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

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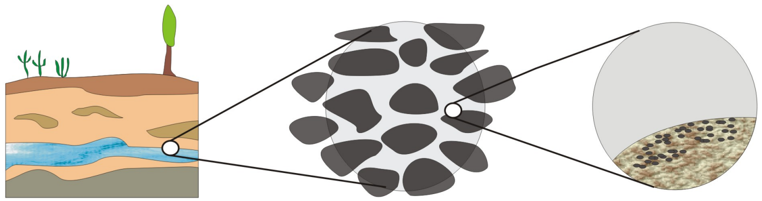
Joint work with F. Hesse, S. Attinger and M. Thullner

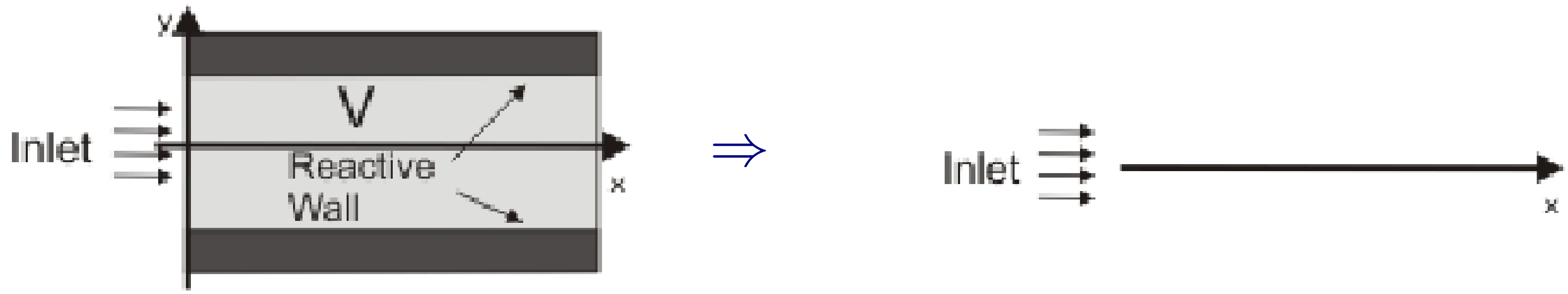
Motivation



- Macroscale simulations based on microscale parameters are normaly overestimating the degradation, which leads to a false prognoze
- 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

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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 contamina … st at the surface

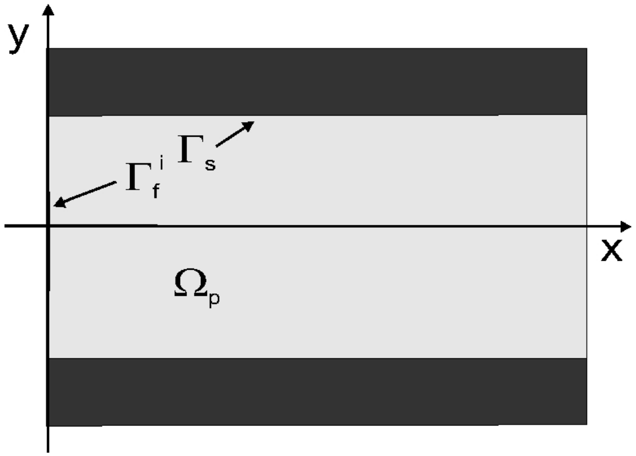
Transition regime

Reaction-limited

- Diffusion is fast compared with the degradation rates
- The process is controlled by reaction

- The effective degradation rates are influenced by diffusion (and convection)!

