Supplementary information

Transport and clogging dynamics of flexible rods in pore constrictions

Berinike Bräsel,[a] Matthias Geiger,[a] John Linkhorst,[a] and Matthias Wessling*[ab]

1 Fluid flow calculation

Fluid flow in the fluid domain Ω_f is solved using the Navier-Stokes equation for an incompressible fluid (1) and the continuity equation (2):

$$\rho_f \frac{\partial u_f}{\partial t} + \rho_f (u_f \cdot \nabla) u_f = -\nabla p + \mu \nabla^2 u_f \ \text{ in } \Omega_f \tag{1}$$

$$\nabla \cdot u_f = 0 \ \text{ in } \Omega_f \tag{2}$$

Here, ρ_f, u_f, and μ are the density, the velocity, and the viscosity of the fluid, respectively, and p denotes the pressure. The coupling of the fluid phase with the particulate phase is realized with the following boundary conditions:

$$u_f = u_p \ \text{ in } \Omega_s \tag{3}$$

$$\sigma \cdot \hat{n} = t_{\Gamma_s} \ \text{ on } \Gamma_s \tag{4}$$

Equation (3) is responsible for transferring the particle's velocity u_p to the fluid velocity field u_f inside the domain of the particle Ω_s. The interface condition in equation (4) describes the fluid stress acting on the particle's interface Γ_s, where σ is the stress tensor of the fluid field, $\hat{n}$ is the outer normal vector, and t_{Γ_s} denotes the traction vector of the fluid acting on the particle. Integration over the particle's interface Γ_s is performed to transfer equation (4) into a force term F_f that considers pressure gradient force and viscous forces of the fluid. In our case, other fluid forces, such as Basset, Saffman, and Magnus forces and gravity effects, are small and therefore neglected.

2 Bonded particle model

For the representation of a flexible rod, we use a multi-sphere model with virtual elastic bonds for connection that was developed by Guo et al.[1] and Schramm et al.[2]. The bond forces are calculated incrementally as follows:

$$dF_n^b = K_n^b d\delta_n^b = \frac{E_b A}{l_b} v_n^r dt \tag{5}$$

$$dF_t^b = K_t^b d\delta_t^b = \frac{G_b A}{l_b} v_t^r dt \tag{6}$$

F_n^b and F_t^b are the normal and tangential forces of the virtual elastic bonds connecting the individual spheres. K_n^b, K_t^b, δ_n^b, δ_t^b, v_n^r, and v_t^r denote the normal and tangential bending stiffness, the normal and tangential (shear) deformation, and the normal and tangential relative velocity between two bonded spheres, respectively. The Young's modulus E_b and the shear modulus G_b of the bond are correlated through the Poisson's ratio $\nu : E_b = 2(1+\nu)G_b$. The bond is assumed to be cylindrical with a radius r_b, a length l_b, and a cross-sectional area $A = \pi r_b^2$. Here, the bond radius r_b is assumed to be the same as the radius of an individual sphere r_p, and the length l_b is the distance between the centers of two connected spheres, which is twice the radius $2r_p$. To account for energy dissipation in the elastic wave propagation through the bonds, a normal and tangential damping force $F_{damp,n}^b$ and $F_{damp,t}^b$ are added:

$$F_{damp,n}^b = 2\beta_{damp} \sqrt{m_p K_n^b} v_n^r \tag{7}$$

$$F_{damp,t}^b = 2\beta_{damp} \sqrt{m_p K_t^b} v_t^r, \tag{8}$$

where β_{damp} is the bond damping coefficient, and m_p is the mass of an individual sphere. In the DEM framework, the trajectory of each sub-sphere within the multi-sphere rod is calculated individually based on the sum of the forces acting on it:

$$m_p \ddot{x}_i = F_n + F_t + F_n^b + F_t^b + F_{damp,n}^b + F_{damp,t}^b + F_b + F_f, \tag{9}$$

