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Numerical simulation of mixing and segregation of granular material

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1. Introduction

Granular materials of various forms are ubiquitous in nature and technology. They exhibit a rich variety of phenomena and, depending on circumstances, can have properties similar to either solids, liquids or gases [1], or behave in a completely different manner. Existing theories of continuous mechanics or statistical physics have only limited applications for description of granular media, and a unified theory encompassing all the granular phenomena is still missing [2, 3]. An ability to describe and predict the conduct of granulated materials is important for technological applications in industry where bulk materials are routinely handled. On the other hand, granular media is an interesting object for theoretical studies because of its intricate phenomenology despite ostensibly simple purely mechanical nature. Numerical simulations can provide a useful insight into the origins of various aspects of this behaviour.

The objective of the present paper is to investigate mixing process inside granular material and the dependency of mixing on the properties of the particle material. Mixing of granular material is sustained by periodic motion of a rectangular bar inside a rectangular container. We observe the segregation and stratification of particles by their sizes and intensity of mixing. Size segregation is a characteristic feature of the moving granular media [4] and it is important, as well as mixing, in industrial handling of granulated materials.

2. Simulation model

A number of models have been applied for describing granular media with a varying degree of success [5]. The discrete element method (DEM) proved to be the most accurate, besides, it is simple to implement. In this method, the motions and collisions of each separate particle are tracked using the equations of classical mechanics. The equations of motion are integrated with a constant step size considerably shorter than the duration of the collision. Particle motion obeys the usual Newton equations

$$\frac{d\boldsymbol{x}_i}{dt}=\boldsymbol{v}_i;\ \frac{d\boldsymbol{v}_i}{dt}=\frac{\boldsymbol{F}_i}{m_i};\ \frac{d\boldsymbol{w}_i}{\mathrm{d}t}=\frac{\boldsymbol{T}_i}{I_i};\ i=\left[1,N\right] \qquad (1)$$

where $\boldsymbol{x}_i$ is the *i*-th particle position; $\boldsymbol{v}_i$ is its velocity; $\boldsymbol{F}_i=\sum_j \boldsymbol{F}_{ij}+m_i\boldsymbol{g}$ is the total force acting upon the *i*th particle; $\boldsymbol{F}_{ij}$ is the force acting upon the *i*-th particle arising from its collision with the *j*-th particle; m_i is the particle mass; $\boldsymbol{g}$ is the acceleration of gravity; $\boldsymbol{w}_i$ is angular velocity; $\boldsymbol{T}_i=\boldsymbol{d}_{cij}\times\boldsymbol{F}_i$ is the torque acting upon the particle, $\boldsymbol{d}_{cij}$ is the collision point vector defined below; I_i is the moment of inertia which is scalar for spherical particles; N is the number of particles. The orientations of particles are not updated because this has no sense for spherical shape.

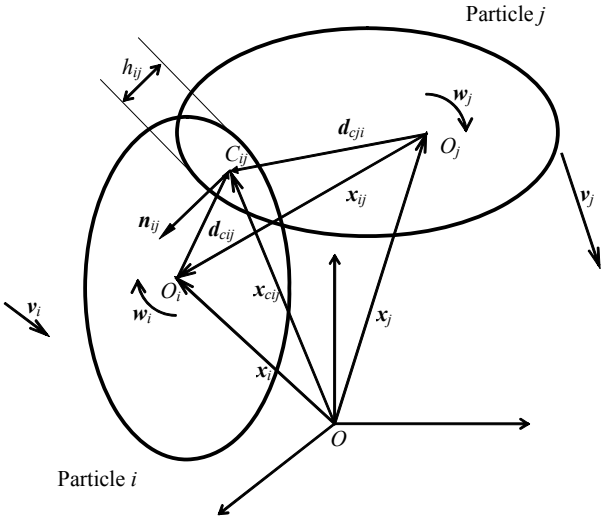

Fig. 1 Geometrical scheme of the elastic interaction between the colliding particles