Mathematical Model (2D Pore Scale Model)



$$
\begin{aligned}
\frac{\partial}{\partial t}c + \mathbf{v}\cdot\nabla c &= D\Delta c \quad \text{in} \quad \Omega_p,\\
D\nabla c\cdot\mathbf{n} &= R(c) \quad \text{on} \quad \Gamma_s,\\
c &= c_0 \quad \text{on} \quad \Gamma_f^i,\\
\nabla c\cdot\mathbf{n} &= 0 \quad \text{on} \quad \Gamma_f^o.
\end{aligned}
$$

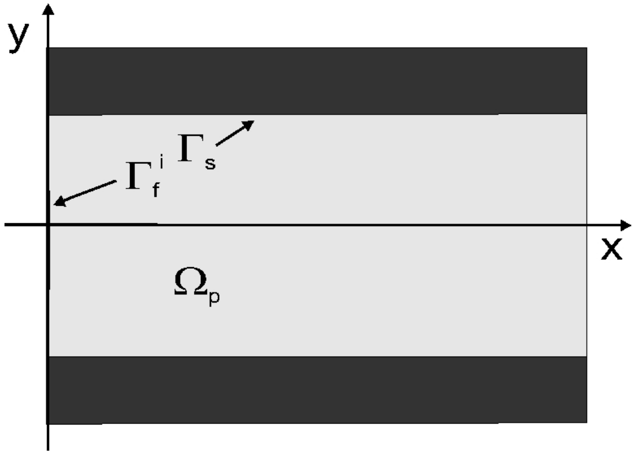
where

$$R(c) = -\frac{k_{\max}\, c}{K_m + c} \text{ or } R(c) = -kc$$

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



$$
\begin{aligned}
\mathrm{Pe}\,\mathrm{v}(\mathrm{y})\frac{\partial}{\partial \mathrm{x}}\mathrm{c} &= D\frac{\partial^2}{\partial y^2}c && \text{in} && \Omega_p, \\
D\nabla c\cdot\mathbf{n} &= R(c) && \text{on} && \Gamma_{\mathrm{s}}, \\
c &= 1 && \text{on} && \Gamma_{\mathrm{f}}^{\mathrm{i}}, \\
\nabla c\cdot\mathbf{n} &= 0 && \text{on} && \Gamma_{\mathrm{f}}^{\mathrm{o}}.
\end{aligned}
$$

where

$$R(c) = -\frac{\Phi^2 c}{1+\frac{c}{K_{\mathrm{m}}}} \text{ or } R(c) = -\Phi^2 c$$

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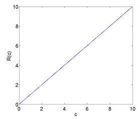
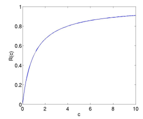
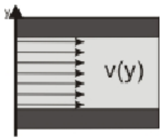
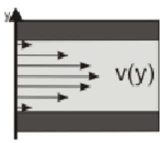
AIM: an 1D upscaled Model

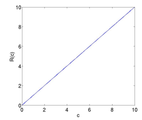
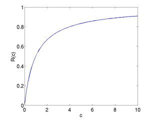
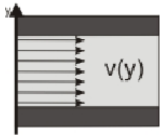
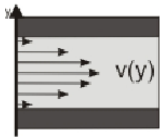
$$
\begin{aligned}
\underbrace{v_{\text{eff}} \frac{\partial}{\partial x} \langle c \rangle_y}_{advection} &= \underbrace{D_{\text{eff}} \frac{\partial^2}{\partial x^2} \langle c \rangle_y}_{diffusion} - \underbrace{R_{\text{eff}}(\langle c \rangle_y)}_{reaction} \quad \text{in} \quad V_x, \\
\langle c \rangle_y &= 1 \quad \text{on} \quad Inlet.
\end{aligned}
$$

- We need to determine the effective coefficients v_{eff}, D_{eff} and R_{eff}.

