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Particle deposition and detachment in capillary sphere packings

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ABSTRACT

Flow simulations in a random sphere packing are used to investigate particulate filtration processes. The local wall shear stress is used to calculate an angular dependent distribution for particle detachment. Simulations of particle deposition by interceptions yield the angular dependent number of impacts. The results from particle detachment calculations and the interception analysis are combined to estimate local particle deposition rates, employing probabilities for detachment and impact. Comparison with X-ray computer tomography of deposited particles within a sphere packing shows good agreement. Therefore, the presented simulation procedure can be used for the design of, e.g., particle filtration apparatus.

1. Introduction

Deep-bed particle filtration is of importance in drinking-water treatment or in oil filters for combustion engines. The local particulate filtration mechanism in general is not yet determinable. There are two counteracting filtration effects: particle impact with deposition and particle detachment. For the latter, Saffman [1] has derived a lift force due to shear flow for spheres moving along a plane. Goldman et al. [2] found solutions for the shear induced forces and torques on a sphere in the low Reynolds regime, as well as translational and rotational forces and torques well below a plane wall. O'Neill [3] derived an exact solution of the linearised Stokes equation for a sphere in contact with a plane, providing the force acting on the sphere in the direction parallel to the plane wall.

A theoretical treatment of the particle deposition dynamics is given, e.g., by Ihme et al. [4]. They considered the mass transfer on the basis of a numerical solution that combines the equation of motion, diffusion and continuity. The trajectory analysis concept, described by Rajagopalan and Tien [5] (see complementary paper of Logan et al. [6]), is able to predict the initial collection rates in filters by taking into account all relevant forces acting between particles and packing matrix. Tufenkji and Elimelech [7] (with a comment of Rajagopalan [8]) present a correlation between various deposition parameters and the single collector efficiency

CFD studies on the fluid flow in packed beds are performed, for instance, by Gunjal et al. [9] who investigate the interstitial flow in periodically packed, rhombohedral and face-centered cubical geometries; their results are in good agreement to experimental as well as to other CFD studies. Tung et al. [10] also performed CFD simulations on ordered packings, but they additionally examine particle deposition by a net force approach similar to that used in this work. The retention of particles in regular cubic packings due to wedging and retention are simulated by Johnson et al. [11]; they found an increase in wedging and retention with decreasing fluid velocity. However, in contrast to these studies based on regular packings, a work of Warren and Stepanek [12] shows that the shear rate in random packings differs considerably from tube flow, which implies that the flow in ordered packings cannot be generalised for random packings.

The currently available computation power enables full 3D trajectory analysis [13]. However, these studies do not take into account the particle detachment, as presented in the work of Hubbe [14]. There, three possibilities of incipient motion of particles as preliminary stage of particle release are noted: sliding, rolling and lifting. Incipient motion depends on the particle–matrix system; for example hard spheres will roll rather than slide, while soft, squared particles will slide rather than roll. Experiments performed by Sharma et al. [15] and by Burdick et al. [16] permit the confirmation of the first relation.

For the rolling particle release mechanism, Bergendahl and Grasso [17] developed a method which depends on thermodynamic and hydrodynamic quantities. A crucial parameter is the contact

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Nomenclature

a	radius of contact circle [m]
$\bar{d}_g$	mean sphere size of the packing [m]
d_p	suspended particle diameter [m]
D_{cyl}	inner diameter of capillary [m]
F_a	adhesion force [N]
F_d	drag force [N]
F_l	lifting force [N]
F_{net}	net force [N]
H	Hamaker constant [J]
H_{imp}	impact frequency
k_f	friction factor
K	Young's modulus [Pa]
L	length of packings [m]
L_{cap}	length of capillary [m]
N_0	number of spheres in the packing
N_{dep}	deposition function
N_{imp}	number of impacts
$P_{dep}(\alpha)$	deposition probability
$P_{det}(\alpha)$	detachment probability
r	radial distance, normal to wall [m]
r_{imp}	particle impact rate
r_{pas}	rate of particles passing the packing
r_p	suspended particle radius [m]
r_g	mean sphere radius of the packing [m]
Re_g	grain Reynolds number
u_0	approaching velocity [m/s]
u_t	tangential velocity [m/s]
v	local velocity [m/s]
W_a	adhesion energy [J]
z_0	reduced radius [m]
α	tilt angle
β	angle of orientation plane
$\dot{\gamma}_w$	wall shear rate [1/s]
δ	particle-wall distance [m]
ϵ	porosity
η_s	single collector efficiency
μ	dynamic viscosity [kg/ms]
ν	kinematic viscosity [m^2/s]
ρ	density [kg/m^3]
τ_w	wall shear stress [kg/ms^2]

