1½-WAY CFD-DEM COUPLING WITH DNSLAB: THE OPTIMAL COMPROMISE BETWEEN MODELING DEPTH AND COMPUTER RESOURCES DEMAND FOR THE 3D SIMULATION OF MICROSCALE FLUID-PARTICLE PROCESSES

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Abstract

Microscale fluid-particle processes, especially such as filtration of solid particles from liquid by porous media, involve the effect of the fluid flow on the particles as well as the effect of the particles on the fluid flow. For the simulation of such processes, where the CFD method is used to model the fluid flow and the DEM method to model particle-particle and particle-structure interactions, several approaches of coupling these two methods can be applied with different modeling depths and demands regarding computer resources. To determine an appropriate approach to simulate a certain fluid-particle process, an essential decision is if and how the effect of the particles on the fluid flow should be taken into account. Doing so with more or less precision will lead to a significantly higher or lower demand of computer resources.

Using the it4e simulation software DNSlab, 1-way, 2-way and recently, as a compromise between 1-way and 2-way, 1½-way CFD-DEM coupling have been implemented and evaluated. The 3 approaches are depicted in Fig. 1.

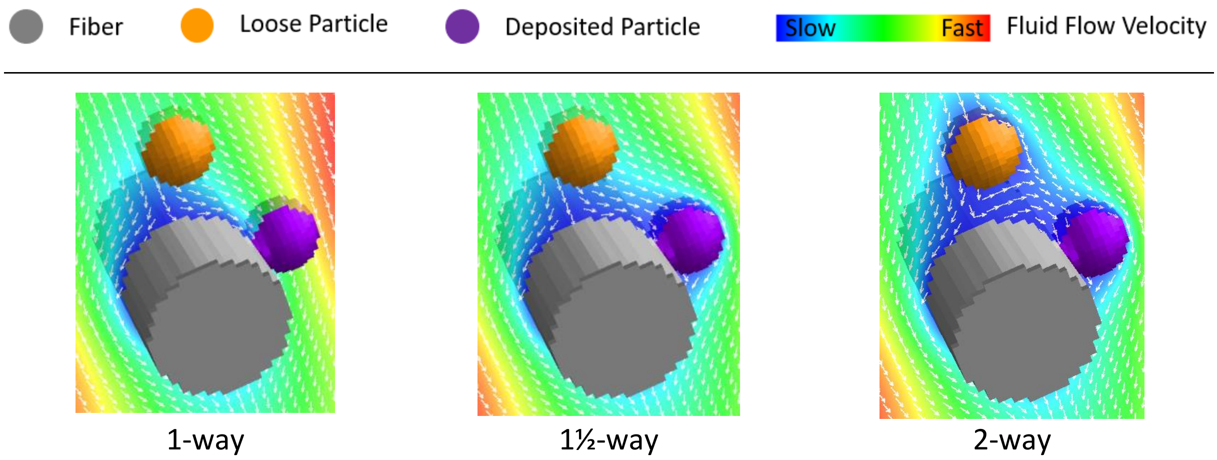


Fig. 1: *Different CFD-DEM coupling approaches in DNSlab. With 1-way coupling, all particles don't affect the fluid flow. With 1½-way coupling, only deposited particles affect the fluid flow. With 2-way coupling, all particles affect the fluid flow.*

In this contribution, the different CFD-DEM coupling approaches in DNSlab are explained and the capabilities of the new 1½-way CFD-DEM coupling method are demonstrated by the simulation of particle deposition at a microfiber nonwoven, filter cake buildup and backwashing with varying particle-particle and particle-structure adhesion forces.