[a] Chemical Process Engineering AVT.CVT, RWTH Aachen University, Forckenbeckstraße 51, 52074 Aachen, Germany. E-mail: manuscripts.cvt@avt.rwth-aachen.de
[b] DWI - Leibniz Institute for Interactive Materials e.V., Forckenbeckstraße 50, 52074 Aachen, Germany.

where F_n and F_t denote the normal and tangential particle-particle and particle-wall contact forces and are calculated with the Hertz contact model[3]. F_b sums up possible body forces, such as gravity, which is neglected in this work. F_f is the particle-fluid interaction force. In addition to the Hertz model, we consider rolling friction and tangential sliding. Rolling friction arises from the small-scale non-sphericity of the particles and is taken into account by using a constant directional torque (CDT) model. A history spring model is chosen to account for the resistance from tangential sliding.[4] The calculation of the moments acting on the spheres and bonds is performed analogously to the force calculation.

3 Stability criteria

In this work, four numerical stability criteria were used to determine the time steps of CFD and DEM and the coupling interval. For the CFD part, the Courant-Friedlich-Lewy (CFL) condition reads[5]:

$$CFL = \Delta t_{CFD} max(\frac{|u|}{\Delta x}) < 1 \tag{10}$$

For the DEM part, the time step is taken as a fraction of 15 % of the Rayleigh time Δt_R, which is defined by:

$$\Delta t_R = \frac{\pi}{2} d_p \sqrt{\frac{\rho_p}{G}} (\frac{1}{0.1631\nu + 0.8766}) \tag{11}$$

where d_p and ρ_p are the diameter and density of the particle, G denotes the shear modulus and ν is the Poisson ratio.
The coupling interval CI resulting from the stability criteria for the CFD and DEM timestep was checked to fulfill[6]:

$$CI \leq min(\Delta t_{pf}, \Delta t_{fp}) \tag{12}$$

$$\Delta t_{pf} \leq \frac{4}{3} \frac{\varepsilon_f}{(1-\varepsilon_f)} \frac{d_p}{C_d} \frac{1}{|u - v_i|} \tag{13}$$

$$\Delta t_{fp} \leq \frac{4}{3} \frac{d_P \rho_P}{C_d \rho_f} \frac{1}{|u - v_i|} \tag{14}$$

where ε_f, ρ_f, and u are the void fraction, the density, and the velocity vector of the fluid. ρ_p and v_i are the density and the velocity vector of the particle. C_d denotes the fluid drag force and is simplified to Stokes flow with $C_D = \frac{24}{Re_p}$.

4 Experimental observations: Materials and methods

The microfluidic chips for the validation experiments were fabricated as described elsewhere[7]. Briefly, a casting mold for channels with a width of 200μm and a height of 20μm was printed with a direct laser writing setup, the Nanoscribe Professional GT+ (Nanoscribe GmbH, Germany). The molds were replicated via soft lithography with Polydimethylsiloxane (Sylgard 184, Mavom GmbH, Germany) at a 10:1 ratio of monomer to crosslinker. The microfluidic chips were bonded to cover slips and coated with an MTS:TEOS coating[8]. For the experiments, the channels were filled with the photoresist IP-L 780 Photoresist (Nanoscribe GmbH, Germany) and loaded to the Nansocribe. The pore constriction was created using in-chip direct laser writing, as described by Lüken et al.[7]. After printing of the pore constriction, tubing was filled with the photoresist IP-L 780 and connected to the chip. Hydrostatic pressure was used to induce a controlled flow of resin through the pore. Particles were fabricated in-situ at the desired location and orientation. Each particle consists of an individual laser trajectory written with a laser power of 50 mW and a scanspeed of 25000μm.

Author Contributions

Berinike Bräsel: Conceptualization, Methodology, Formal analysis, Investigation, Data Curation, Writing - Original Draft, Visualization, Project administration.
Matthias Geiger: Investigation, Data Curation, Writing - Original Draft, Visualization.
John Linkhorst: Conceptualization, Writing - Review & Editing, Project administration, Supervision.
Matthias Wessling: Conceptualization, Writing - Review & Editing, Resources, Project administration, Supervision, Funding acquisition.

Conflicts of interest

There are no conflicts to declare.

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