On Coupled Particle Level and Filter Element Level Simulation for Filtration Processes

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1. Introduction

Mathematical modeling and computer simulations can assist engineers in designing new filter media and filter elements. Often, modeling and simulation assists the filter media design at microscale (pore and particle scale), whereas, at macroscale (filter element scale) it assists the filter element design. In fact, in many cases the processes at microscale and macroscale are interdependent, and a consideration of the coupled micro and macro models is needed. Moreover, the microscale simulations can provide the macroscopic models with important parameters, e.g. deposition rate, changes in permeability due to the loading, etc. In this way a complete design cycle of filter media and filter element can be performed, embedding all studies in the virtual material design concept. Earlier, Fraunhofer ITWM has presented algorithms and software, independently for simulations on the micro scale, see, e.g. [1, 2], and macro scale, see, e.g., [3, 4]. The goal of this paper is to discuss two approaches where the coupled micro and macro scale simulations are used in CAE.

In the first case, coupled simulation on micro- and macro- scales is discussed. The approach is based on a fractional time step discretization, with subproblems being solved consecutively on the micro and macro scales. The macro scale parameters, permeability and absorption rate, are consecutively upscaled from solutions of micro scale problems. The macroscopic solution at each time step is downscaled to provide input velocity and particles distribution for the micro scale simulations. The changes in the microstructure are monitored in selected locations of the filter media in order to provide proper information for the upscaling procedure.

In the second case, the microscale simulations are used to determine the coefficients for the macroscopic equations, thus significantly reducing the amount of the required measurements data.

Below, we shortly present the macro scale and the micro scale models, and discuss their advantages and disadvantages. Next, we discuss the above mentioned approaches for coupled simulation on the micro and macro scales.

2. Macro scale model

As shown in the figure, on the macro scale, the Navier Stokes-Brinkmann system is coupled with a macroscopic equation for the concentration of particles where $\vec{u}$, p and

C are the velocity, the pressure and the concentration of dirt particles, respectively. For more details, please refer to [3, 4].

(1) $$\frac{\partial \vec{u}}{\partial t} - \nabla \cdot (\tilde{\mu} \nabla \vec{u}) + (\rho \vec{u}, \nabla)\vec{u} + \mu K^{-1} \vec{u} + \nabla p = \vec{f}$$ (momentum balance equation)

(2) $$\nabla \cdot \vec{u} = 0$$ (continuity equation)

(3) $$\frac{\partial C}{\partial t} + (\vec{u}, \nabla C) = D \Delta C - \frac{\partial M}{\partial t}$$ (transport equation)

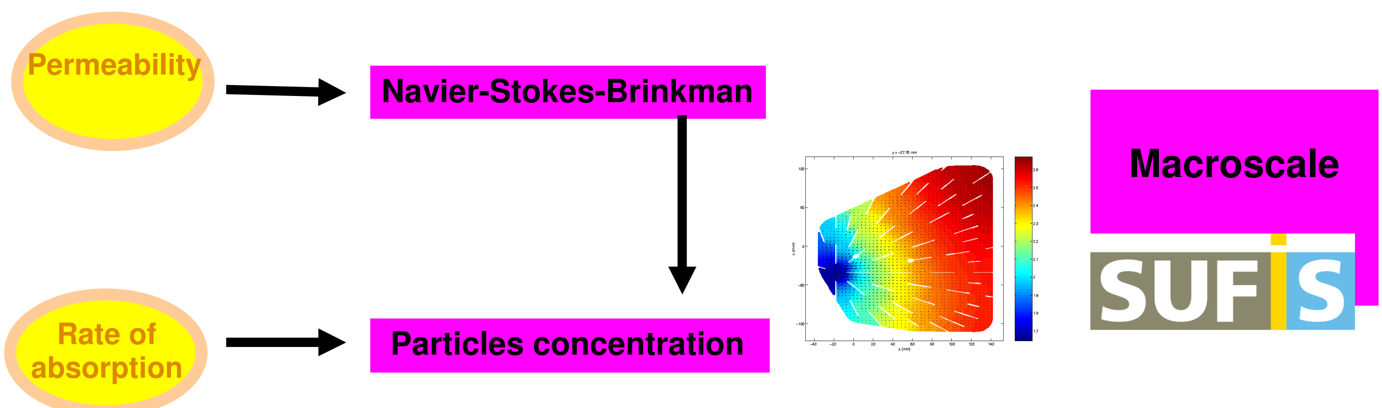
Here one can consider different assumptions for the deposition rate, in particular,