Keywords: Fluid-Particle Separation, Simulation, CFD, DEM, Porous Media, Microscale

1. CFD-DEM 1-way coupling

CFD-DEM 1-way coupling (Fig. 2) has been implemented by using a steady-state flow field which can be computed either by a Finite Differences or alternatively by a Lattice-Boltzmann scheme. Then the motion of the particles is modeled by the DEM method, where the local flow velocities at the particle positions are taken into account by the drag respectively resistance force which acts from the flow field on the particles. The advantage of this approach is that the resolution of the computational grid for the flow calculation and the particle sizes can be chosen more or less independently from each other, and that the flow field can be computed independently from the particles, which results in a low demand of computer resources. The disadvantage of this approach is that the effect of the particles on the fluid flow is neglected.

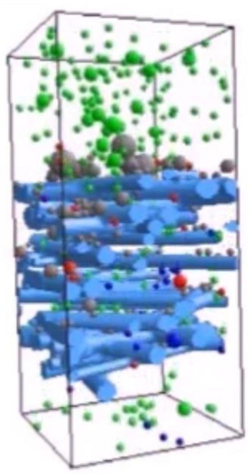
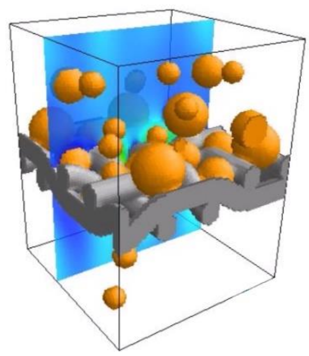


Fig. 2: *1-way coupled CFD-DEM simulation of the deposition of solid polydisperse particles at a nonwoven, showing particle adhesion and detachment at varying flow velocities. See the animation at https://youtu.be/dO1Sz-KwiCA*

2. CFD-DEM 2-way coupling

A CFD-DEM 2-way coupling (Fig. 3) approach has been implemented by coupling the DEM method with the Lattice-Boltzmann method, where the volume displacement and the momentum transfer from the particles to the fluid are taken into account by applying velocity boundary conditions on the moving surface of the particles. The benefit of this approach is that the transient flow field around each particle is resolved and that the effect of the particles on the fluid flow is modeled down to the last detail. On the other hand, a high resolution of the computational grid for the flow computation is required to resolve the particles, and the flow field must be updated at each DEM time step, which results in a high demand of computer resources.

Fig. 3: *2-way coupled CFD-DEM simulation of the deposition and backwashing of solid polydisperse particles at a wire mesh. Each particle is regarded as an obstacle for the fluid flow. See the animation at https://youtu.be/GJCfA586eTA.*



3. CFD-DEM 1½-way coupling

To overcome the disadvantage of the high demand of computer resources of the CFD-DEM 2-way coupling approach, but still to include the effect of *deposited* particles on the fluid flow, the so-called CFD-DEM 1½-way coupling method has been developed. At this, the steady-state flow field is only updated when a particle or a small number of particles is deposited or detached, so that the most essential effects of the particles on the fluid flow by pore clogging, filter cake buildup and particle re-entrainment are reproduced; but, in comparison to the 2-way coupling approach described above, at a much lower computing power demand.

In the following, the capability of the CFD-DEM 1½-way coupling method to reproduce various types of filtration processes with variable emphasis on depth filtration or cake filtration including backwashing is demonstrated by an example of the separation of solid particles from water at a microfiber nonwoven.

The nonwoven structure model consists of cylindrical fibers with 15 µm diameter and has a porosity of 80%, with a resolution of the grid for the flow computation of 80x80x315 voxels and voxel length 2 µm. A dispersion of two fractions of spherical particles with diameters 10 and 20 µm in water passes through the nonwoven from top to bottom with an average flow velocity of 0.02 m/s. Using a hard sphere model for the DEM part of the simulation, the adhesion forces between particles and fibers and between particles and particles have been varied between 1 and 10 nN. Coefficients of sliding and static friction were set to 0.5 and 0.9. For each variant, the separation of 750 particles has been simulated in 150.000 DEM time steps with 1 µs per time step, which corresponds to 0.15 s real time for each simulation run. After 100,000 time steps respectively 0.1 s real time, the flow direction has been reversed for backwashing. During each simulation, the flow field was updated about 80 times due to a changed flow profile by attached or detached particles, using the Finite Differences CFD method to solve the Stokes equations. The overall computing time for each simulation has been about 4.5 hours on a low cost office PC with a Ryzen 3 3200 processor (4 CPU cores at 3.6 GHz) and used about 1 GB DDR4 memory. Both numerical schemes, CFD and DEM, have been running parallelly on the 4 CPU cores.

