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The Soil as a Bioreactor: Reaction-Diffusion Processes and Biofilms

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Abstract: The fate of organic substances in soil strongly depends on biological processes. These biological processes are shaped by microorganisms, which occur in soil pores, either in suspension or as biofilms inside and outside soil aggregates. Biofilms alter the pore geometry while growing which directly influences the soil water flow field and hence the convective transport of organic substances. In this paper we present a model of the bioreactor soil at the pore scale under saturated conditions comprising coupled fluid flow, transport, reaction, sorption, and biofilm dynamics. The spatio-temporal development of the biofilm is altering properties such as viscosity, diffusion coefficient and degradation rates. The degradation potential of organic substances was analyzed by considering the influence of microbes on their breakthrough behavior.
The model results underline that biological processes exert a major influence on the fate of organic substances in soil.

Keywords: environmental fate, degradation, microorganisms, pore scale, Navier-Stokes

1. Introduction

Soil is a complex medium consisting of inorganic and organic, living and non-living, solid, fluid and gaseous substances. Organic non-living substances occur in soil naturally or anthropogenically applied e.g. through farming. Soil is commonly conceived as a bioreactor for organic substances because transport through and degradation in the soil strongly depend on biological processes. These biological processes are shaped by microorganisms, which occur in soil pores, either in suspension or as biofilms inside and outside soil aggregates [16, 8]. Biofilms are bacterial populations that are enclosed by extracellular polymeric substances (EPS) matrix. Its populations may contain several bacteria species [8]. Biofilms may alter the pore geometry, until clogging them, while growing [12]. This alteration directly influences the soil water flow field [15] and hence the convective transport of organic substances. In this paper we present a model of the bioreactor soil at the pore scale under saturated conditions comprising coupled fluid flow, transport, reaction, sorption, and biofilm dynamics.

2. Governing Equations

Subsequently, we list the governing equations of all relevant processes. Implementations and related initial and boundary conditions can be found in the subsequent section.

Water

The water flow in soil pores under saturated conditions was described by Navier-Stokes equations for incompressible flow [3, 6, 5, 9, 14, 17, 19]

$$\begin{aligned} &\rho\frac{\partial v}{\partial t} + \rho(v\cdot\nabla)v = -\nabla p + \mu\nabla^2 v + F \\ &\rho\nabla\cdot v = 0 \\ &F = \rho\cdot g \end{aligned} \quad (1)$$

with fluid density ρ [kg m^{-3}], velocity v [m s^{-1}], pressure p [Pa], dynamic fluid viscosity μ [Pa s] and external forces F [N m^{-3}]. The component of the external force F is the gravity component, with its gravitational acceleration g [m s^{-2}].

Substrate

The substrate transport is dependent on soil water movement and diffusion. The process was described by convection-diffusion-reaction-equation [e.g. 2, 4, 6, 5 and 7]

$$\begin{aligned} &\frac{\partial c}{\partial t} + \nabla\cdot(-D\nabla c) + \nabla(v\cdot c) = f \\ &f = -r_{\max}\frac{c}{K_S + c}\cdot X \end{aligned} \quad (2)$$

with substrate concentration c [g m^{-3}] and molecular diffusion D [m^2 s^{-1}]. The convective flux ($v\cdot c$) couples substrate dynamics and water flow (Eq. (1)). The sink term f contains the substrate degradation by microorganisms (next section).

The substrate can be sorbed by soil particles. It was described by the Langmuir equation on the particle boundaries

$$\frac{\partial q}{\partial t} = k_a \cdot c \cdot (q_{\max} - q) - k_d \cdot q \qquad (3)$$

with actually occupied receptors q [mol m^{-2}], adsorption rate k_a [m^3 mol^{-1} s^{-1}], molecule concentration c [mol m^{-3}] in the bulk fluid, maximum number of binding sites q_{max} [mol m^{-2}] and desorption rate k_d [s^{-1}] [21].

Microorganisms

Microorganisms in soil are able to degrade organic substances. Their population dynamics was described as substrate dependent growth with diffusive expansion. The growth rate r is substrate limited and is described with Monod kinetics [13, 18 and 20]

$$\frac{\partial X}{\partial t} + \nabla \cdot (-D_X \nabla X) = r_{\max} \frac{c}{K_S + c} \cdot X \qquad (4)$$

with microorganism/biofilm density X [kg m^{-3}], biofilm diffusion coefficient D_X [m^2 s^{-1}] which was assumed to be dependent on biofilm density, maximum growth rate r_{max} [s^{-1}], and Monod constant K_S [kg m^{-3}].