The scheme of collision between two particles is shown in Fig. 1. Although only spherical particles were used in the calculations described here, the scheme shows a more general case of ellipse-shaped particles. Particle deformations during collisions are approximated by a partial overlap of their geometric shapes, with the overlap depth h_{ij}. The position of colliding particles i and j in space and their motion is defined by the radii-vectors $\boldsymbol{x}_i$, $\boldsymbol{x}_j$ of their centres O_i, O_j, linear velocities $\boldsymbol{v}_i, \boldsymbol{v}_j$ and angular velocities $\boldsymbol{w}_i$, $\mathbf{w}_j$. The relative position of the colliding particles is $\boldsymbol{x}_{ij}=\boldsymbol{x}_i-\boldsymbol{x}_j$. The point of contact C_{ij} is located in the middle of the overlap area and its radius-vector is x_{cij}. The unit vector n_{ij} is normal to the contact surface and directed toward the particle i, $\boldsymbol{n}_{ij}=-\boldsymbol{n}_{ji}$. The vectors $\boldsymbol{d}_{cij}$ and $\boldsymbol{d}_{cji}$ specify the position of the contact point C_{ij} with respect to the centres of the particles i and j: $\boldsymbol{d}_{cij}=\boldsymbol{x}_{cij}-\boldsymbol{x}_i$. Relative velocity of the

particles at the contact point is defined as $\boldsymbol{v}_{ij} = \boldsymbol{v}_{cij} - \boldsymbol{v}_{cji}$, $\boldsymbol{v}_{ij} = -\boldsymbol{v}_{ji}$, where $\boldsymbol{v}_{cij} = \boldsymbol{v}_i + \boldsymbol{w}_i \times \boldsymbol{d}_{cij}$, $\boldsymbol{v}_{cji} = \boldsymbol{v}_j + \boldsymbol{w}_j \times \boldsymbol{d}_{cji}$ are the velocities of the particles i and j at the contact point. Normal and tangential components of the relative velocity are expressed as $\boldsymbol{v}_{n,ij} = \left(\boldsymbol{v}_{ij}\,\boldsymbol{n}_{ij}\right)\boldsymbol{n}_{ij}$, $\boldsymbol{v}_{t,ij} = \boldsymbol{v}_{ij} - \boldsymbol{v}_{n,ij}$, respectively. Tangential forces act at the contact point. The colliding particles can slip with respect to each other in tangential direction by the distance $\delta_{t,ij}$, which is referred to as the integrated slip and is defined by $\delta_{t,ij} = \left|\int \boldsymbol{v}_{t,ij}(t)dt\right|$. As the particles slip, the value of $\delta_{t,ij}$ increases until the tangential force exceeds the force caused by static friction, and after that, the tangential force component is defined by dynamic friction. The resulting expressions for the normal and tangential components of the forces arising from the collision between the i-th and j-th particles read as follows

$$\left.\begin{aligned} \boldsymbol{F}_{ij}^{n} &= k_n r_{ij} h_{ij} \boldsymbol{n}_{ij} - m_{ij}\gamma_n \boldsymbol{v}_{ij}^{n} \\ \boldsymbol{F}_{ij}^{t} &= -\boldsymbol{t}_{ij}\, min\left[\mu\left|\boldsymbol{F}_{ij}^{n}\right|, \left|-\gamma_t m_{ij}\boldsymbol{v}_{ij}^{t} - k_t \boldsymbol{\delta}_{ij}^{t}\sqrt{r_{ij}h_{ij}}\right|\right] \end{aligned}\right\} \qquad (2)$$

where $k_n = \frac{4}{3}\cdot\frac{E}{2(1-\nu)}$; E is the elastic modulus of the particle material; ν is Poisson's ratio; $r_{ij} = \frac{r_i\, r_j}{r_i + r_j}$, $m_{ij} = \frac{m_i\, m_j}{m_i + m_j}$ are normalized radius and normalized mass; h_{ij} is overlap depth of the particle shapes during collisions [5]; $\boldsymbol{n}_{ij}$ and $\boldsymbol{t}_{ij}$ are normal and tangential vectors at the contact point; γ_n and γ_t are normal and tangential (shear) dissipation coefficients; $\boldsymbol{v}_{ij}^{n}$ and $\boldsymbol{v}_{ij}^{t}$ are normal and tangential components of the relative velocity of the colliding particles; μ is dynamic friction coefficient; $k_t = \frac{8}{3}\cdot\frac{G}{2-\nu}$; G is shear modulus; $\boldsymbol{\delta}_{ij}^{t} = \left|\int \boldsymbol{v}_{ij}^{t}\,\mathrm{d}t\right|$ is the slip of the contact point over the surfaces of the colliding particles, integrated over the total duration of collision. The simulations described below used the time-driven DEM implementation which is described in more detail in [5, 6]. The equations of motion (1) were integrated using the 6th-order Gear predictor-corrector scheme [7].

