SIMULATION IN MAGNETIC FIELD ENHANCED CENTRIFUGATION

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ABSTRACT

High Gradient Magnetic Separation (HGMS) uses magnetic wire filters for the separation of magnetizable particles from fluid. Simulation of the process allows understanding, prediction and optimization of magnetic separation. Magnetic and mechanic forces between the particles are calculated using the Discrete Element Methode (DEM). The magnetic force of the wire is implemented additionally.
Simulation of the particles shows that parameters like particle and wire magnetization influence the structure of the deposit built on the wire. Needle-shaped agglomerates appear in case of strong interparticulate magnetic forces, while high external forces create a compact layer of particles on the support.

KEYWORDS

Centrifugation; Selective Bioseparation; High Gradient Magnetic Separation; Simulation;

1. Introduction

A possibility for the separation of proteins is the use of a packed bed with protein-binding functionalisation. Still, column packing in a homogenous way is cost-intensive and prone to packing problems like inhomogenous fluid resistance in the cross section. Another option is the immobilization of the functionalisation on magnetic particles. The use of magnetic particles permits an easier process control compared to a packed bed by an easy exchange of the functionalisation. Additionally difficult process steps like column packing do not play a role in the use of magnetic particles. The process depends on the functionalized surface. Therefore the large specific surface of particles down to nanometer scale allows a low total mass of particles in the process. Still high particle amounts in the scale of 10 - 50 g/l are realistic in many processes. Another application for magnetic particles consists in their use as a carrier for catalyzing substances. This is an alternative to immobilizing catalyzers in a classic packed bed.

High Gradient Magnetic Separation (HGMS) uses magnetic forces for the separation of magnetic particles out of fluid. Magnetic forces allow selective separation in combination with high separation efficiency and high volume flow. A challenge is still the realization of a continuous process, because most HGMS devices need to be backflushed batch-wise after separation. Another challenge is the uniform use of magnetic filter. In many cases, the HGMS cells plug close to the inlet. In this case selectivity is reduced due to cake filtration caused by magnetic matter blocking the complete cross-section area.

A possibility to clean the magnetic filter during the process is Magnetically Enhanced Centrifugation (MEC). In this case a star-shaped magnetic filter is installed in a centrifuge, which itself is in the center of a magnet creating an axial field in the centrifuge. Wires are cleaned simultaneously during separation by centrifugation. The deposit of particles on the wires and the forces holding particles on the wires depend on the centrifugal velocity and the magnetic forces [1].

All these processes depend on the properties of magnetic particles [2]. The understanding and the influence of the different parameters on the particle behavior is important to use them efficiently in processes. Simulations have already been done by Satoh [3]. Our approach consists in simulating the particle behavior with respect to the influence of a constant magnetic background field, in particular in HGMS.

2. Theory

To simulate the microscopic particle behavior, mechanic and magnetic forces are implemented in a commercial Discrete Element software. We assume magnetic and mechanic forces to be important, besides fluid forces which are neglected in this approach. Van-der-Waals, electrostatic and fluid friction force (Stokes) are not shown in this paper. Fluid friction reduces the velocity of particle motion, but the final result is similar.

Magnetic forces

The magnetic force depends on the volume V_P and magnetization M_P of the particle or respectively its magnetic moment μ_P and the gradient of the magnetic field H:

$$\boldsymbol{F}_m = \mu_0 \mu_\mathrm{P} \nabla H = \mu_0 V_\mathrm{P} M_\mathrm{P} \nabla H \tag{1}$$

μ_0 is the permeability constant. The force $\boldsymbol{F}_m$ of ferromagnetic wires in saturation on a particle in cylindric coordinates r and θ has already been solved analytically [2]:

$$\boldsymbol{F}_{m,r} = -\mu_0 V_\mathrm{P} M_\mathrm{P} M_W \frac{a^2}{r^3}\left(\frac{M_W}{2H_0}\frac{a^2}{r^2} + \cos(2\theta)\right) \tag{2}$$

$$\boldsymbol{F}_{m,\theta} = -\mu_0 V_\mathrm{P} M_\mathrm{P} M_W \frac{a^2}{r^3}\sin(2\theta) \tag{3}$$

where M_W is the wire magnetization, H_0 the background field and a the wire diameter. In this case the magnetic permeability of the surrounding fluid is assumed to be much lower than the permeability of wire and particle.