Fig. 4 and 5 show the resulting distribution of the deposited particles after 0.1 s (before backwashing) and after 0.15 s (after backwashing) for the varied adhesion forces in comparison.

Fig. 6 shows the corresponding volume fractions of the deposited particles as a function of the vertical distance to the inflow area at the top of the model.

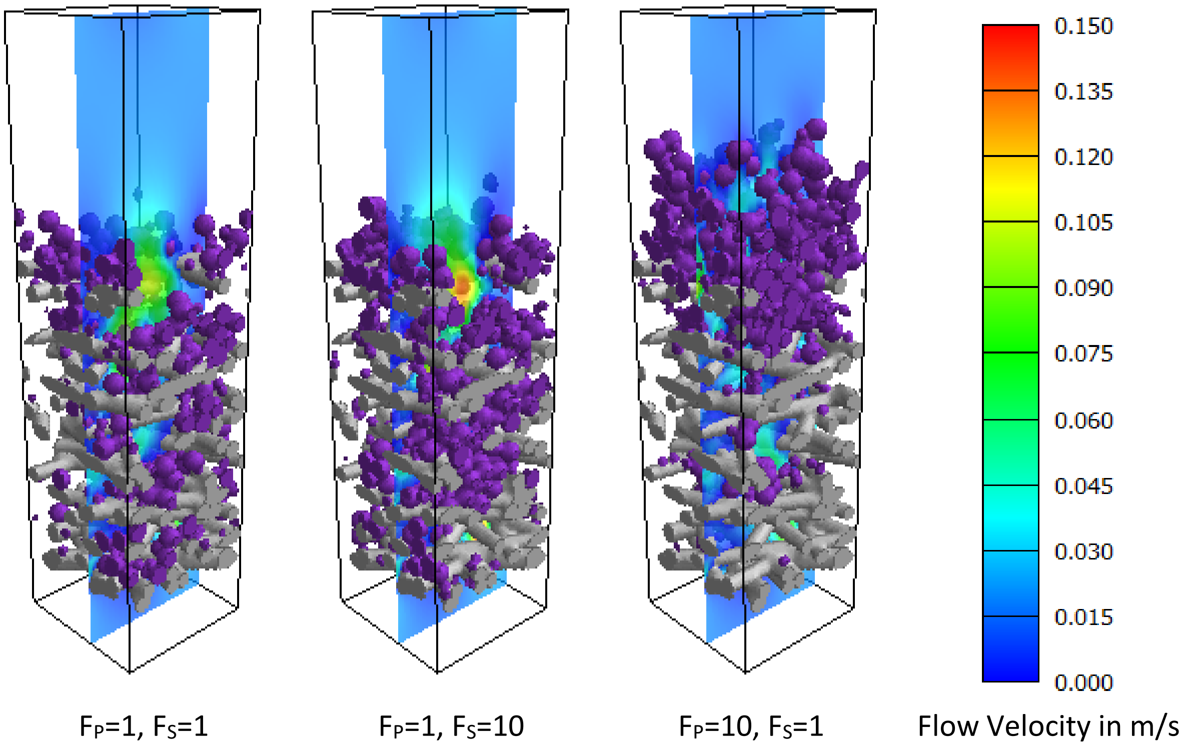


***Fig. 4:** Simulated distribution of deposited particles **before backwashing** for varied adhesion forces between particles and particles (F_P) and between particles and fiber structure (F_S). The adhesion forces are given in nN.*