The main feature that sets the granular medium apart from the model of an ideal gas is that kinetic energy is lost during collisions due to dissipation, unlike in the case of an ideal gas. Therefore, for the process to continue, mechanical energy of the granular medium must be continuously replenished by stirring it using a periodically moving bar. The system consists of a rectangular box whose size is 0.2 m×0.4 m×0.2 m containing $N = 1600$ spherical particles of various sizes with random distribution of particle depths for particles of different sizes.

The model system at the initial time is shown on Fig. 2, a. The particles of different sizes are distributed randomly over the volume occupied by the granular medium (the packed bed). Typical trajectories of three arbitrarily selected particles during the simulation period are shown in Fig. 2, b. Fig 2, c shows the positions of particles at 190 s from the start of simulation, when the moving bar is at its right-most position. The final situation at the end of the simulation is shown on Fig. 2, d. The distribution of particle sizes was random (white noise, Fig. 3) in the range of the radii between 0.005 and 0.015 m. The density of the particle material was ρ = 700 kg/m^3. At the left side of the box there is a moving bar comprised of two rectangular walls (horizontal and vertical). The width of the bar is equal to the width of the box. The bar moves from its left-most position along the x axis over the distance of 0.1 m with the constant velocity of 0.01 m/s, then retracts back to its initial position with the same velocity, and then the process repeats itself. The total simulation time was 200 s. Periodic forward and backward motion of the bar stirs the particles which results in inhomogeneous distribution of the particles of different sizes over the volume filled with the particles. The simulations were performed for three different values of dynamic friction coefficient of the particle material: μ = 0.2, 0.5 and 0.8.

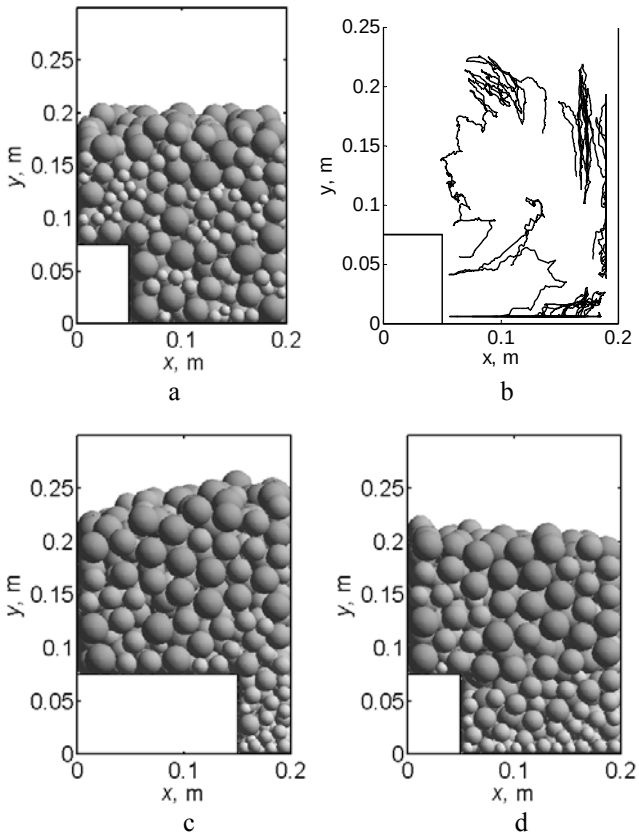

Fig. 2 Initial (a) position of the particles at t = 0 s in the box, the trajectory of motion of three random particles during the mixing process (b), the particle positions at t = 190 s when the moving bar is at its right-most position (c), and positions of the particles in the box at t = 200 s (d)