The forces $F_{m,ij}$ between two particles i and j are approximated by a dipole-dipole approach [3]:

$$\boldsymbol{F}_{m,ij} = -\frac{3\mu_0\mu_{\mathrm{P}i}\mu_{\mathrm{P}j}}{4\pi} * \frac{1}{{r_{ij}}^4}\left[-(\boldsymbol{n}_i * \boldsymbol{n}_j) + 5(\boldsymbol{n}_i * \boldsymbol{t}_{ij})(\boldsymbol{n}_j * \boldsymbol{t}_{ij})\boldsymbol{t}_{ij} - \{(\boldsymbol{n}_j * \boldsymbol{t}_{ij})\boldsymbol{n}_i + (\boldsymbol{n}_i * \boldsymbol{t}_{ij})\boldsymbol{n}_j\}\right] \tag{4}$$

μ_{Pi} *and* μ_{Pj} are the magnetic moments of the two particles, r_{ij} the magnitude of the distance between the two particle centers, $\boldsymbol{t}_{ij}$ is the unit vector denoting the direction from particle center i to particle center j, and $\boldsymbol{n}_i$ and $\boldsymbol{n}_j$ are the unit vector denoting the direction of the magnetic moment of particle i and j respectively. In case of a magnetic field in x-direction and the particles being aligned in the same direction, equation (4) can be simplified. We neglect as well torques of the particles:

$$\boldsymbol{F}_{m,ij} = -\frac{3\mu_0\mu_{\mathrm{Pi}}\mu_{\mathrm{Pj}}}{4\pi}\frac{1}{r_{ij}^4}\begin{pmatrix}(5 * t_X{}^2 - 3)t_X \\ (5 * t_X{}^2 - 1)t_Y \\ (5 * t_X{}^2 - 1)t_Z\end{pmatrix} \tag{5}$$

The components of the unit vector $\boldsymbol{t}_{ij}$ are t_X, t_Y and t_Z.

Mechanic forces

The normal force on magnetic particles is in a spring-damper model [4]:

$$\boldsymbol{F}_{n,ij} = k_n\delta^{3/2}\boldsymbol{t}_{ij} - \eta_{ij} * \boldsymbol{v}_{rel,n,ij} \tag{6}$$

The coefficient k_n depends on the Young Modulus and radius of the particles. The overlapping δ of the particle spheres measures the rejecting spring force. This soft sphere model requires low time steps, because the overlapping of two particles at high time steps might be large causing hugh forces and hence instable simulations. The parameter η_{ij} depends on the mass, stiffness and the restitution of the particle. The damping part depends on the relative velocity of the two particles $\boldsymbol{v}_{rel,n,ij}$, and leads to convergence of particle velocities of magnetically attracting particles over a certain number of time steps. As tangential force $\boldsymbol{F}_{t,ij}$, we only consider friction using a damper model. $\mathbf{v}_{\mathrm{rel,t,ij}}$ is the relative velocity in tangential direction. Slow particle motion in tangential direction is not hindered by sticking. Particles are considered to be smooth:

$$\boldsymbol{F}_{t,ij} = -\eta_{ij} * \boldsymbol{v}_{rel,t,ij} \tag{7}$$

As a consequence of interparticulate forces, particles may only agglomerate in field direction, while there is a repulsive zone around the particle eliminating agglomeration in different directions (see Figure 1).