Different scenarios

Reaction / Velocity	First-order 	Monod 
uniform 	$v = 1$ $R(c) = -\Phi^2 c$	$v = 1$ $R(c) = -\frac{\Phi^2 c}{1+c/K_{\mathrm{m}}}$
parabolic 	$v = 1.5\left(1 - y^2\right)$ $R(c) = -\Phi^2 c$	$v = 1.5\left(1 - y^2\right)$ $R(c) = -\frac{\Phi^2 c}{1+c/K_{\mathrm{m}}}$

First-order kinetics and uniform velocity profile

Reaction / Velocity	First-order 	Monod 
uniform 	$v = 1$ $R(c) = -\Phi^2 c$	$v = 1$ $R(c) = -\frac{\Phi^2 c}{1+c/K_{\mathrm{m}}}$
parabolic 	$v = 1.5\left(1-y^2\right)$ $R(c) = -\Phi^2 c$	$v = 1.5\left(1-y^2\right)$ $R(c) = -\frac{\Phi^2 c}{1+c/K_{\mathrm{m}}}$

First-order kinetics and uniform velocity profile

- The effective averaged equation reads:

$$\mathrm{Pe}\,\frac{\partial}{\partial \mathrm{x}}\langle \mathrm{c}\rangle_{\mathrm{y}} = -\Phi^2_{\mathrm{eff}}\langle \mathrm{c}\rangle_{\mathrm{y}}\,,$$

- Effective degradation rate

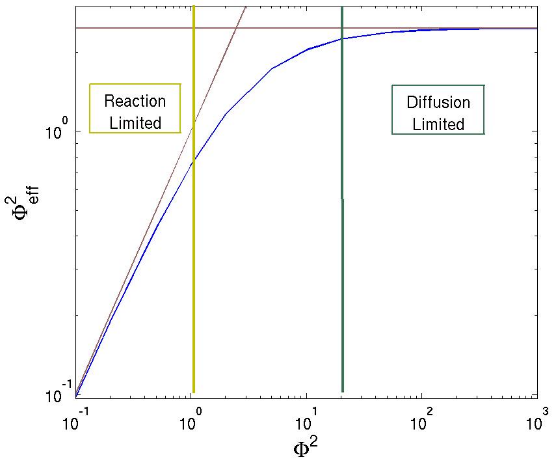
$$\Phi^2_{\mathrm{eff}} = \eta\Phi^2$$

with

$$\eta = \frac{c_{|y=1}}{\langle c\rangle_y}$$

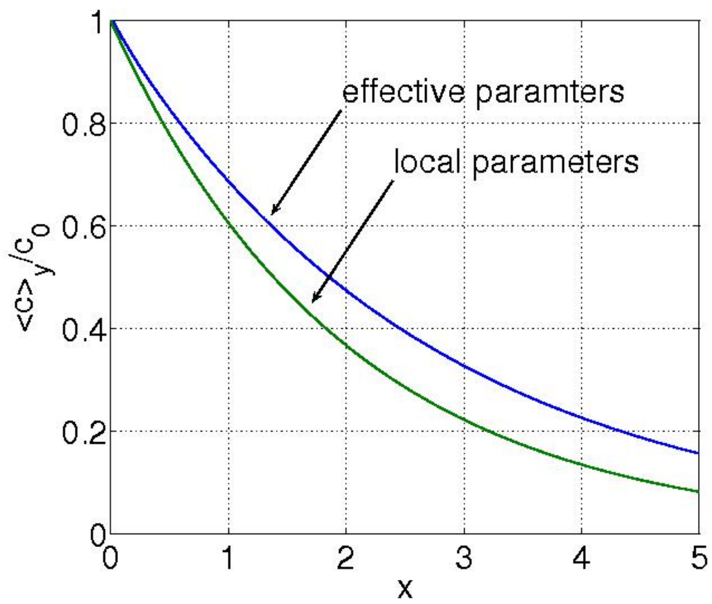
- $c_{|y=1}$ is the bioavailable concentration, whereas $\langle c\rangle_y$ the y-averaged one.