Motion of the particles exhibits certain patterns that can be visualized by means of velocity fields in the planes transverse to the x, y, z axes (Fig. 4). The particle velocities averaged over the simulation time and over the direction transverse to the corresponding plane are plotted. As it can be expected, the fastest motion takes place in the

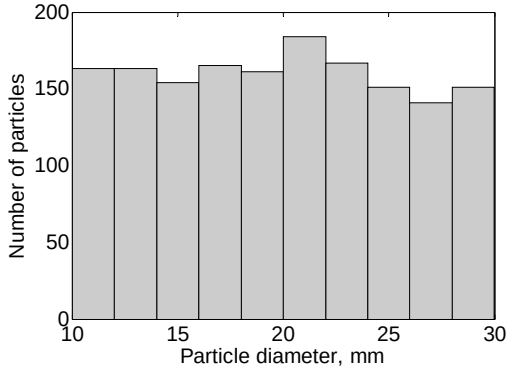

Fig. 3 Histogram of distribution of particle sizes

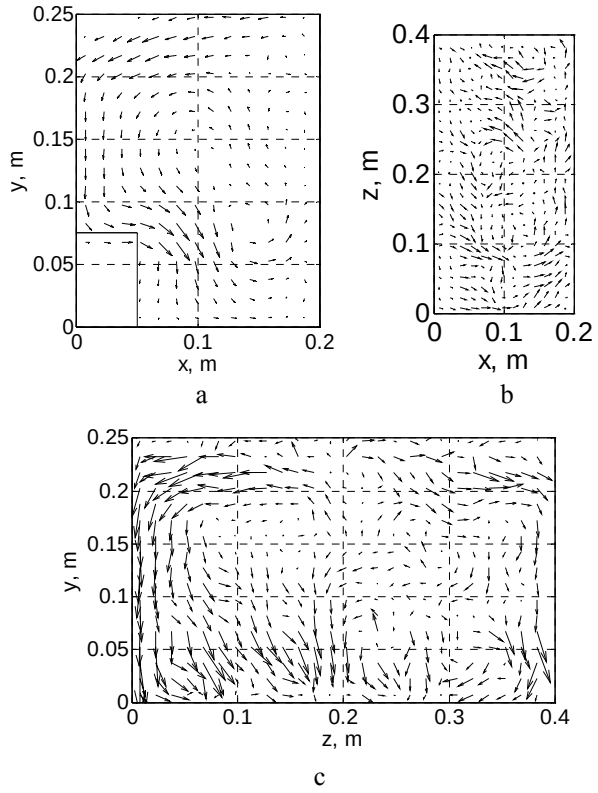

Fig. 4 Fields of particle velocities averaged over the simulation time in the *x*-*y* (a), *x*-*z* (b) and *y*-*z* planes (c)

x-*y* plane near the edge of the moving bar. The maximum average velocity in *x* and *y* directions is of 10^{-3} m/s order, and the particles move in a characteristic vortex-like pattern around the perimeter consisting of the box walls, facets of the moving bar and the upper free surface of the packed bed. Smaller vortices can be observed near the right-most position of the bar edge and above the bar. Patterns of the mean velocity field are seen also in *x*-*z* plane. The mean velocity of particles transfer on *x*-*z* plane is less intense (of the order of $2\text{-}3\cdot10^{-4}$ m/s) and is influenced by non-uniformity of the packed bed and the bounding walls. More detailed analysis of the velocity fields can provide a more thorough understanding of general characteristics of particles transfer in a moving granular material; however, it was beyond the scope of present research.