3. Use of COMSOL Multiphysics

The model was implemented in COMSOL Multiphysics 4.2 using the subsurface flow module. The water flow velocities were described with Navier-Stokes equations for incompressible fluids and laminar flow. Biofilm population dynamics was implemented as partial differential equation with substrate depending growth and diffusive spread. Transport and reaction of the organic substance were modeled by a convection-diffusion-reaction-equation. The ordinary differential equation (3) was solved for sorption [21] on the soil particle boundaries. The spatio-temporal development of the biofilm is altering material properties of pore space such as viscosity, diffusion coefficient and degradation rates.

The model was implemented on two different geometries (**Figure 1**), a simple rectangle pore space and a complex pore space defined through particles. Furthermore, a number of microbial case studies were implemented.

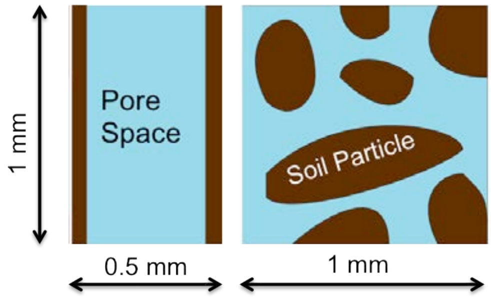

Figure 1. Pore and soil particle geometries.

Subsequently, we describe all initial and boundary conditions and specify the microbial study cases.

Water

The inflow and outflow boundary condition and the initial conditions were described with pressure resulting from gravitational forces. No slip condition is set at all other boundaries.

Substrate

The upper boundary condition assumed to be a fixed concentration c_{IN} until the specific time t_{S}. The lower boundary condition is an outflow condition:

$$-n \cdot (-D \nabla c) = 0 \qquad (5)$$

with normal vector n. The initial concentration in pore space was 0 mol m^{-3}.

Equation (3) was solved on particle boundaries as was done in e.g. [21].

Sorption was modeled as a time dependent outward flux onto soil particle boundaries. The substrate transport boundary condition is

$$(-D \nabla c) + \nabla (v \cdot c) = -J_n$$
$$J_n = \frac{\partial q}{\partial t} \qquad (6)$$

with normal boundary flux J_n.

Microorganisms

In contrast to [10] biofilm spread D_X was implemented as a Heavyside function at 9 kg m^{-3} of X.

The boundary conditions were set as no flux conditions in all three cases.

A: Microorganisms in suspension

The microorganisms were in suspension in soil water and were able to degrade the substrate. It was assumed that the microorganisms were present in the whole pore space and do not expand in space ($D_X = 0$). Therefore equation (4) was solved in the domain that represents the pore space. The initial bacteria density was 5 kg m^{-3}.

B: Biofilm inside soil aggregates

The biofilm was inside the soil aggregates. In soil it is able to degrade the substrate through transport processes inside the aggregates. In our model the population dynamics of such biofilm were implemented as weak partial differential equation on the particle boundaries. The initial biofilm density was 5 kg m^{-3}.
This substrate sink was implemented as time dependent outward flux onto particle boundaries as it is described for adsorption in equation (6).

C: Biofilm outside soil aggregates

The biofilm outside the aggregates was treated as porous medium [11]. It was assumed that water flows through the biofilm. Its density is supposed to represent a flow resistance. This mechanism was implemented as a local change of fluid viscosity proportional to the local biofilm density

$$\mu = \begin{cases} \mu_w & X \le \mu_w \\ m \cdot X & else \end{cases} \quad (7)$$

with viscosity of water μ_W [Pa s] and an impact factor m [m^2 s^{-1}]. The higher the biofilm density, respectively the fluid viscosity, is, the lower is the local flow velocity.
The biofilm was able to degrade the substance. It is assumed that diffusive substrate transport is possible through the biofilm region. The molecular diffusive coefficient differs in biofilm region from bulk fluid [1]. The EPS and only small tunnels for water flow resulting in a much smaller molecular diffusion coefficient than for bulk fluid.
Two cases were studied, a non-spreading biofilm (C1), $D_X = 0$, and a spreading biofilm (C2), $D_X > 0$. The initial biofilm density was implemented as a two dimensional Gaussian distribution with its peak on particle boundary (**Figure 2**).