(4) $$\frac{\partial M}{\partial t} = \alpha C$$

or (see, e.g., [5])

(5) $$\frac{\partial M}{\partial t} = \alpha \left(1 - \frac{M}{M_0} \right) C$$

Here M stands for the amount of the concentration of the deposited particles.



Note that $\vec{u}$, C, K and α, denoting the velocity, the permeability and the absorption rate of the filter media, serve as binding parameters for coupling the macro scale simulations with the micro scale simulations. In general, a macro scale model can be successfully used for simulating filtration processes at the level of a filter element. The permeability and the absorption rate need to be determined from measurements, if micro scale simulations are not available. Such an approach is discussed in [4]. Determining the permeability and absorption rate opens new horizons for a better understanding of filtration processes.

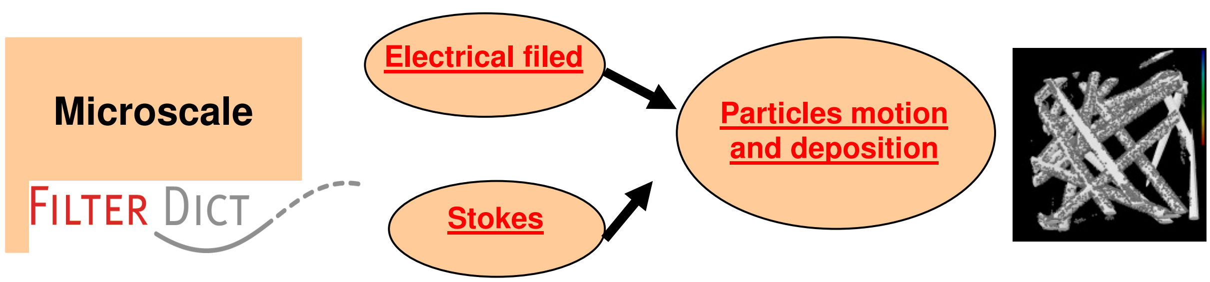
3. Micro scale model

The microscopic model for the motion and deposition of particles is described by a stochastic ordinary differential equation. For further details, please refer to [1, 2]

$$
\begin{aligned}
& d\vec{u} = -\gamma \times \left(\vec{u}(\vec{x}) - \vec{u}_0(\vec{x}) \right) dt + \frac{Q\vec{E}_0(\vec{x})}{m} dt + \sigma \times d\vec{W}(t) \\
& d\vec{x} = \vec{v} dt \\
& \gamma = 6\pi\rho\mu \frac{R}{m} \\
& \sigma^2 = \frac{2k_B T \gamma}{m} \\
& \langle dW_i(t), dW_j(t) \rangle = \delta_{ij} dt
\end{aligned}
\tag{6}
$$

Here $\vec{x}$, $\vec{u}$, R and m denote the position, velocity, radius and mass of particle, respectively. Further, $\vec{u}_0$, ρ and μ denote the fluid velocity, density and viscosity. Additionally, t denotes the time, whereas T, k_B and $d\vec{W}(t)$ denote the ambient temperature, Boltzmann constant and 3d probability (Wiener) measure.

In general, the capacity of today's computers does not permit the solution of these equations in a full filter element. The equations provide a very good option for local simulations in a small part of the filtering medium, but the variations at the level of the filtering element can not be captured in this case. In this context, coupling such micro scale simulations for selected filter medium locations, with the macro scale simulations for the complete filter element, will allow us to get more accurate simulation results.