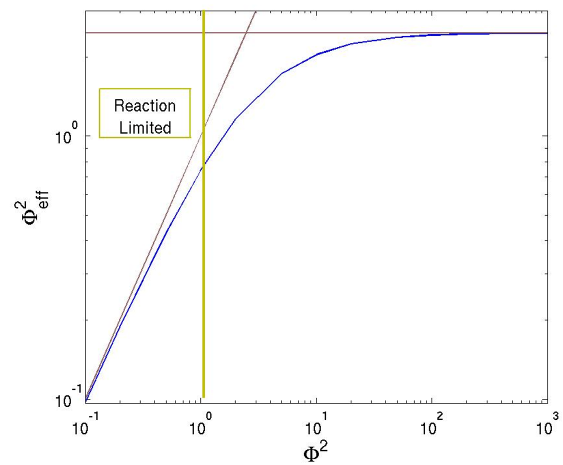
First-order kinetics and uniform velocity profile



- For small Φ^2 the global and local behavior is coupled (*reaction-limited regime*).
- For large Φ^2 the global reaction rate Φ^2_{eff} saturates (*diffusion-limited regime*).

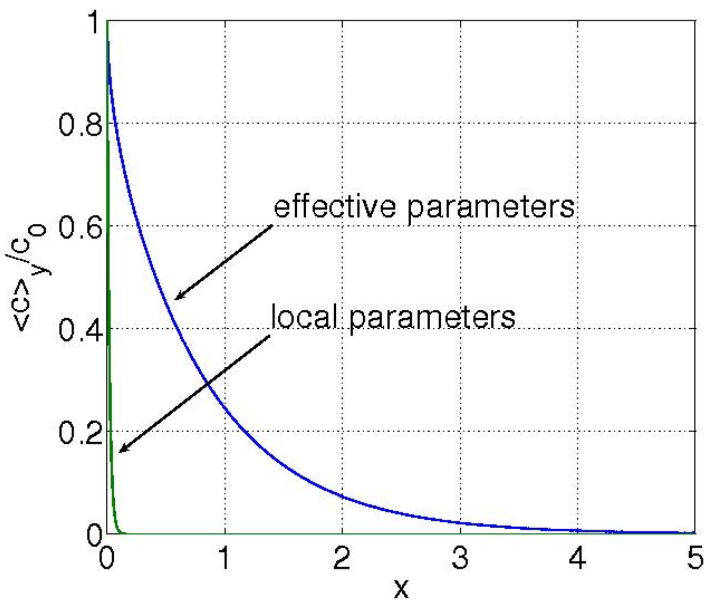
Diffusion limited regime

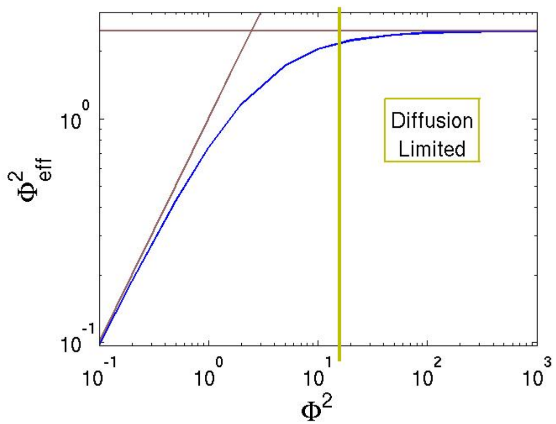




- In the *reaction-limited regime* quantitatively differences of both curves.

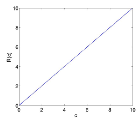
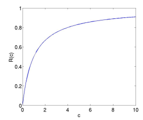
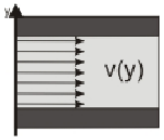
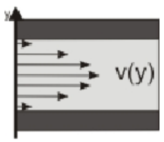
Diffusion-limited regime





- In the *diffusion-limited regime* both curves are far apart.