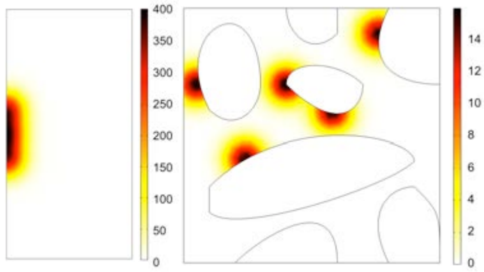

Figure 2. Initial biofilm distribution outside soil aggregates in both geometries.

4. Results & Discussion

The degradation potential of organic substances was analyzed by considering the behavior of microorganisms. Hereto, we considered the influence of microbial suspension, biofilm and its growth on the breakthrough behavior of organic substances. In addition, the effect of microorganisms within soil aggregates was considered. Finally, the model was implemented on a complex geometry.
The breakthrough curves (**Figure 3**) of all three microbial study cases show the impact of microbial life depending on considered state. The bacteria in suspension have nearly no effect on breakthrough behavior of organic substances. The spreading biofilm reduces the maximum outflow concentration and stores substrate, longer in the observed pore, because of the reduced substrate transport properties. The biofilm within the aggregates has the highest impact on the maximum outflow concentration. It degrades the substance completely on the particle boundaries hence no desorption phenomena can be observed in the breakthrough curve after stopping the injection.

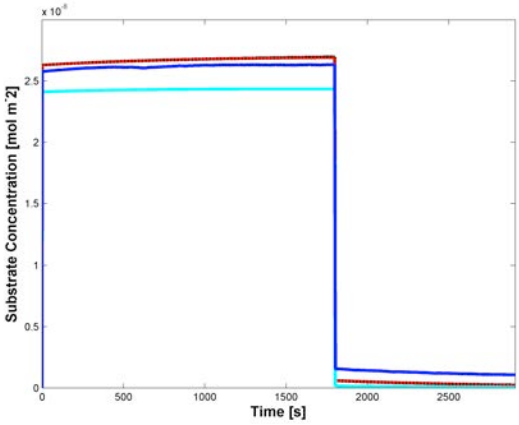

Figure 3. Breakthrough curves evaluated on the outflow boundary. Black: pore without microorganisms, dotted red: bacteria in suspension (A), cyan: biofilm within aggregates (B), blue: spreading biofilm (C2).

The difference between the spreading and the non-spreading biofilm can be observed in the breakthrough curves (**Figure 4**). The substrate degradation reduced during the injection, and substrate concentration nearly reached the maximum of the curve without microorganisms. The substrate decrease took a longer time than in the system with spreading biofilm. Thus the degradation potential of spreading biofilm is higher.

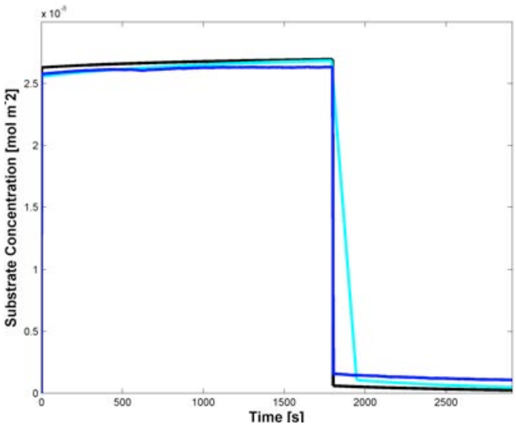

Figure 4. Breakthrough curves evaluated on the outflow boundary. Black: pore without microorganisms, cyan: non-spreading biofilm (C1), blue: spreading biofilm (C2).