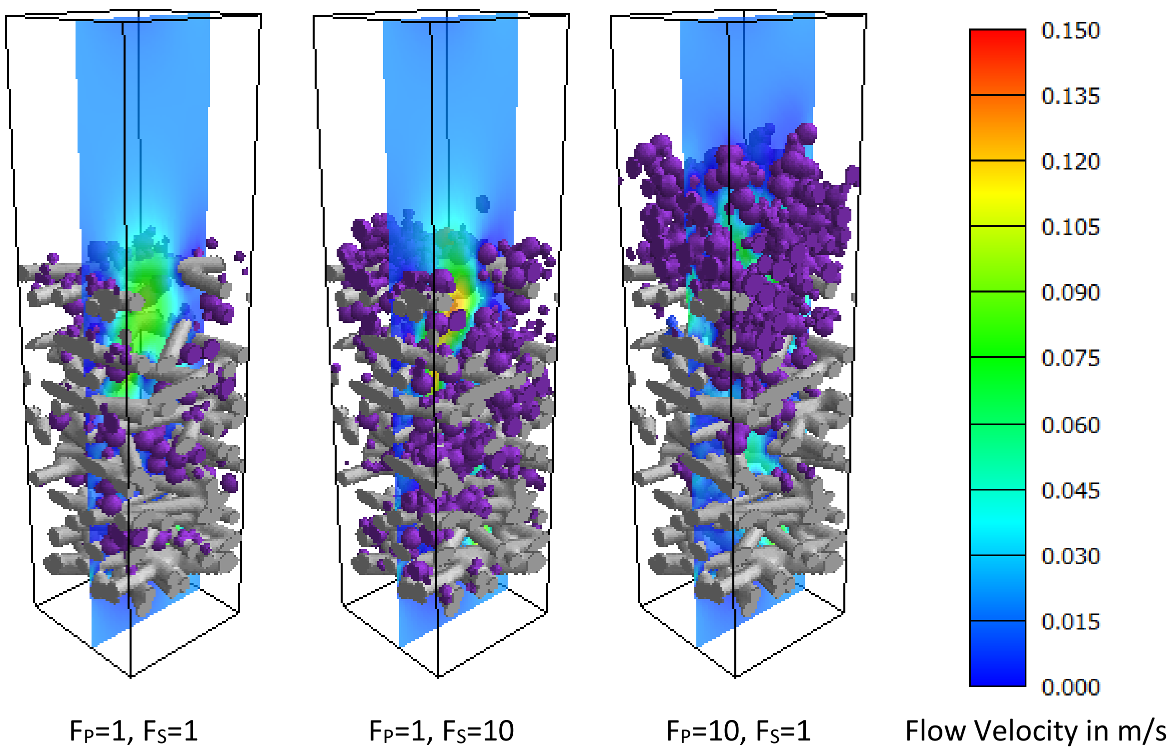


***Fig. 5:** Simulated distribution of deposited particles **after backwashing** (same units and color scale as in Fig. 4).*