Uniform velocity profile and Monod kinetics

Velocity \ Reaction	First-order 	Monod 
uniform 	$v = 1$ $R(c) = -\Phi^2 c$	$v = 1$ $R(c) = -\frac{\Phi^2 c}{1+c/K_{\mathrm{m}}}$
parabolic 	$v = 1.5\left(1 - y^2\right)$ $R(c) = -\Phi^2 c$	$v = 1.5\left(1 - y^2\right)$ $R(c) = -\frac{\Phi^2 c}{1+c/K_{\mathrm{m}}}$

Uniform velocity profile and Monod kinetics

- The effective averaged equation reads:

$$\mathrm{Pe}\,\frac{\partial}{\partial \mathrm{x}}\langle \mathrm{c}\rangle_{\mathrm{y}} = -\frac{\Phi_{\mathrm{eff}}^2 \langle \mathrm{c}\rangle_{\mathrm{y}}}{1+\langle \mathrm{c}\rangle_{\mathrm{y}}/\mathrm{K_m}},$$

- Effective degradation rate

$$\Phi_{\mathrm{eff}}^2 = \eta\Phi^2 \text{ und } K_{m,\mathrm{eff}} = K_m/\eta$$

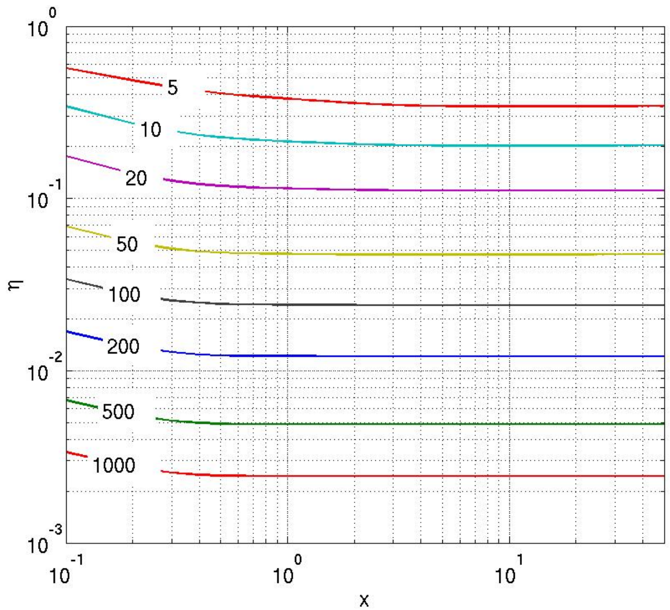
with

$$\eta = \frac{c_{|y=1}}{\langle c\rangle_y}$$

- $c_{|y=1}$ is the bioavailable concentration, whereas $\langle c\rangle_y$ the y-averaged one.

Uniform velocity profile and Monod kinetics

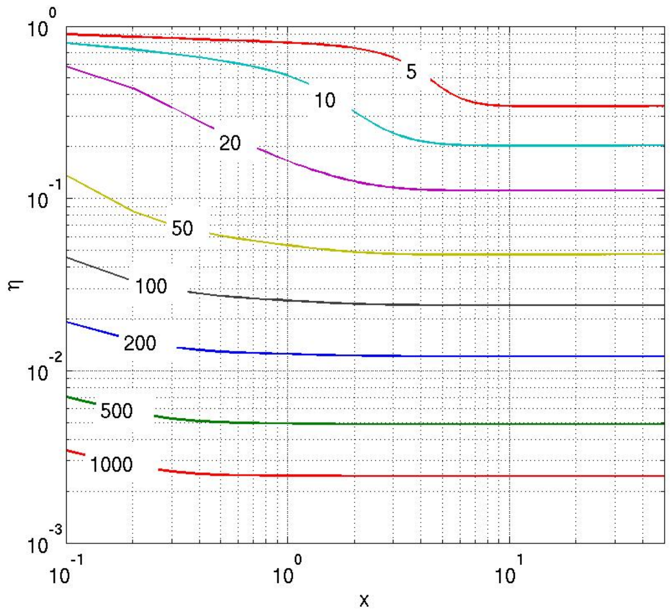
$$K_m = 1$$



- For $K_{\rm m} > c$ behavior of η is similar to first-order reaction.

