/V = 0 \) the porosity equals \( \varepsilon = 0.42 \), whereas at the point \( V_r/V = 1 \) it is \( \varepsilon = 0.58 \) and determined by the adhesion force between impurity particles.

Fig. 3 depicts the results of calculating the dependence of the fluid clarification degree, \( M \), on the particle size ratio, \( R/r \). Here, \( M = (n_1/n_2) \times 100 \% \), \( n_1 \) is the number of impurity particles retained by the filter, \( n_2 \) is the number of impurity particles passed from the upper face of the cube. Curve 1 corresponds to the calculation without adhesion (\( K_{\text{ad}} = 0 \)) and Curve 2 shows the calculation taking adhesive interaction into account. As follows, in the absence of adhesion the impurity particles whose size is \( r = R/20 \) are almost not trapped by the sand layer with a thickness of 0.1 m. Taking into account adhesive interaction results in trapping 58% of the impurity particles whose size is \( r = R/10 \) and 2% for the particles whose size is \( r = R/35 \) using the sand layer with a thickness of 0.1 m.
To improve the degree of clarification of water containing particles of a smaller size, it is necessary to increase the thickness of the sand layer or to use appropriate surfactants to enhance the adhesion interaction between particles.

As seen in Fig. 4, the solid line shows the results of calculating the porosity of the layer along the container when the adhesive force between particles, a particle and the wall of the container was not taken into account. At the wall of the container the porosity is equal to unity because a particle contacts the surface at this point. Further, the porosity is observed to be fluctuating up to five particle radii. The dotted line in the figure shows the experimental values of the porosity for the bulk layer borrowed from [8]. Comparison of the calculated and experimental results shows their qualitative agreement. When filtering mine waters, the space between sand particles is filled with smaller coal slurry particles, with the thickness of the near-wall layer being determined by the latter ones. In using sand filters in the coal industry, the influence of the near-wall layer can be neglected since its thickness is much smaller than that of the filter.

The filter is governed by the total pressure drop in the deposited, blocking and pure sand layers [9]. The layer of sand lying below the blocking one performs no filtering function, but it increases the pressure drop, thereby increasing the energy consumption of sewage treatment plants. Therefore,
solving the task of clarifying fluid from a polydisperse ensemble of solid particles, it is necessary to consider this factor.

Numerical implementation of the problem was performed using the computer program PORA [10] on the multiprocessor cluster SKIF-CYBERIA.

6. Conclusions
The calculation method proposed allows one to consider the process of filtration of fluid at the level of discrete particles and pores, to determine the degree of clarification of mine waste water containing fine coal slurry particles and to optimize the degree of filter loading depending on the filtrate parameters and the operating mode of treatment facilities. The results obtained can be used for designing bulk filters.

References
[1] Zhuzhikov V.A. Fil'trovanie: teoriya i praktika razdeleniya suspensiy [Filtration: theory and practice of suspension separation]. Moscow: Khimiya, 1971. 441 p.
[2] Wakeman R.J., Tarleton E.S. Filtration: equipment selection, modeling and process simulation. Oxford, UK; New York: Elsevier Advanced Technology, 1999. 446 p.
[3] Zhu H.P., Zhou Z.Y., Yang R.Y., Yu A.B. Discrete particle simulation of particulate systems: theoretical development // Chemical Engineering Science. 2007. Vol. 62, is. 13. P. 3378-3396.
[4] Zhu H.P., Zhou Z.Y., Yang R.Y., Yu A.B. Discrete particle simulation of particulate systems: a review of major applications and findings // Chemical Engineering Science. 2008. Vol. 63, is. 23. P. 5728-5770.
[5] Nesse Th., Dueck J., Dyachenko E. Simulation of filter cake porosity in solid/liquid separation // Powder Technology. 2009. Vol. 193. P. 332-335.
[6] Dyachenko E.N., Dueck J. G. Computer simulation of porous layers based on the method of discrete elements // Journal of Engineering Physics and Thermophysics. 2013. Vol. 86, is. 6. P. 1315-1327.
[7] Israelachvili J. Intermolecular and surface forces. San Diega: Academic Press, 1955. 450 p.
[8] Brayer H. Grundlagen der Einplazen and Mehrphasenstromunge. Aarau, Switzerland: Sauerlander, 1971. 955 p.
[9] Vasenin I.M., Dyachenko N.N., Dyachenko L.I. Osvetlenie shakhtnykh vod na sloe peska [Clarification of mine water by filtering it through a sand bed] // Isvestiya Vysshikh Uchebnykh Zavedenii. Gornyi Zhurnal. 2004. Vol. 6. P. 50-54.
[10] Dyachenko E.N., Minkov L.L. Raschet formirovaniya nasypnogo sloya iz polidispersnykh chastits staticeskim metodom [Calculation of bulk layer formation from polydisperse particles by the static method]. Computer Program Patent, no. 2013615471 issued by Pospatent (June 10, 2013).