Universiteit Utrecht

"UPSCALING REACTIVE TRANSPORT USING PORE-NETWORK MODEL"

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Introduction

The main objective of this research is to provide insight in, and quantitative relations for upscaling reactive transport in porous media. This will be done with the aid of computational upscaling.

Single tube computations (cylindrical tube)

we consider numerical simulations in a single tube assuming equilibrium adsorption at its wall. Equation 1 is the dimensionless micro-scale transport equation:

$$\frac{\partial c}{\partial t}+2(1-r^2)\frac{\partial c}{\partial z}=\frac{1}{Pe}\left[\frac{\partial^2 c}{\partial z^2}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)\right] \quad (1)$$

With the following dimensionless boundary condition at r = 1:

$$\frac{\partial c}{\partial r}=-Pe\ .\ \mathrm{kd}\ .\frac{\partial c}{\partial t}$$

We have solved this differential equation numerically to get average breakthrough curve in a single pipe (Figure 1).
At one scale up, we assumed macro-scale kinetic adsorption (Equation 2):

$$\frac{\partial \bar{c}}{\partial t}+\frac{\partial \bar{c}}{\partial z}=\frac{1}{Pe^*}\frac{\partial^2 \bar{c}}{\partial z^2}-K_{\mathrm{det}}(K_D\bar{c}-\bar{s}) \quad (2)$$

$$\frac{\partial \bar{s}}{\partial t}=K_{att}\bar{c}-K_{\mathrm{det}}\bar{s}$$

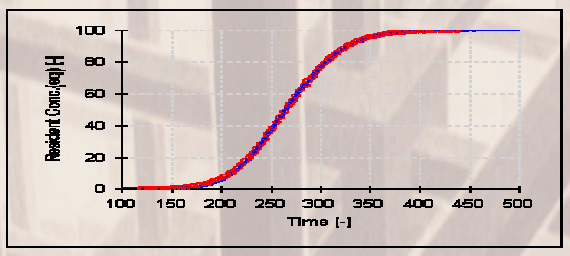

Fig 1. breakthrough curves obtained by solving equation 1 using input parameters: kd=1.0, Pe*=12 (red circles) and fitting to the solution of equation2 (blue line).

Relation between micro and macro scales:

By fitting the breakthrough curve of average concentration ,equation 1, to the analytical solution of macro-scale equation 2, we found corresponding k_{det} and k_{att} for micro-scale K_d and Pe (Figure 1). For macro scale Peclet number we used the Taylor dispersion formula:

$$\frac{1}{pe^*}=\frac{1}{pe}+\frac{pe}{48} \quad (3)$$

Doing this numerical simulation for different micro-scale k_d and Pe (to find the corresponding macro-scale k_{det} and k_{att}) we found the relation between micro-scale and corresponding macro-scale parameters (Figure 2). Equations 4 and 5 are showing these relations.

$$K_D=\frac{3.7(1-e^{-2kd})(1+4kd)}{9.0} \quad (4)$$

$$K_{\mathrm{det}}=\frac{9.0}{(1+4kd)\ \mathrm{Pe}^{0.95}} \quad (5)$$

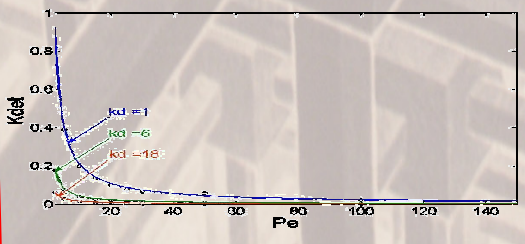

Fig 2. macro-scale K_{det} as a function of micro-scale Pe (a) and Kd (b)

Pore-network modeling of reactive solute transport:

In the next step, we have used the pore-network model to upscale reactive parameters. After construction of network (consisting of different bore-throat sizes, so different velocities) we have used equation 4 and 5 to calculate reactive parameters for each pore-throat in the pore-network (Figure 3). Then we have simulate solute transport with kinetic adsorption inside the network to get the breakthrough curve at the outlet (Figure 4).

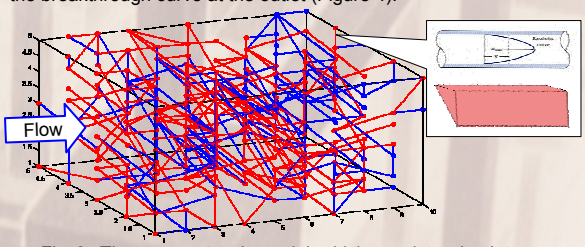

Fig 3. The pore-network model which used to simulate reactive solute transport. With cross section either circular or triangular.

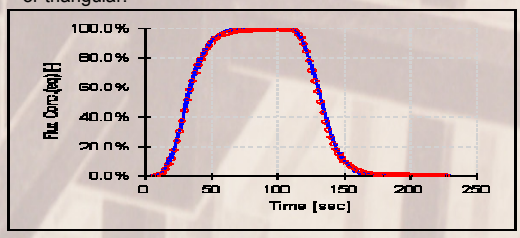

Fig 4. flux-averaged concentration breakthrough curve at the outlet of the pore-network.

Single tube computations (triangular cross section)

We simulated solute transfer in corner fluid filaments. To get the velocity field we solved stokes equation by finite-element method. Then the resulting velocity field is used to simulate convection diffusion in corner fluid. Figure 5 shown the velocity field and figure 6 show the resulting solute concentration field and breakthrough curve of average effluent concentration.

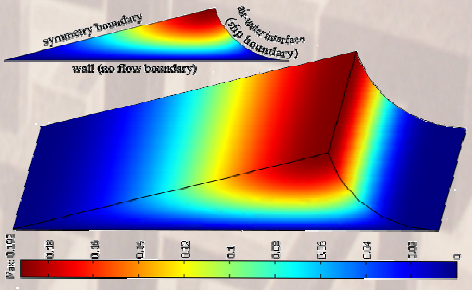

Fig 5. velocity filed in a 2D domain and a 3D domain with the same cross section and mesh structure.

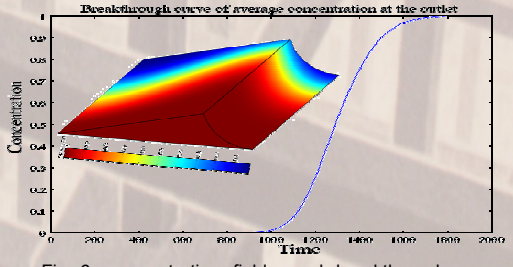

Fig 6. concentration field and breakthrough curve of average effluent concentration.

Results & Conclusions

By upscaling reactive transport parameters we found that:
If we have linear equilibrium adsorption at the scale of pore walls, we get linear kinetic adsorption at larger scale
kinetic adsorption parameters are found to be a function of local-scale adsorption and Peclet number.
reactive transport at core scale can be modeled with our pore-scale network model.