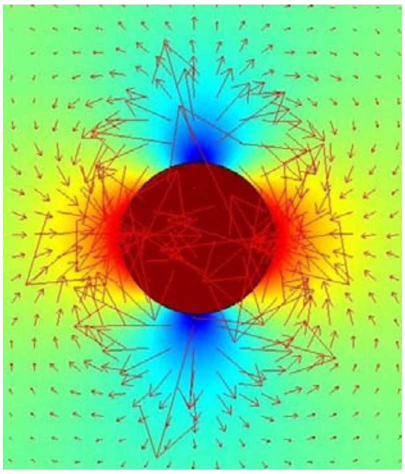

Figure 1: FEM-simulation of the magnetic field and its gradient

3. Methods

The simulation has been realized in the commercial Discrete Element Program EDEM of the company DEM Solutions Ltd. The graphics and the base calculation engine were used, but our own models have been implemented using User Defined Libraries to implement the mechanic and magnetic forces.

A particle magnetization of 480 000 A/m² has been set for magnetite. The wire magnetization of ferromagnetic steel of 1 278 200 A/m² has been set. The particle diameter is 2 µm, except for the simulation shown in Fig. 3. The particles' Poisson ratio is 0.3, the shear modulus 7.93e10 Pa, and the density is 5 200 kg/m³. A challenge in the simulation of magnetic forces is the fact that the magnetic field change of particles is non-linear. The basic equations are only valid for interaction between two particles. The field distortion of two particles close to each other is significantly different from the distortion of each particle isolated. As a consequence needles of three or more particles are instable, i.e. particles in the middle of the needle are pushed out of the needle by the particles at the ends of the chain. In our simulation the force of distant particles being caught in the same agglomerate has been eliminated. In the specific agglomerated state only the magnetic attraction of particles in contact is taken into account. This is an approximation, but we assume it to be sufficient to gain physical results. An alternative would be to calculate the magnetic field and its forces at each time step by a Finite Elements Method, which is out of proportion of our computational power.

4. Results and discussion

In the simulations the particles actually agglomerate – depending on several parameters – in needle-shape and are attracted by the wires, where they build deposits. Fig. 2 shows a picture taken from the test centrifuge during the process of Magnetically Enhanced Centrifugation. The particles form a rough surface on the wires. Opposite to each wire, a particle deposit is on the wall of the centrifuge.

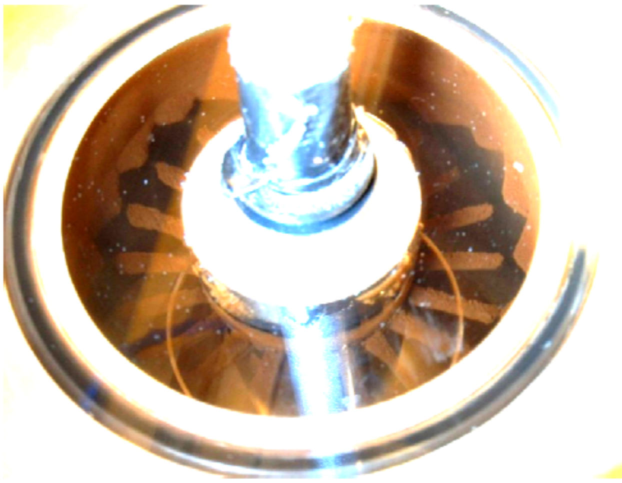

Figure 2: Deposit during the process in MEC in the first prototype; photo taken using a stroboscope; the rough surface of the particles on the wire is well visible;

Fig. 3 shows a simulation of large particles building needles which attach to the wires. The wire diameter is 1 mm, the particles have a diameter of 100 µm. In this specific simulation the magnetization of the wire has been chosen 1/70 of its actual value.