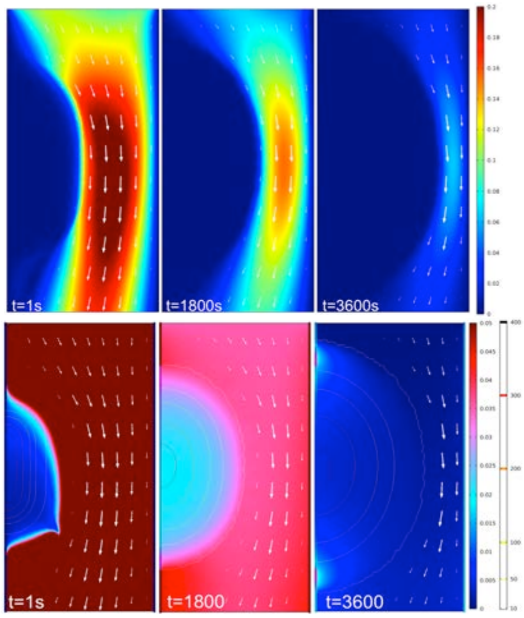

Figure 5. Velocity field (above) and substrate concentration profiles (below) at three different times with spreading biofilm.

The impact of the biofilm on the velocity field and concentration profile for three times is shown in **Figure 5**. Maximum velocities decreased while biofilm was spreading. The substrate concentration within the biofilm is very low because of degradation and smaller transport velocities. Where biofilm density is low, substrate was able to be adsorbed, respectively desorbed. The latter is bioavailable and could be degraded.
Concentration profiles of the second geometry are shown in **Figure 6**. The impact of velocity field is higher than in a single pore. Pores were clogged and transport properties changed by biofilms. The more complex the geometry and biofilm distribution is the more the flow field is affected and hence the substrate transport and reaction.

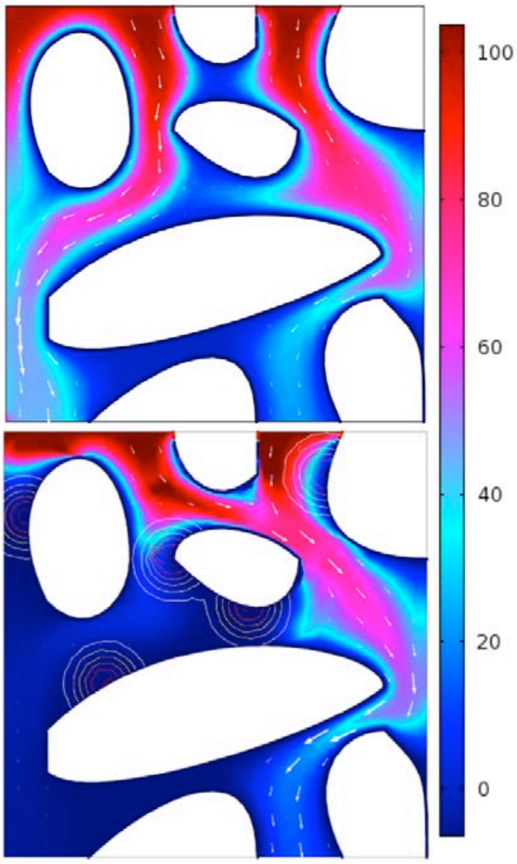

Figure 6. Substrate concentration profiles with (lower) and with spreading biofilm (t = 60 s).

5. Conclusions

The model results under saturated conditions at pore scale showed that biological processes exert a major influence on the fate of organic substances in soil. The degradation through microorganisms shapes the breakthrough behavior of organic substances at pore scale. The geometry of pore space altered by biofilm growth has remarkable impact on the flow field.

All simulations were implemented under saturated conditions. Future work has to consider unsaturated conditions. In addition, a sensitivity analysis of inflow velocities and inflow concentrations and durations will be evaluated.

6. References

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7. Appendix

Table 1: Parameter used within the microbial study cases.

Parameter	Value
D_X	2.31 10^{-13} m^2 s^{-1}
m	0.1 Pa s
r_{max}	6.94 10^{-5} s^{-1} A, C: 6.94 10^{-4} s^{-1}
D	1.16 10^{-6} m^2 s^{-1} C: 1.16 10^{-6} m^2 s^{-1} (fluid) 1.16 10^{-9} m^2 s^{-1} (biofilm)
k_a	10^{-3} m^3 mol^{-1} s^{-1}
k_d	10^{-3} s^{-1}
q_{max}	1 mol m^{-2}
c_{IN}	0.11 mol m^{-3}
K_S	0.01 mol m^{-2}
t_c	1800 s