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Discrete-continuum multiscale model for transport, biomass development and solid restructuring in porous media

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ABSTRACT

Upscaling transport in porous media including both biomass development and simultaneous structural changes in the solid matrix is extremely challenging. This is because both affect the medium's porosity as well as mass transport parameters and flow paths. We address this challenge by means of a multiscale model. At the pore scale, the local discontinuous Galerkin (LDG) method is used to solve differential equations describing particularly the bacteria's and the nutrient's development. Likewise, a sticky agent tightening together solid or bio cells is considered. This is combined with a cellular automaton method (CAM) capturing structural changes of the underlying computational domain stemming from biomass development and solid restructuring. Findings from standard homogenization theory are applied to determine the medium's characteristic time- and space-dependent properties. Investigating these results enhances our understanding of the strong interplay between a medium's functional properties and its geometric structure. Finally, integrating such properties as model parameters into models defined on a larger scale enables reflecting the impact of pore scale processes on the larger scale.

1. Introduction

Soils' functions are intimately linked to their heterogeneous and dynamically evolving three-dimensional structure. Particle (dis-)aggregation under the influence of microbial activity and biofilm growth or decay within soils (or porous media in general) strongly influences their characteristic properties such as porosity, mass transport parameters, e.g. effective diffusivity, or flow paths. Determining the evolution of such properties in space and time is demanding both at the pore scale and at the laboratory or field scale. In addition, accessing three-dimensional imaging data of porous structures in combination with their inhabiting biomass at a high spatial resolution remains challenging. As a consequence, the mathematical modeling of the quantitative relationship between structure and its functional properties based on theoretical concepts is desirable across scales.

To date researchers have developed a variety of biofilm models, also formulated at different scales, ranging from continuum models and models based on cellular automaton methods (CAM) to individual based models (Wang and Zhang, 2010). In combination with experiments, the cellular automaton method has successfully been used to describe the structural development of biofilm at the pore scale (Tang and Valocchi, 2013; Tang et al., 2013). In this method straightforward biomass spreading rules are prescribed, which allow a very flexible formulation of geometric changes, potentially also including stochastic aspects. However, aiming to understand flow and transport in the soil at larger scales, pure pore-scale simulations are impractical due to high computational costs.

To cross scales the following research has been undertaken in the context of biofilms. In Golfier et al. (2009) and Orgogozo et al. (2010) a volume averaging technique was applied to an equilibrium and a non-equilibrium continuum pore-scale model for transport in biofilm and fluid with interphase mass transfer and biologically-mediated reactions. In Peszynska et al. (2015) a continuum flow model was fully coupled with a continuous biomass-nutrient growth model and the Darcy conductivity was calculated. In doing so for each time step the computational results of the flow model were upscaled using volume averaging techniques. Further upscaling methods have been applied to problems including biofilm development. However, tracking the evolving biofilm interface is in general very complex to handle. In van Noorden et al. (2010) biofilm growth in a thin strip was investigated and an effective model was derived using formal two-scale asymptotic expansion in a level-set framework. The same methods were applied to a more sophisticated model in Schulz and Knabner (2012). Moreover, for the resulting effective model, existence and uniqueness of weak solutions were shown. In Tang et al. (2015) a hybrid model was developed, coupling pore-scale subdomains and continuum subdo-

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Table 1
Model parts.

Cell states	Sticky agent (α)	Cells' alterations	Components	Components' alterations
solid (s)	yes	jumping	–	–
fluid (f)	not on fluid-fluid interfaces	passively movable	nutrient (O_2)	strong diffusion, consumption by bacteria and sticky agent
			bacteria (Bac)	strong diffusion, nutrient consumption, transformation to biomass
bio (b)	yes	spreading	nutrient (O_2)	weak diffusion, consumption by biomass, bacteria, sticky agent
			bacteria (Bac)	weak diffusion, nutrient consumption, integration to biomass
			biomass (B)	nutrient consumption, generation from bacteria, growth and decay

mains by means of the Mortar method. Hereby, the biofilm development was simulated at the pore scale by means of the cellular automaton method.

With regard to changes in the soil's structure, in Crawford et al. (2012) the feedback between structure and microbial activity was investigated. There, stabilizing sticky agents, which stem from biological activity and enhance the binding of soil particles, were investigated and their affinities calculated. However, the focus was placed on the self-organization of soil-microbe systems by means of stabilizing agents and not on the volume effects that are created by growing or decaying biomass.

