Upscaling of the Reaction-Advection-Diffusion Equation in Porous Media with Monod-Like Kinetics

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Joint work with F. Hesse, S. Attinger and M. Thullner
Motivation

- Macroscale simulations based on microscale parameters are normally overestimating the degradation, which leads to a false prognosis.
- There is therefore a strong need for effective, macroscale degradation rates.
- For the zero- or first-order degradation, the derivation of effective parameters is well understood. Not the same can be said about Monod-like kinetics.
OBJECTIVE

- Starting with the 2D pore scale model to derive an 1D model by upscaling in the transversal direction

- To determinate effective rates for Monod-like degradation

- To consider the effect of bioavailability on upscaling
Bioavailability

Diffusion-limited regime:

- Diffusion is low compared with the degradation rates
- The contaminant is degraded very fast at the surface
Bioavailability

Diffusion-limited regime:
- Diffusion is low compared with the degradation rates
- The contaminant is degraded very fast at the surface

Reaction-limited regime:
- Diffusion is fast compared with the degradation rates
- The process is controlled by reaction
Bioavailability

**Diffusion-limited regime:**
- Diffusion is low compared with the degradation rates
- The contaminant is degraded very fast at the surface

**Reaction-limited regime:**
- Diffusion is fast compared with the degradation rates
- The process is controlled by reaction

**Transition regime**
- The effective degradation rates are influenced by diffusion (and convection)!
Mathematical Model (2D Pore Scale Model)

\[
\frac{\partial}{\partial t} c + \mathbf{v} \cdot \nabla c = D \Delta c \quad \text{in} \quad \Omega_p,
\]

\[
D \nabla c \cdot \mathbf{n} = R(c) \quad \text{on} \quad \Gamma_s,
\]

\[
c = c_0 \quad \text{on} \quad \Gamma_f^i,
\]

\[
\nabla c \cdot \mathbf{n} = 0 \quad \text{on} \quad \Gamma_f^o.
\]

where

\[
R(c) = -\frac{k_{\text{max}} c}{K_m + c} \quad \text{or} \quad R(c) = -kc
\]
Simplifications

- The system is made dimensionless
- We consider steady state
- We neglect the longitudinal diffusion
- The velocity has a component only in the flow direction
(simplified) Mathematical Model

\[ \text{Pe} \ v(y) \frac{\partial}{\partial x} c = D \frac{\partial^2}{\partial y^2} c \quad \text{in} \quad \Omega_p, \]

\[ D \nabla c \cdot n = R(c) \quad \text{on} \quad \Gamma_s, \]

\[ c = 1 \quad \text{on} \quad \Gamma_f^i, \]

\[ \nabla c \cdot n = 0 \quad \text{on} \quad \Gamma_f^o. \]

where

\[ R(c) = -\frac{\Phi^2 c}{1 + \frac{c}{K_m}} \quad \text{or} \quad R(c) = -\Phi^2 c \]
AIM: an 1D upscaled Model

\[ \nu_{\text{eff}} \frac{\partial}{\partial x} \langle c \rangle_y = D_{\text{eff}} \frac{\partial^2}{\partial x^2} \langle c \rangle_y - R_{\text{eff}}(\langle c \rangle_y) \quad \text{in} \quad V_x, \]

\[ \langle c \rangle_y = 1 \quad \text{on} \quad \text{Inlet}. \]

- We need to determine the effective coefficients \( \nu_{\text{eff}}, D_{\text{eff}} \) and \( R_{\text{eff}} \).
### Different scenarios

<table>
<thead>
<tr>
<th>Velocity</th>
<th>Reaction</th>
<th>Monod</th>
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<tbody>
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First-order kinetics and uniform velocity profile

• The effective averaged equation reads:

\[
P_e \frac{\partial}{\partial x} \langle c \rangle_y = -\Phi_{\text{eff}}^2 \langle c \rangle_y,
\]

• Effective degradation rate

\[
\Phi_{\text{eff}}^2 = \eta \Phi^2
\]

with

\[
\eta = \frac{c|_{y=1}}{\langle c \rangle_y}
\]

• \(c|_{y=1}\) is the bioavailable concentration, whereas \(\langle c \rangle_y\) the \(y\)-averaged one.
First-order kinetics and uniform velocity profile

• For small $\Phi^2$ the global and local behavior is coupled (reaction-limited regime).

• For large $\Phi^2$ the global reaction rate $\Phi^2_{\text{eff}}$ saturates (diffusion-limited regime).
Diffusion limited regime

- In the *reaction-limited regime* quantitatively differences of both curves.
In the diffusion-limited regime both curves are far apart.
### Uniform velocity profile and Monod kinetics

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The effective averaged equation reads:

\[
\text{Pe} \frac{\partial}{\partial x} \langle c \rangle_y = -\frac{\Phi^2_{\text{eff}} \langle c \rangle_y}{1 + \langle c \rangle_y / K_m},
\]

Effective degradation rate

\[
\Phi^2_{\text{eff}} = \eta \Phi^2 \quad \text{und} \quad K_{m,\text{eff}} = K_m / \eta
\]

with

\[
\eta = \frac{c|_{y=1}}{\langle c \rangle_y}
\]

\(c|_{y=1}\) is the bioavailable concentration, whereas \(\langle c \rangle_y\) the \(y\)-averaged one.
Uniform velocity profile and Monod kinetics

\[ K_m = 1 \]

- For \( K_m > c \) behavior of \( \eta \) is similar to first-order reaction.
Uniform velocity profile and Monod kinetics

\[ K_m = 0.1 \]

For \( K_m \lesssim c \) nonlinearities increase.
Uniform velocity profile and Monod kinetics

\[ K_m = 0.01 \]

- Constant approximations for effective parameters through fitting.
Uniform velocity profile and Monod kinetics

- Fitting for $\eta$ is not able to reproduce behavior in the transition regime.
• With two parameters the characteristic is well preserved.
### Parabolic velocity profile

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Parabolic velocity profile

- **Idea:** variable separation

\[ c(x, y) = \sum_{i \geq 1} c_i(x) \Psi_i(y) \]

- **Effective equation for the first mode** \( c_1 \)

\[
\begin{aligned}
\nu_{\text{eff}} \frac{\partial}{\partial x} c_1 &= D_{\text{eff}} \frac{\partial^2}{\partial x^2} c_1 - R_{\text{eff}}(c_1) \quad \text{in} \quad V_x, \\
\langle c \rangle_y &= 1 \quad \text{on} \quad \text{Inlet}.
\end{aligned}
\]

- The averaged concentration is approximated by \( c_1 \langle \Psi_1 \rangle_y \).
• Higher reaction rate emphasize the effect of velocity profile.

The effective velocity \( v_{\text{eff}} \) saturates for high values of \( \Phi^2 \).
• Weak dependency of the dispersivity from reaction rate.
• The effective dispersivity $D_{\text{eff}}$ saturates for high values of $\Phi^2$
• Same fitting procedure as with uniform velocity can be applied.

• Slightly different behavior is observed.
Summary

• We considered a 2D pore scale model for advective-diffusive-reactive transport of a contaminant

• A dimension reducing upscaling model is presented

• The special case of degradation following Monod kinetics is treated

• Constant effective parameters are determined through numerical fitting