Uniform velocity profile and Monod kinetics

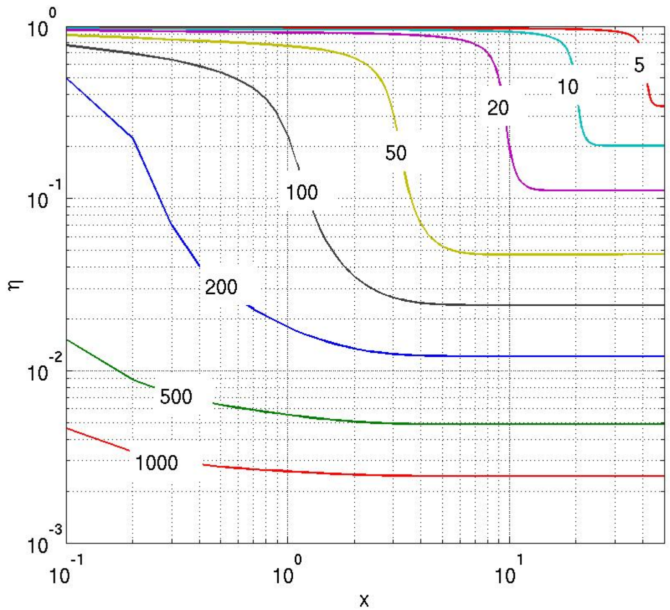
$$K_m = 0.1$$



For $K_{\mathrm{m}} \lesssim c$ nonlinearities increase.

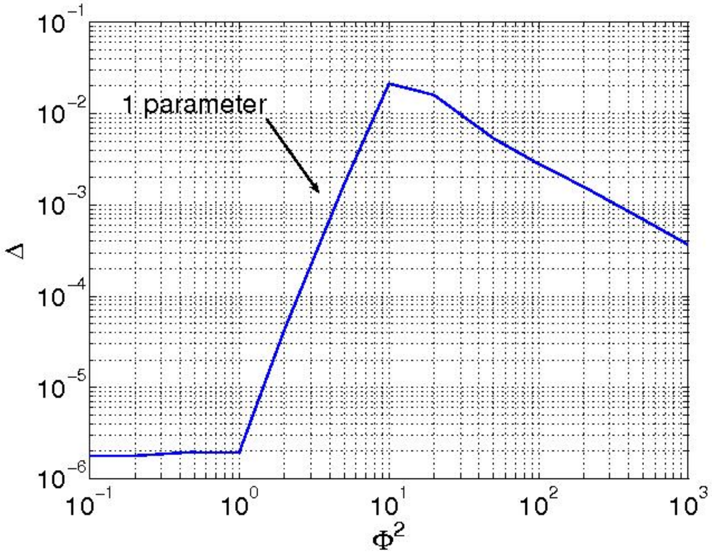
Uniform velocity profile and Monod kinetics

$$K_m = 0.01$$



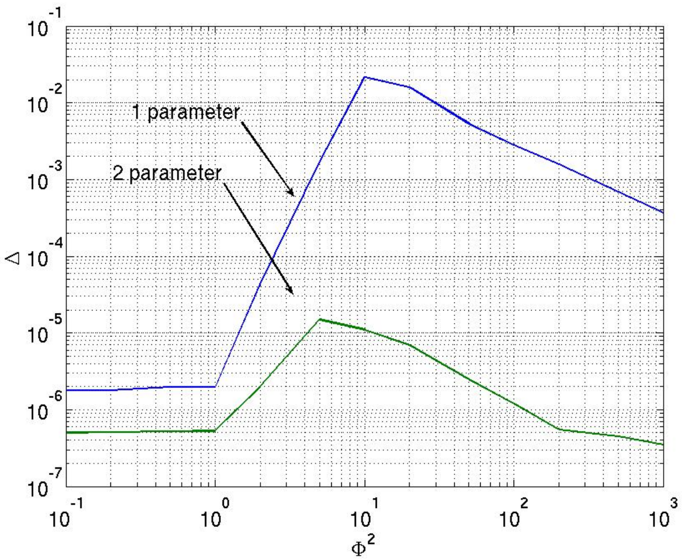
• Constant approximations for effective parameters through fitting.