In this research, we combine both of the aforementioned processes – biomass development and structural changes in the solid originating from stabilizing sticky agents – in a comprehensive pore-scale model. To that end, a combined discrete–continuum approach is envisaged which omits the explicit tracking of interfaces as it is necessary in level-set approaches. The diffusion of mobile bacteria, possibly transforming into immobile biomass, and nutrients (e.g. oxygen) are prescribed by means of partial differential equations (PDEs) which are numerically solved using the local discontinuous Galerkin (LDG) method (Cockburn and Shu, 1998; Frank et al., 2015). Likewise, the surface concentration of a sticky agent tightening together solid or bio cells (in the cellular automaton context) is considered. However, the underlying time-dependent computational domain, i.e. the distribution of a solid, bio cells, and a fluid is determined discretely by means of a cellular automaton method.

One main objective of this research is to examine the strong interplay between functional properties and geometric structure. To that end standard homogenization results are used to compute the soil's characteristic properties such as porosity or effective diffusion tensors for the resulting complex and time-dependent geometries. Several scenarios are numerically evaluated in two space dimensions and the results are discussed thoroughly. Here, particular attention is paid to the impact of the concurrently occurring biomass development and solid restructuring.

Another focus of this paper is to further evaluate the model's applicability at larger scales. Consequently, a weakly coupled multiscale simulation scenario is investigated. In this setting the impact of the potentially changing yet microscopic geometry on macroscopic effects is discussed carefully.

The paper is structured as follows: In Section 2, we establish the underlying mathematical model, i.e. the differential equations for the development of nutrients, bacteria and sticky agents, and carry out the jumping/spreading rules for bio and solid cells. Finally, we define the effective parameters applying the findings from homogenization theory. In Section 3 several simulation results are shown and the effective parameters, particularly their dependence on the underlying geometry, are discussed. Moreover, a weakly coupled hybrid model is set up and investigated numerically. In Section 4 our results are summarized and prospective research proposals given.

2. Geometric setting, mathematical model, and methods

In this section, we discuss the fundamental mathematical model and aspects of its numerical discretization and implementation. The model contains prototype model parts as listed in Table 1, since in this stage our focus lies on the illustration of the model's capability rather than on the detailed recreation of experiments. Particularly, we aim at highlighting the impact of the solid's geometric structure and biomass growth/decay on the porous medium's porosity, the possible reduction of the effective diffusion tensors, and finally the alteration of flow paths. However, we do not consider fluid flow explicitly and limit ourselves to only two mobile prototype species termed bacteria and nutrient. Extensions to a fully coupled biomass–fluid model, multispecies biomass, or several mobile species are possible – c.f. the discussion in Section 4.

Our model includes a combination of discrete and continuum parts: A CAM is used to capture geometric and structural changes. The cellular automaton consists of a quadratic domain Y with periodic boundary ∂Y being covered by a regular grid containing N^2 rectangular cells Y^i with faces ∂Y^i. At first, one of the following three cell states is (randomly) assigned to each of the cells: "bio" (b), "fluid" (f), or "solid" (s), c.f. Fig. 1. The cells in principle correspond to physical particles and are assumed to have the same size and shape. The union $\bigcup_i Y_b^i$ of the bio cells is denoted by Y_b, the union $\bigcup_i Y_f^i$ of the fluid cells by Y_f, and the union $\bigcup_i Y_s^i$ of the solid cells by Y_s with boundary ∂Y_s (on which in addition to the periodic boundary conditions on ∂Y no flux boundary conditions for the bacteria and nutrient are prescribed), c.f. Fig. 1. In each time step a redistribution of solid and biomass is defined according to spreading/jumping rules (see Section 2.3) and the fluid is defined as the remainder: $Y_f = Y \setminus (\bar{Y}_s \cup \bar{Y}_b)$. Within the union of fluid and bio cells that are both defined by the respective states of the associated cells, the continuum parts of the model come into play. Here, (eventually coupled, partial) differential equations are solved for the transported nutrient (e.g. oxygen), bacteria, and the immobile biomass. Likewise, an ordinary differential equation is considered for the sticky agent, possibly being present on $\bigcup_i \partial Y_s^i \cup \bigcup_i \partial Y_b^i$ and holding together bio and/or solid cells – c.f. Sections 2.2 and 2.3.

2.1. Model parts

Within our model, we essentially consider the following prototypical time- and space-dependent model parts:

1. an inert solid (s) whose cells are held together by some sticky agent (α),
2. a fluid (f), e.g. water, at rest containing one prototype of diffusing bacteria (Bac) and one prototype of diffusing nutrient (O_2), e.g. oxygen,
3. and bio cells (b) in which the nutrient and bacteria also diffuse, however, with lower diffusivity than in the fluid (reduced by 80% as assumed in Tang and Valocchi, 2013). Moreover, biomass is created if the bacteria exceed a certain predefined threshold in the fluid, it decays and grows depending on the availability of the nutrient and bacteria in the bio cells. Along that line fluid cells may be transformed into bio cells.

Finally, the nutrient is consumed by biomass, bacteria, and the sticky agent which additionally holds together the bio cells.