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Upscaling of the advection–diffusion–reaction equation with Monod reaction

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ABSTRACT

The need for reliable models for the reactive transport of contaminants in the subsurface is well recognized. The predictive power of these models is determined by the accurate description of bioavailability of contaminants to microorganisms in porous media. Among many other factors influencing bioavailability, diffusive mass transfer processes may limit the substrate availability at the pore scale and hence reduce the effective degradation rate considerably. In this study we used a combination of analytical and numerical methods to upscale surface catalyzed Monod-type reaction rates within a single pore, to obtain effective rate expression at a larger scale. Results show that in the upscaled description Monod kinetics lead to a concentration dependent transition between a reaction and diffusion-limited regime. Strictly, the effective rate repression does not follow Monod-type kinetics. However, we can present appropriate effective parameters relations, which provide an acceptable approximation of degradation dynamics using an effective Monod-type reaction rate.

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1. Introduction

Anthropogenic groundwater contamination is a severe problem in many industrialized countries. *Ex situ* remediation means, such as pump-and-treat systems, are often neither technically nor financially feasible due to the size of the contaminated sites. For many organic carbon compounds *in situ* bioremediation, either passive or enhanced, has shown to be a cost-effective alternative. Enhanced bioremediation uses the ability of subsurface microorganisms to degrade organic contaminants [55].

The biodegradation of groundwater contaminants has been extensively investigated, both in the field and in the laboratory. However, due to the complex interplay of microbial, chemical and physical processes occurring in groundwater, a direct quantification of *in situ* biodegradation is often hard to achieve. In order to judge the effectiveness of biodegradation on contaminated sites the experimental characterization is often combined with numerical simulations using reactive transport models (e.g. [36,4,10,40]). Yet, their predictive power is restricted by the accuracy of the implemented process descriptions.

The extrapolation of laboratory results on microbial degradation processes to *in situ* biodegradation processes in the field and the incorporation of these processes in reactive transport simulations are – among many other aspects – challenged by finding an adequate description of the bioavailability of the substrate [20,51]. Factors controlling the bioavailability include the physico-chemical structure of the substrate [8,22], physical occlusion by small pores [32,58,27] or mineral coatings [45], and macroscopic mixing processes [12,50]. Most importantly, the bioavailability of a dissolved contaminant in porous media is highly affected by mass transfer processes at the pore or sub-pore scale. The activity of microorganisms is controlled by substrate concentrations in their immediate vicinity [19,47,23]. In porous media microorganisms primarily reside on the surface of the solid matrix (Fig. 1, right part). Microscopic transport processes within each pore must provide the supply of the contaminant from the bulk pore water to the location of the microbial cells. This transport limits bioavailability, besides any of the other processes mentioned above, which might impose an additional restriction to bioavailabilty. As a consequence, the bioavailable concentration, to which microorganisms are exposed to, may differ considerably from the average concentration measured at the macroscale [43,33].

To understand the limitations of macroscopic degradation rates by such pore-scale mass fluxes, research has focused on simple representations of the pore space [3,28,30]. Looking at the pore scale it can be shown that the effective reaction rate can be significantly reduced when pore-scale diffusion becomes a limiting factor for bioavailability [3,9,16,25,34]. However, the reaction rate in most of these studies was assumed to follow first-order kinetics with respect to the concentration of the degraded species. In case of microbially catalyzed reaction first-order kinetics valid for low

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Nomenclature

Latin

A	amplitude of Ψ
c	concentration of the solute
c_0	concentration at Γ_f^i
c_{bio}	bioavailable concentration
c_{ref}	reference concentration
C	macroscale concentration
D	microscale diffusion coefficient
K_m	half-saturation constant
L_{ref}	reference length scale
$\mathscr{L}$	microscale differential operator
$\mathbf{n}$	unit vector normal to Γ_s
Pe	Péclet number
q_{max}	maximum conversion rate
R	general reaction rate
$\mathbf{v}$	microscale fluid velocity
V	pore-scale average velocity