3. Characterization of mixing

The approach to characterization of mixing of particles in granular media stems from the theory of turbulence in fluid dynamics [8]. It is assumed that the velocity of each particle $\boldsymbol{v}_i$ can be split into its mean value $\boldsymbol{V}_i$ and the fluctuating part $\boldsymbol{v}_i'$

$$\boldsymbol{v}_i'(t) = \boldsymbol{v}_i(t) - \boldsymbol{V}_i(t) \tag{3}$$

The mean velocity is defined by averaging the particles surrounding the given particle within a certain preset volume

$$\boldsymbol{V}_i(t) = \frac{\sum_{j=1}^{N} \boldsymbol{v}_j(t)\delta\left(\left|\boldsymbol{x}_j - \boldsymbol{x}_i\right| \le R_V\right)}{\sum_{j=1}^{N} \delta\left(\left|\boldsymbol{x}_j - \boldsymbol{x}_i\right| \le R_V\right)} \tag{4}$$

where R_V is the radius of the selected volume surrounding the *i*-th particle, and a logical function is introduced

$$\delta(\text{condition}) = \begin{cases} 1, \text{ condition is satisfied} \\ 0, \text{ otherwise} \end{cases} \tag{5}$$

The fluctuating velocity shows how quickly the *i*-th particle changes its position with respect to the surrounding particles. By averaging $\boldsymbol{v}'^2_{x_n}$ over the simulation volume, the time-dependent mixing parameters are introduced

$$\Pi_{x_n}(t) = \sqrt{\frac{1}{N}\sum_{i=1}^{N} \boldsymbol{v}'^2_{x_n,i}(t)}, \; n = 1,2,3 \tag{6}$$

$$\Pi(t) = \sqrt{\Pi_x^2(t) + \Pi_y^2(t) + \Pi_z^2(t)} \tag{7}$$

where the coordinate axes are denoted as $x_1 \equiv x$, $x_2 \equiv y$, $x_3 \equiv z$. Averaging over the total simulation time $[t_1, t_2]$, where $t_1 = 0$ s, $t_2 = 200$ s, yields the total mixing parameters during the entire simulation period

$$P_{B,x_n} = \sqrt{\frac{1}{t_2 - t_1}\int_{t_1}^{t_2} \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{v}'^2_{x_n,i}(t)\,dt} = \\ = \sqrt{\frac{1}{t_2 - t_1}\int_{t_1}^{t_2} \Pi_{x_n}(t)\,dt} \tag{8}$$

$$P_B = \sqrt{P_{B,x}^2 + P_{B,y}^2 + P_{B,z}^2} \tag{9}$$

The segregation is estimated quantitatively as the change of vertical positions of the particles during simulation period depending on particle sizes. Particles whose radii are within the upper 20% of the total interval of the particle radii are considered "large" ($r_i = [0.013, 0.015]$ m), and those with the radii within the lower 20% of the total interval are considered "small" ($r_i = [0.005, 0.007]$ m). The average vertical position of particles whose radii are in the interval $r_1 \le r_i \le r_2$ is defined as

$$\left\langle y_{r_1,r_2}(t) \right\rangle = \frac{\sum_{i=1}^{N} y_i(t)\delta(r_1 \le r_i \le r_2)}{\sum_{i=1}^{N} \delta(r_1 \le r_i \le r_2)} \tag{10}$$

The changes of the average vertical position $\langle y_i \rangle$ of "small" and "large" particles are compared to the change of the average vertical position of all the particles (including large and small ones).

4. Simulation results and discussion

Segregation of the particles can be seen by comparing Figs. 2, a and d. Evidently, smaller particles tend to sink downwards and accumulate near the bottom after 200 s simulation period. Fig. 5 shows the change of the

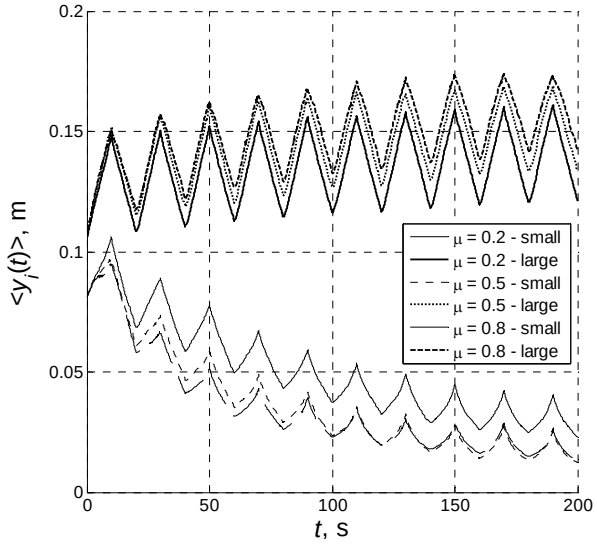

Fig. 5 Evolution of average vertical positions $\langle y \rangle$ of small and large particles with different dynamic friction coefficient

