Multiscale modelling in separation processes: particle interactions, homogenisation and the role of gradients

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Filters involved processes occurring in multiple scales and, as a result, we require multiscale models to capture their behaviour. For example, what are the effects of the pore distribution or fibre-contaminant interactions on the overall filter performance? In this talk I will discuss methods to incorporate discrete-level features such as these into macroscopic models for the contaminant concentration across the filter. These are based on partial differential equations, which have the advantage over microscopic models that are easy to solve and analyse in terms of the model parameters.

Though the methods are general, I plan to discuss the particular case of diffusion in a porous medium consisting of a collection of impenetrable spheres. I will present two different approaches for calculating the effective diffusion coefficient as a function of the microstructure. The first is a deterministic approach for quasi-periodic media based on the method of multiple scales, which works at any porosity; the second is a stochastic approach for random media based on matched asymptotic expansions which is limited to low porosities but has the advantage that the porous matrix can be dynamic and interactions with the contaminant can be very general.

As future work, I'm interested in comparisons of my homogenised PDE models with experiments and/or microscopic monte carlo simulations. Moreover, I'm interested in applications of Bayesian inference to parametrise the models, and the inverse problem of finding the optimal filter (that is, model parameters defining the filter) to fit a given filtration challenge. Finally, I'm also interested in separation or segregation processes, where we have multiple particle types that we want to separate (as opposed to one type of particles being fixed, the filter matrix). Can we use methods from filtration to tackle these systems?