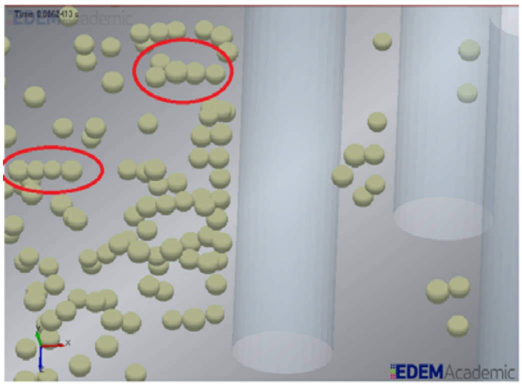

Figure 3: 100 µm particles agglomerating in needle-shape on a 1mm wire

Fig. 4 shows the different influence of particle magnetization and wire magnetization for particles of 2 µm diameter on a 1 mm wire. In the left picture the magnetization of steel was set for the wire. The particles form a compact layer on the wire. Interparticulate forces are not strong enough to influence the form of the layer. In the right picture the magnetization was reduced by a factor 70. Particles agglomerate in a highly porous way in needle-shape. Lateral to each needle, a specific distance is kept due to repulsing magnetic forces. A consequence is the fact that the porosity of the filter cake of magnetic particles is a function of the magnetization of wires and particles M_P / M_W.

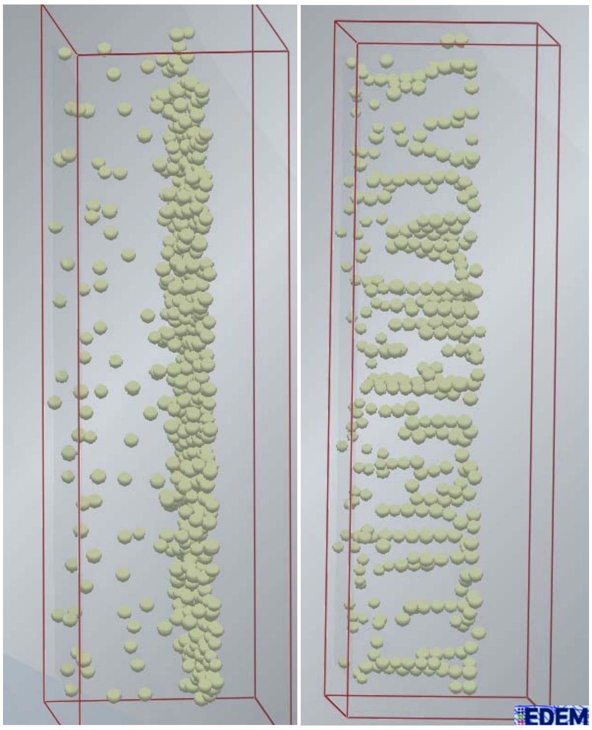

Figure 4.1 - 4.2: Particle deposit in a similar simulation different by a factor 70 in the wire magnetization: a dense deposit (left) and needles at a distance (right); not shown is the wire surface where the particles stick to;

A comparison of the forces in Fig. 5 shows that for the materials we use in our experiments, agglomeration occurs for low particle distances and hence high concentrations. In the high magnetic field of the wire, the shape of the deposit is still influenced mainly by the wire, not by the individual particles. We expect in the deposit of particles lower layers to form a compact layer, but upper layers to agglomerate in needle-shape. In general, the analytic comparison is in agreement with the simulation results shown above.