average vertical position $\langle y \rangle$ of small and large particles. The smaller particles tend to move toward the bottom, while the larger ones flow to the top. Jagged shape of the curve corresponds to the motion of the bar. Segregation is more intense at higher values of the dynamic friction coefficient, and this dependence is more pronounced for larger particles. However, as the stirring bar moves forward and backwards, the height of the volume occupied by the particles (packed bed) changes. Therefore, it is reasonable to introduce the average height of this volume $H_{PB}(t)$ and to normalize vertical positions of the particles by $H_{PB}(t)$, in order to discriminate the vertical motion of individual particles from the motion of entire packed bed as a whole

$$\langle Y(r_1, r_2, t) \rangle = \frac{\langle y(r_1, r_2, t) \rangle}{H_{PB}(t)} \tag{11}$$

Fig. 6 shows the changes of average depth of the packed bed H_{PB} during the process, and the evolution of vertical positions of the particles normalized to the depth of the packed bed is shown in Fig. 7.

Mixing is more intense for higher values of the dynamic friction coefficient, and more intense mixing results in faster segregation. Evolutions of time-dependent mixing coefficients $\Pi(t)$ follow the motion of the stirring bar (Fig. 8). The dependence of the overall mixing coefficients P_{B,x_n} upon dynamic friction coefficient μ is shown in Fig. 9. However, there is still no definite explanation for

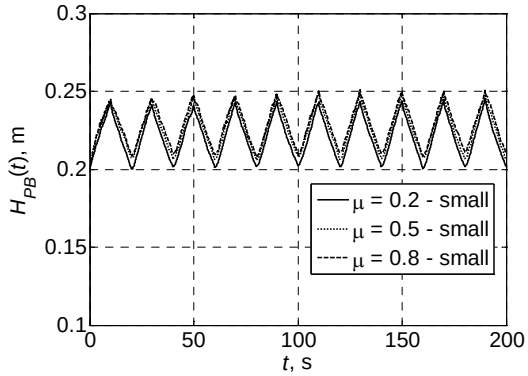

Fig. 6 Evolution of average depth of the packed bed

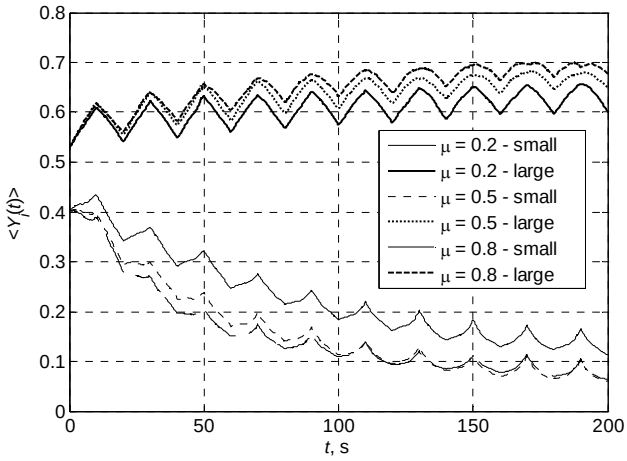

Fig. 7 Evolution of normalized average vertical positions $\langle Y \rangle$ of small and large particles with different dynamic friction coefficients

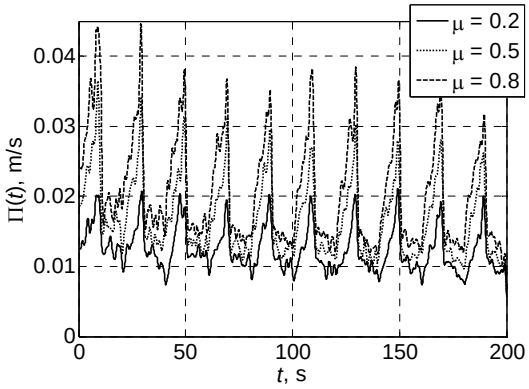

Fig. 8 Evolution of time-dependent mixing parameter $\Pi(t)$ for different values of dynamic friction coefficient μ