radius which determines the moment required for incipient rolling. This is calculated by one of the models treating the contact deformation on the adhesion force, like that of Johnson, Kendall and Roberts (JKR) or Derjaguin, Muller and Toporov (DMT) (see Soltani and Ahmadi [18] for a comparison of different particle adhesion models). The particle release mechanism due to sliding is described by Tien and Ramarao [19] together with a modelling method. The key parameter here is the friction factor of the particle and the wall material. The effect of surface roughness on the particle deposition is treated by Hoek and Agarwal [20], who therefore founds an increasing deposition probability due to a decrease of the repulsive interaction energy.

Yoon et al. [21] reported particle filtration processes as observed by an optical measurement setup. Their results indicate a distinction between irreversible deposited contact retardation and a reversible surface retardation with subsequent reentrainment after attachment. Straining due to trapping in the pore throats is another effect of particle retention; however this is not included in colloid attachment theory [22]. Although straining is obviously an important effect in quantitative filtration theory, it is not necessary to

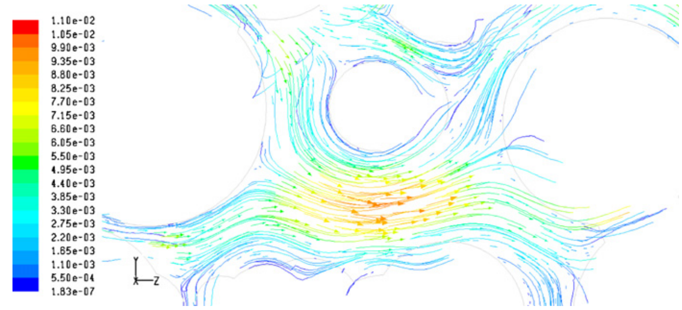

Fig. 1. Fluid velocities in a sphere packing with porosity $\epsilon_0 = 0.434$ and superficial velocity $Re_g = 2.75$.

regard this effect for the investigation concerning the local deposition rate on a model sphere, where the particle position due to straining occurs everywhere on the model sphere with the same probability. This circumstance also holds in a random sphere packing.

The basis of this work is the calculation of the fluid flow in a sphere packing with high local resolution. Firstly, an averaged wall shear rate can be estimated which depends on the position (tilt angle α) of a unit sphere. The wall shear rate causes a drag force on an attached particle depending on α from which, in combination with adhesion and lift forces, a detachment probability can be calculated.

Secondly, the locally resolved fluid flow can be used for a particle tracking analysis which yields, as far as a suspended particle hits somewhere on the sphere packing, the impact position. Additionally, the number of particles passing the packing without any collision delivers the passing rate.

The results of detachment probabilities and impact rates can be combined to give an angle depending deposition function. Together with the passing rate, the integral collector efficiency can be estimated.

2. Local fluid flow simulations

Detachment of particles in a deep bed filter originates due to shear forces near the walls. The local wall shear stress will be calculated by commercial CFD tools in combination with evaluation algorithms written by the authors.

The first step is to generate random sphere packings with geometrical properties close to real packings. This is performed by the use of the algorithm of Jodrey and Tory [23]. In the next step, the fluid flow in the abstract sphere structure will be computable after a 3D meshing and subsequent calculation of the fluid flow using a CFD software package (Gambit and Fluent, ANSYS Corp.; Gunjal et al. [9] mentioned above have shown the applicability of this software and, therefore the volume of fluid method). Due to the low Reynolds number of the flow in the small voids of the packings, a laminar model together with the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm is used for the fluid flow calculation. A section of the complex fluid flow can be seen in Fig. 1.

The resulting fluid flow data are distributed on an irregular grid. A 3D interpolation of the velocities in the mesh cells around discrete points, which are located on lines defined by the corresponding sphere centers, delivers shear stresses on well defined positions. The orientation of these lines depends on different angles in respect to the direction of superficial flow (see Fig. 2 for definitions). The angles α and β are used instead of the angles in standard spherical coordinate systems θ and ϕ, respectively, to avoid mistakes. The resulting quantities used in this work depend on the tilt angle α and are mean values of the complete packing, averaged over different planes defined by plane angle β and averaged over all spheres.