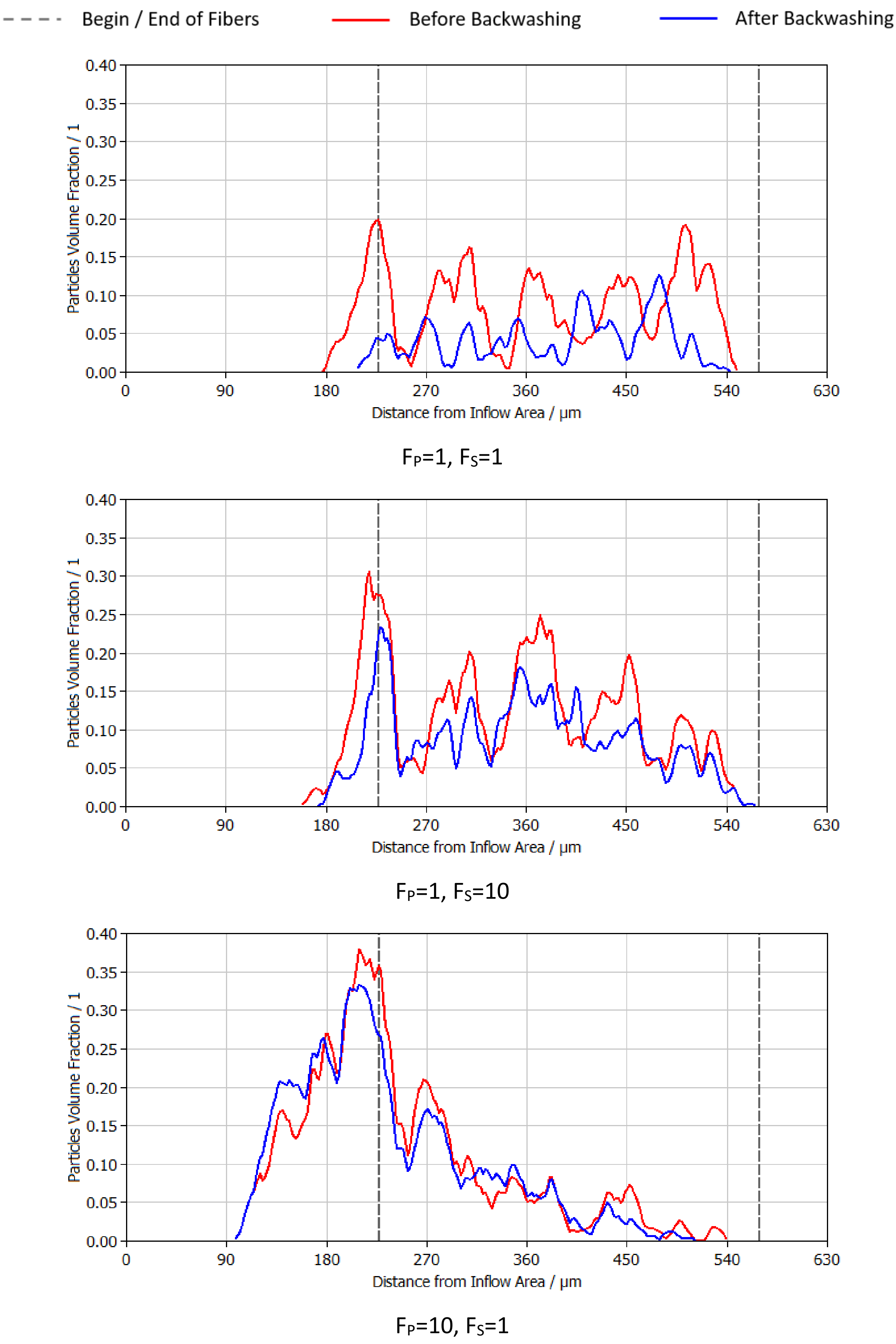


Fig. 6: *Comparison of volume fractions of particles as a function of the distance to the inflow area for the simulations shown in Fig. 4 and 5.*

As expected, the variant with the smallest adhesion forces displayed at the **top of Fig. 6** shows the smallest filter cake and the greatest backwashing effect. A greater adhesion of the particles to the fiber structure results in a greater total deposited particle mass and a smaller backwashing effect as shown at the **center of Fig. 6**. When the adhesion force between particles is greater than the adhesion force between particles and fibers (shown at the **bottom of Fig. 6**) it results in the greatest total deposited particles mass, the greatest filter cake and the smallest backwashing effect.

4. Conclusion

The CFD-DEM 1½-way coupling approach allows to reproduce microscale deposition and detachment of particles including backwashing. By DEM contact models like hard sphere with adhesion forces, sliding and static friction, various fluid-particle-structure systems with different penetration depths, filter cake structures and backwashing properties can be modeled. The required computer resources are within a range which allow simulation runs in the order of magnitude of a few hours, for scientific as well as for industrial applications.

5. References

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