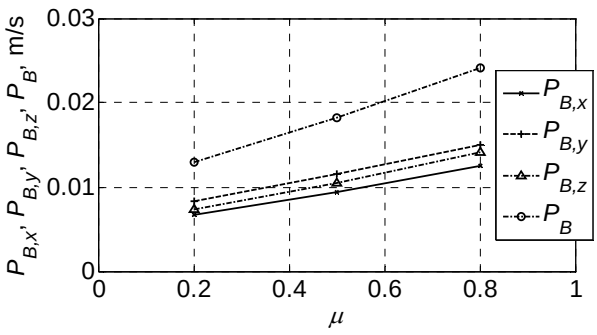

Fig. 9 Total mixing coefficients P_B versus dynamic friction coefficient μ

the dependence of mixing intensity upon the dynamic fric tion coefficient. This dependence is analogous to that observed in fluid dynamics where mixing is more intense for more viscous fluids. Clarification of this problem for granular matter requires further research.

5. Conclusions

Numerical simulation of mixing and segregation of granular material put to motion by a moving bar was performed using the discrete element method for different values of dynamic friction coefficient of the granules. Mixing is more intense at higher values of the dynamic friction coefficient, and consequently more intense mixing results in faster and more distinct segregation. This result is similar to the case of hydrodynamics where mixing is more intense in more viscous fluids, but this dependence for the granular material requires further investigations.

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GRANULIUOTŲ MEDŽIAGŲ MAIŠYMOSI IR SEGREGACIJOS SKAITINIS MODELIAVIMAS

R e z i u m ė

Diskrečiųjų elementų metodu skaitiškai ištirtas granuliuotos medžiagos, susidedančios iš apvalių įvairaus dydžio dalelių, maišomų periodiškai judančiu laipteliu, maišymasis ir segregacija. Parodyta, kad maišymosi metu granuliuotą medžiagą sudarančios sferinės dalelės pasiskirsto netolygiai: mažesnės susirenka konteinerio apačioje, o didesnės kyla į viršų. Tokio išsiskirstymo (segregacijos) greitis priklauso nuo maišymosi, kuris yra intensyvesnis, esant didesniam dinaminės trinties tarp dalelių koeficientui. Tokia priklausomybė panaši kaip ir skysčių maišymosi atveju, kai maišymosi intensyvumas yra didesnis esant didesnei klampai, bet granuliuotų medžiagų šiai priklausomybei nustatyti reikia detalesnių tyrimų.

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NUMERICAL SIMULATION OF MIXING AND SEGREGATION OF GRANULAR MATTER

S u m m a r y

Mixing and segregation of granular material, consisting of spherical particles of various sizes, stirred by a periodically moving bar was simulated numerically, using the discrete element method. It was shown that smaller particles of the granulated material tend to sink to the bottom while the larger particles rise to the top. The segregation process depends on mixing, which is more intense for higher values of the dynamic friction coefficient of the particle material. This dependence is similar to the case of hydrodynamics where mixing is more intense in more viscous fluids, but more thorough understanding of this dependence for the case of granular matter requires further investigations.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ПЕРЕМЕШИВАНИЯ И СЕГРЕГАЦИИ ГРАНУЛИРОВАННОГО МАТЕРИАЛА

Р е з ю м е

Используя метод дискретных элементов, численно исследованы процессы перемешивания и сегрегации в гранулированной среде, состоящей из сферических частиц разных диаметров, приводимых в движение периодически движущейся ступенью. Показано, что перемешивание приводит к расслоению частиц по величине, причем перемешивание происходит более интенсивно при больших значениях коэффициента динамического трения. Эта зависимость похожа на случай гидродинамики, где перемешивание происходит более интенсивно в более вязкой жидкости, но детальное выяснение этой зависимости в гранулированной среде требует дальнейших исследований.

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