One parameter fit



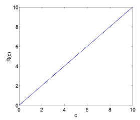
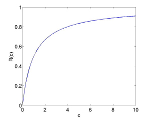
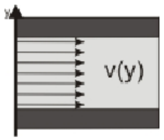
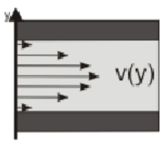
- Fitting for η is not able to reproduce behavior in the transition regime.

Two parameter fit



- With two parameters the characteristic is well preserved.

Parabolic velocity profile

Velocity / Reaction	First-order 	Monod 
uniform 	$v = 1$ $R(c) = -\Phi^2 c$	$v = 1$ $R(c) = -\frac{\Phi^2 c}{1+c/K_\mathrm{m}}$
parabolic 	$v = 1.5\left(1 - y^2\right)$ $R(c) = -\Phi^2 c$	$v = 1.5\left(1 - y^2\right)$ $R(c) = -\frac{\Phi^2 c}{1+c/K_\mathrm{m}}$

Parabolic velocity profile

- Idea: variable separation

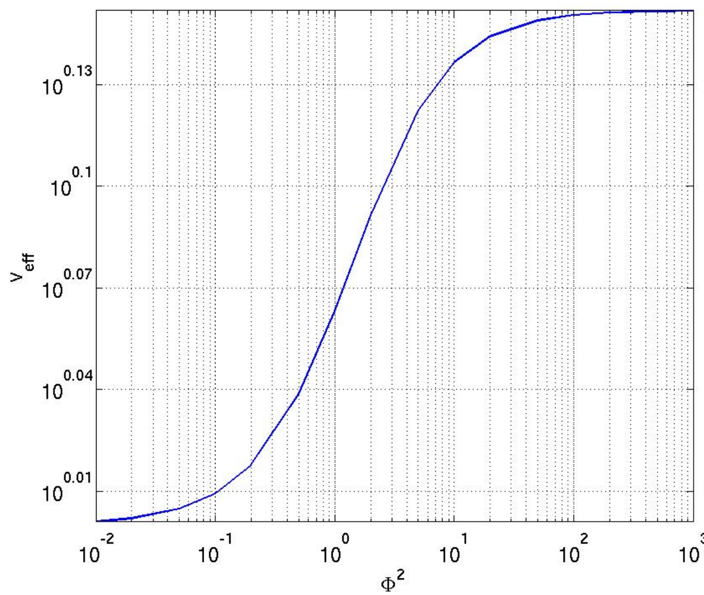
$$c(x,y) = \sum_{i \geq 1} c_i(x)\Psi_i(y)$$

- Effective equation for the first mode c_1

$$\begin{aligned} \underbrace{v_{\text{eff}} \frac{\partial}{\partial x} c_1}_{advection} &= \underbrace{D_{\text{eff}} \frac{\partial^2}{\partial x^2} c_1}_{diffusion} - \underbrace{R_{\text{eff}}(c_1)}_{reaction} \quad \text{in} \quad V_x, \\ \langle c \rangle_y &= 1 \quad \text{on} \quad Inlet. \end{aligned}$$