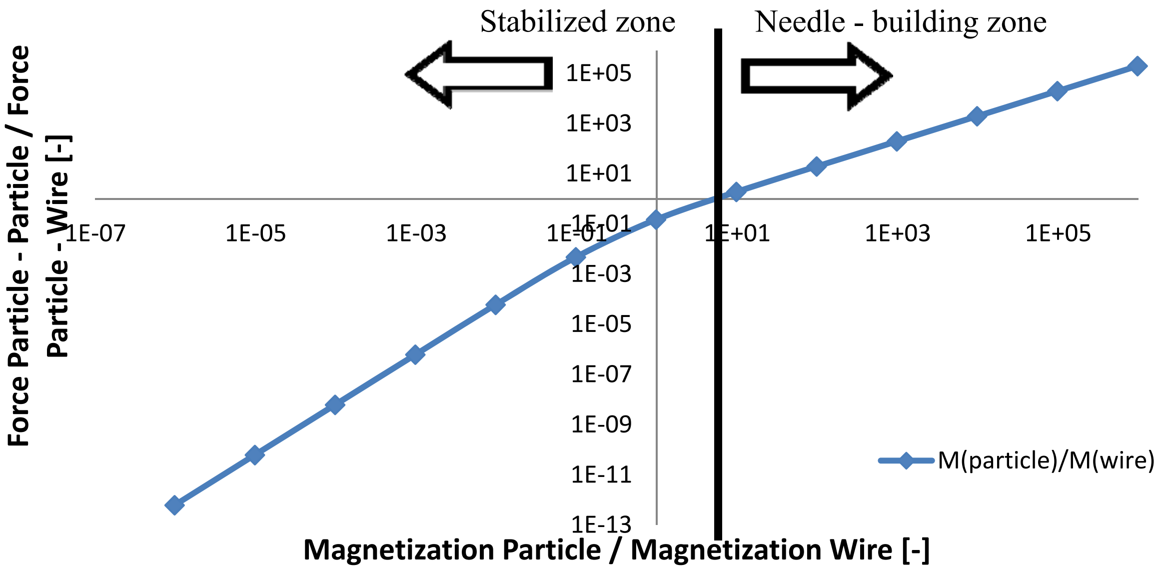

Figure 5: Interparticulate forces normed by wire attraction forces over the magnetization of particle and wire; purely analytic; 2 µm particle,1 mm wire diameter; 1mm particle wire distance; 10 µm particle – particle distance;

5. Conclusion

The simulation of magnetic and mechanic forces common in HGMS processes is possible. Dipole – dipole forces were implemented, and simulate the behavior of particles close to wires. The simulation delivers interesting results on the structure of the particle deposit. The simulation of magnetic particles close to magnetic wires allows calculating the influence of different parameters on the structure and porosity of the deposit. A low wire magnetization causes highly porous deposit on the wire in needle-shape, due to repulsing forces laterally of the needles.

6. Outlook

To simulate as well the kinetics of the process the implementation of fluid forces and of the DLVO theory is necessary as well. This allows as well the simulation of the efficiency of the HGMS device.

An interesting aspect is the same order of magnitude of electrostatic force and magnetic interparticulate force. This is the case for a low proportion of magnetisable matter in the particle and hence low magnetization of the particle compared to pure magnetite. The coating of particles with silica or polymer influences as well the particle behavior.

Furthermore the approach allows the simulation of rheological behavior. The behavior of magnetic suspensions is unique. The viscosity of these suspensions depends on the magnetic background field, the shear direction relative to the field and the magnetization of the particles. The viscosity of magnetic suspensions is highly isotropic and can be controlled externally by changing the magnetic field.

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Formulae signs

a	[m]	wire radius
F_m	[N]	magnetic force
H	[A/m]	magnetic field
H_0	[A/m]	magnetic background field
M_P	[A/m]	magnetization particle
M_W	[A/m]	magnetization wire
$\boldsymbol{n}_i$, $\boldsymbol{n}_j$	[-]	unit vector of the magnetic moment of the particle *i* and *j*
r	[m]	magnitude of the distance vector from wire center to particle center, cylindrical coordinate
r_{ij}	[m]	magnitude of the vector from particle *i* to particle *j*
$\boldsymbol{t}_{ij}$	[-]	unit vector from particle *i* to particle *j*, $\boldsymbol{t}_{ij}=\boldsymbol{r}_{ij}/r_{ij}$
t_X, t_Y, t_Z	[-]	Components of $\boldsymbol{t}_{ij}$
$v_{rel,n,ij}$	[m]	Normal component of relative particle velocity
$v_{rel,t,ij}$	[m]	Tangential component of relative particle velocity
v_0	[m/s]	Fluid velocity
V_P	[m³]	volume particle
η_{ij}	[kg/s]	damper parameter
μ_0	[V s / A m]	permeability constant
μ_P	[A m²]	magnitude of the magnetic moment
θ	[-]	angle, cylindrical coordinate

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