4. Algorithm for coupling the simulations on the micro scale and macro scales

The processes on different scales are certainly not independent from each other: the micro scale geometry changes due to the deposited particles, thereby affecting the macroscopic parameters such as permeability and absorption rate, because they depend on the microscale solutions. On the other hand, changes in the macroscopic velocity influence the microscopic solution because the ratio between the velocity and the other forces changes. In the proposed coupling approach, we solve the macroscopic equations within the complete filter element, while micro scale equations are solved only at selected locations of the filtering medium. The used fractional time step discretization means that within one time step, macro scale and micro scale equations are consecutively solved, with a proper exchange of information in between these semi-steps. A sketch of one time step of the coupling procedure is as follows.

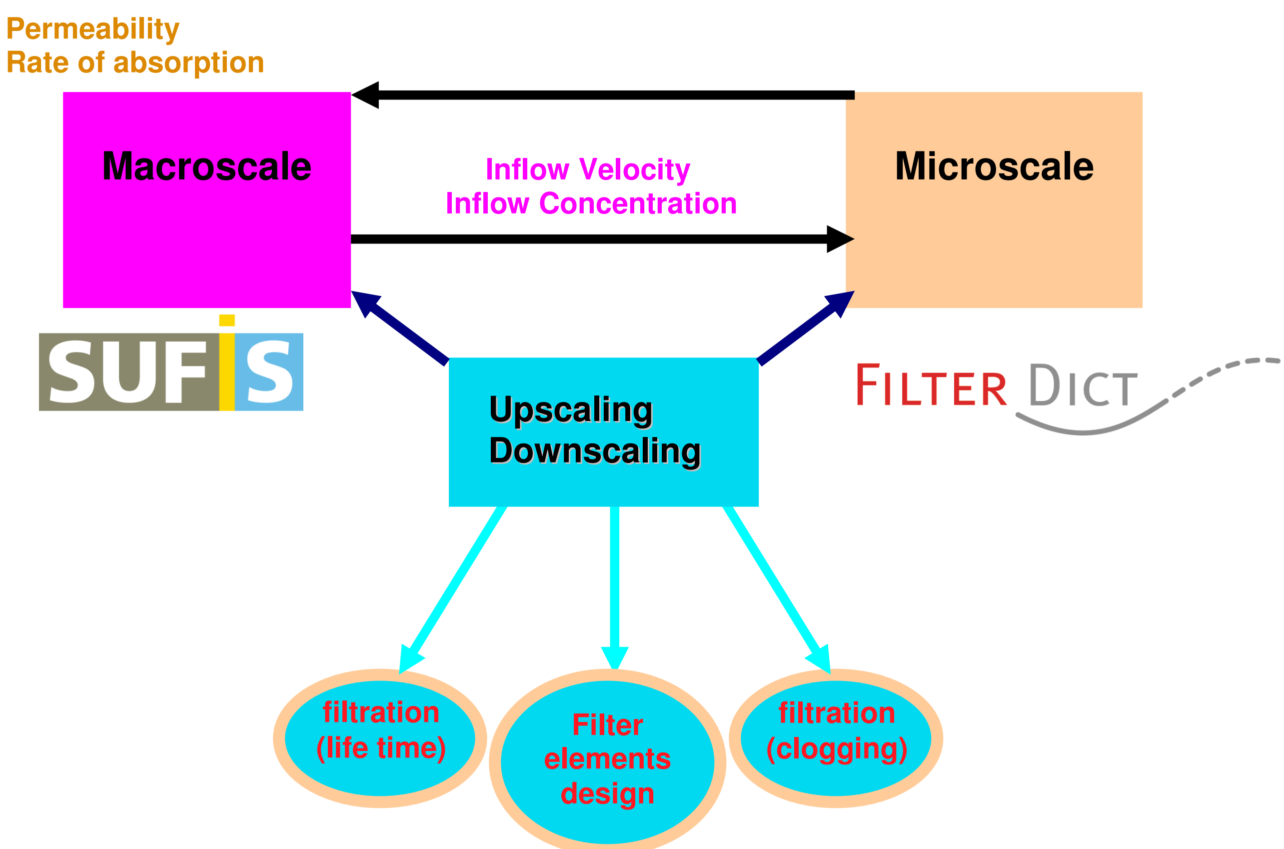
1. At the selected locations of the filtering porous media, local Stokes problems, as well as stochastic ODEs describing the movement and deposition of particles, are solved;