Greek

η	scaling coefficient
Γ_f	boundary of Ω with the fluid
Γ_f^i	inlet of Ω_p
Γ_f^o	outlet of Ω_p
Γ_s	boundary of Ω with the solid
Φ^2	Thiele modulus
Ψ	transversal part of solution c
λ	eigenvalue of Ψ
τ_{ij}	coupling constant between mode i and j
Ω	whole domain
Ω_p	pore domain

Miscellaneous

$\langle\cdot\rangle$	averaged quantity
$\tilde{\cdot}$	deviation quantity
$\hat{\cdot}$	scaled quantity
$\cdot^{eff}$	upscaled parameter
$\cdot^{eqv}$	constant approximation for $\cdot^{eff}$
$\cdot_i$	ith mode

concentrations only [6]. In reality, the biodegradation of organic contaminants often follows Monod-type kinetics [35]. Recently, Wood et al. [56] have performed investigations assuming a Monod-type reaction rate within a single pore. They derived upscaling rules in the cases of either very low or very high substrate concentration. However, by comparing their upscaled equation with numerical simulations in a complex array of pores they got a mismatch for concentrations in the range of the Monod-half-saturation constant.

In this work we use a channel geometry comparable to [25,3] but consider a Monod-type reaction rate for the reactive surface of the pore. We chose this simple geometry in order to be able to make use of analytical tools in the upscaling process. With our approach we aim to verify: (i) whether the upscaled reaction rate laws can be sufficiently described by Monod-type kinetics, and whether the problems reported by Wood et al. can be resolved and if yes: (ii) how the parameters of such macroscopic Monod kinetics can be linked to microscopic reaction rate parameters that are valid at the local scale. The results obtained in this study for pore-scale systems may provide the base for interpreting results from laboratory column experiments. With further upscaling steps and additionally taking into account large scale heterogeneities, our results can be applied for describing biodegradation efficiency at the field scale.

In the following sections of this paper we will first introduce the conceptual approach used in this study including the underlying equations, the geometric representation of the pore system, and the applied numerical schemes and upscaling concepts (Section 2). This is followed by the description of the analytical tools used to obtain explicit solutions for the microscale problems and effective equations for the macroscale continuum (Section 3). Analytical and numerical results are presented and discussed in Section 4 and final conclusions for the scaling behavior of bioavailabilty controlled Monod-type reactions are given in Section 5.

2. Conceptual model

This section describes the conceptual approach used in this study. This includes the governing equations describing transport and degradation of a reactive species as well as the pore geometry these equations are applied to. Furthermore, the applied upscaling concepts and numerical schemes are introduced.

2.1. Mathematical description

In the following we will derive the mathematical model for reactive transport at the pore scale. Starting with a general description we will introduce appropriate scaling units and apply a few simplifications before stating the definite mathematical description.

The scale of interest is that of a single pore (Fig. 2). All flow and transport processes are taking place in the fluid phase Ω, only. For a single pore, the boundaries of the fluid phase domain can be separated into a fluid–solid interface Γ_s and a fluid–fluid interface Γ_f.

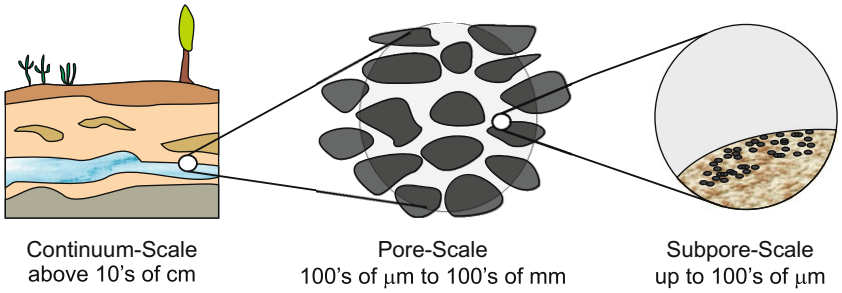

Fig. 1. Schematic of the complexity of the subsurface and the variety the different scales involved.

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