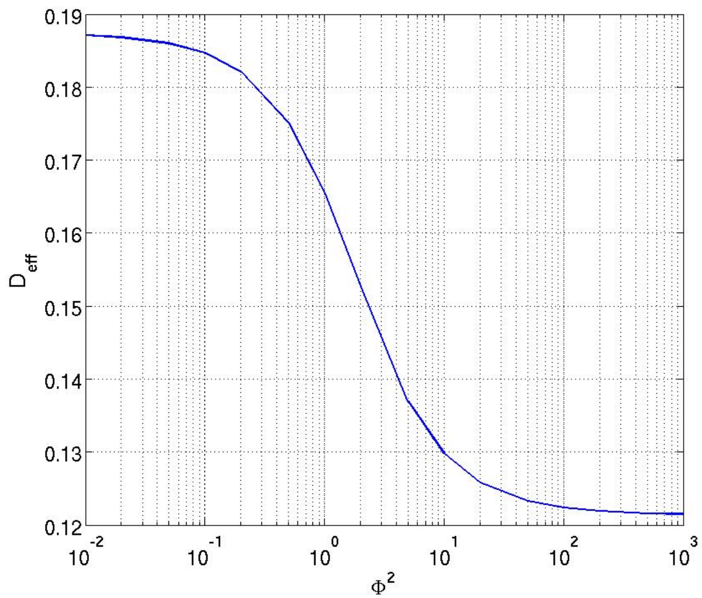
- The averaged concentration is approximated by $c_1 \langle \Psi_1 \rangle_y$.

Effective velocity



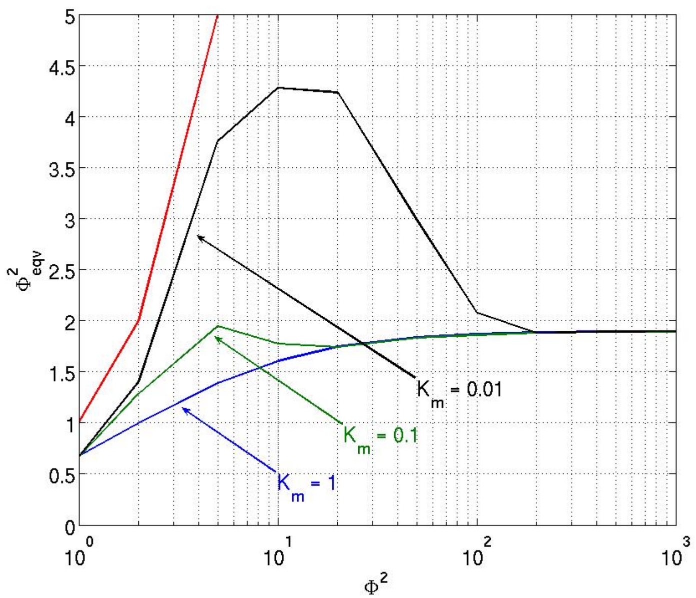
- Higher reaction rate emphasize the effect of velocity profile.
- The effective velocity v_{eff} saturates for high values of Φ^2

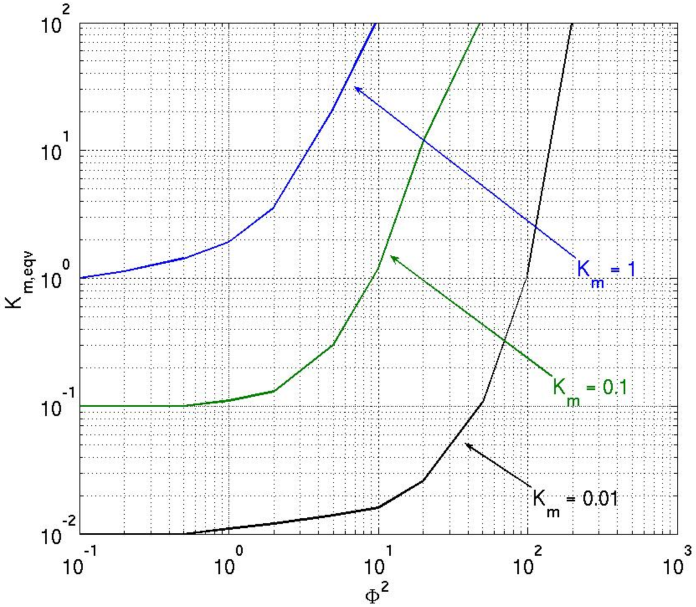
Effective diffusion



- Weak dependecy of the dipersivity from reaction rate.
- The effective dispersivity D_{eff} saturates for high values of Φ^2

Monod kinetics





- 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 determinated through numerical fitting