2. Based on a consecutive upscaling procedure, these results are used to update permeability and the absorption rate in the selected locations;

3. A proper interpolation procedure is used to calculate proper permeability and absorption rate in the full porous medium;

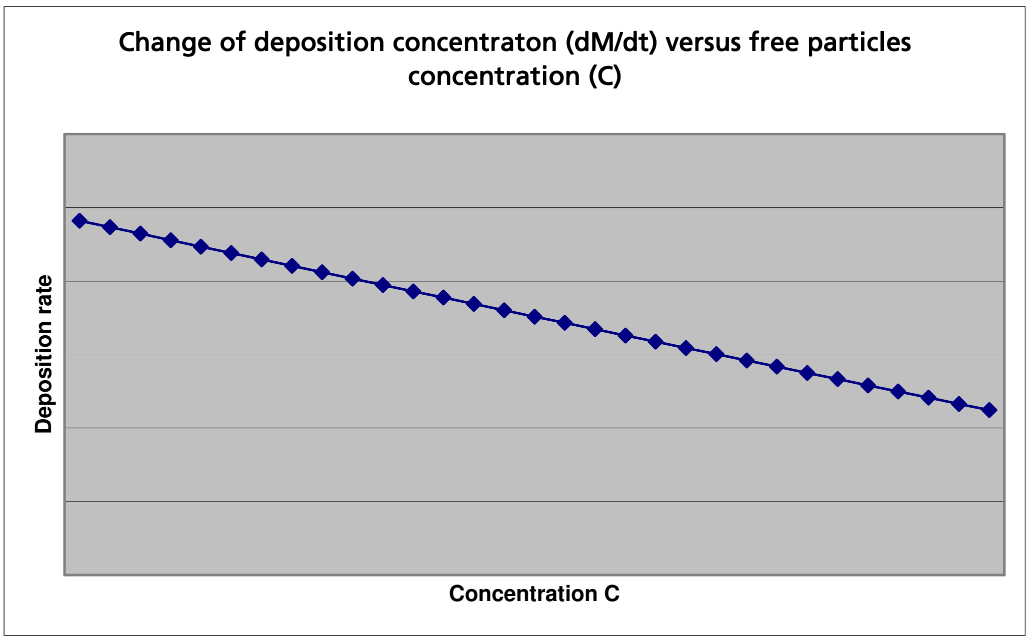
4. The updated permeability and absorption rate are used to perform a semi time step with the macroscopic algorithm;

5. The velocities and the concentration of particles are downscaled in order to provide input for the micro scale computations at the next time step.



5. Macroscale parameters via microscale simulations

Parameters α, M_0 in Eqs.(4),(5), in general, can be determined from measurements of the efficiency of the filter media or complete filter element, such as multipass or TFEM tests. These measurements however, are expensive, and partial substitution by computer simulations allow us to reduce the costs and to shorten the time for new designs. At each time moment, the microscale simulation (see, e.g., [1,2], or www.geodict.com) provides detailed information about the amount (concentration) of free particles and of the deposited particles, In this way, parameters α, M_0 in Eqs.(4),(5) can be determined, or new relations instead of Eqs.(4),(5) can be discovered. The Fig. below shows a plot allowing to determine α from Eq.(4). The results concern filtration of transmission oil (small concentration of particles, no change in permeability). More results will be included in the Conference presentation.



6. Conclusion

Undoubtedly, the interplay between macro scale and micro scale simulations reflects the true nature of filtration processes. A concentration equation is introduced as an extension to the previously used macro model in SuFiS, serving as the binding equation to couple micro scale and macro scale simulations. We have presented an idea that enables this coupling between multiple scales with the help of a systematic iterative procedure of updating parameters appropriately on the level of both scales. This further gives an insight to the time-dependent clogging of filter media for those finite regions of the filter where micro fibrous structures were resolved. With proper interpolation and approximation procedures, this further provides a new platform for attaining approximates for filter efficiency and filter clogging to enhance the design of innovative filters.

References

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