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

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N. Ray, A. Rupp & A. Prechtel

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Nadja Ray, Andreas Rupp, Alexander Prechtel*  
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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.

*Applied Mathematics I, Department of Mathematics, Friedrich-Alexander Universität Erlangen-Nürnberg, Cauerstr.11, 91058 Erlangen, Germany, ray@math.fau.de
(CAM) to individual based models [16]. In the applied sciences, the cellular automaton method has widely been used to describe the structural development of biofilm at the pore scale. In this method straightforward biomass spreading rules are prescribed, which allow a very flexible formulation of geometric changes, potentially also including stochastic aspects. Various spreading rules for multispecies biofilm are available in the literature. However, many of them lead to strong internal mixing if different biomass species are present. A comparison between different spreading rules was made in [11]. 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 [7] and [8] 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 [9] 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 [14] 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 [10]. Moreover, for the resulting effective model, existence and uniqueness of weak solutions were shown. In [12] a hybrid model was developed, coupling pore-scale subdomains and continuum subdomains 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 [4] 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 rather than on the impact of volume effects.

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 [3, 6]. 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 underlying geometry 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 to highlight 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 rectangular domain \( Y \) with periodic boundary \( \partial Y \) being covered by a regular grid containing \( (NX)^2 \) rectangular cells \( Y_i \) with faces \( \partial Y_i \). 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. Figure 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 \( \partial Y_s \) (on which in addition to the periodic boundary conditions on \( \partial Y \) no flux boundary conditions for the bacteria and nutrient are prescribed), c.f. Figure 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: \( Y_f = Y \setminus (Y_s \cup Y_b) \). 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. Section 2.2 and Section 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 \((\alpha)\),
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 [11]). 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. We emphasize that the sticky agent is possibly present at the solid cells’ interfaces (i.e. solid-solid, solid-bio, and solid-fluid interfaces) and bio cells’ interfaces (i.e. bio-bio, bio-fluid, and bio-solid interfaces), but not at the fluid-fluid cells’ interfaces. We recapitulate the model parts and their specific features in Table 1.

2.2 Continuum model parts

Within the continuum part of the model, c.f. Table 2, differential equations are solved for the nutrient and the bacteria, both of which diffuse in the fluid and bio cells. More precisely, diffusion–reaction equations for the transport of the nutrient concentration \(c_{O_2}\) and the bacteria concentration \(c_{Bac}\), c.f. Equations (1), (2), are considered. We emphasize here that the differential equations are defined in the time-dependent domain \(Y_f \cup Y_b\), c.f. Table 1 and Figure 1. The molecular diffusivities for the nutrient are denoted by \(D_{O_2,b}\) and \(D_{O_2,f}\) within the bio cells and fluid and for the bacteria by \(D_{Bac,b}\) and \(D_{Bac,f}\) within the bio...
<table>
<thead>
<tr>
<th>Cell states</th>
<th>Sticky agent (α)</th>
<th>Cells’ alterations</th>
<th>Components</th>
<th>Components’ alterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>solid (s)</td>
<td>yes</td>
<td>jumping</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>fluid (f)</td>
<td>not on fluid-fluid interfaces</td>
<td>passively movable</td>
<td>nutrient (O₂)</td>
<td>strong diffusion, consumption by bacteria and sticky agent</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>bacteria (Bac)</td>
<td>strong diffusion, nutrient consumption, transformation to biomass</td>
</tr>
<tr>
<td>bio (b)</td>
<td>yes</td>
<td>spreading</td>
<td>nutrient (O₂)</td>
<td>weak diffusion, consumption by biomass, bacteria, sticky agent</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>bacteria (Bac)</td>
<td>weak diffusion, nutrient consumption, integration to biomass</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>biomass (B)</td>
<td>nutrient consumption, generation from bacteria, growth and decay</td>
</tr>
</tbody>
</table>

Table 1: Model parts.

cells and fluid, respectively. Note that both diffusivities $D_{O₂}$ and $D_{Bac}$ are discontinuous since they are reduced by 80 % in the bio cells.

\[
\partial t c_{O₂} - \nabla \cdot D_{O₂,f/b} \nabla c_{O₂} = \text{source} - \text{sink} \quad \text{in } Y_f \cup Y_b, \quad (1a)
\]

\[
-D_{O₂,f/b} \nabla c_{O₂} \cdot \nu = 0 \quad \text{on } \partial Y_s. \quad (1b)
\]

\[
\partial t c_{Bac} - \nabla \cdot D_{Bac,f/b} \nabla c_{Bac} = \text{source} - \text{sink} \quad \text{in } Y_f \cup Y_b, \quad (2a)
\]

\[
-D_{Bac,f/b} \nabla c_{Bac} \cdot \nu = 0 \quad \text{on } \partial Y_s. \quad (2b)
\]

Note that the domain $Y$ is periodic which, in particular, implies periodic boundary conditions for the nutrient and bacteria on $\partial Y$. Moreover, appropriate initial conditions are prescribed to close the problem and to potentially ensure the presence of the nutrient and bacteria at time $t_0 = 0$. For each simulation scenario, they will be specified in Section 3 if necessary.

In the following, we discuss the transformation of bacteria into biomass, its growth and decay, the evolution of the sticky agent’s concentration, and the consumption of the nutrient which is inherent to both processes. In this sense, internal sources or sinks are included in the model equations (1) and (2). More precisely, the nutrient sinks which are related to its consumption by the sticky agent, bacteria, and biomass, and the transformation of the bacteria into biomass, i.e. a sink for bacteria, are discussed below.

First, the transformation of a fluid cell into a bio cell is accompanied with the generation of biomass from bacteria, its growth, and its decay. The transformation of a fluid cell $Y_f^i$ into a bio cell $Y_b^i$ occurs if the bacteria exceed a certain threshold $\int_{Y_f^i} c_{Bac,max} dx$ in the respective cell, i.e. if

\[
\int_{Y_f^i} c_{Bac} dx > \int_{Y_f^i} c_{Bac,max} dx.
\]
Then, the bacteria completely transform into biomass and their concentration $c_{Bac}$ becomes zero in this cell, c.f. (4). Simultaneously, the biomass concentration $c_B$ takes a constant value within the newly created biomass cell $Y^i_b \leftarrow Y^j_i$ as defined in (3). Note that, on the contrary, bio cells turn into fluid cells if the biomass concentration reaches zero.

$$
c_B = \frac{1}{|Y^i_b|} \int_{Y^i_b} c_{Bac} \, dx \quad \text{in } Y^i_b, \quad (3)
$$
$$
c_{Bac} = 0 \quad \text{in } Y^i_b. \quad (4)
$$

Within the bio cells $Y^i_b$ a generation of biomass from bacteria takes place. Moreover, biomass and bacteria growth by means of the nutrient takes place in the bio cells $Y^i_b$ and in the bio and fluid cells $Y^i_b \cup Y^j_f$, respectively.

$$
\partial_t c_B = f_{\text{growth/decay}, B}(c_B, c_{O_2}) + f_{\text{increase}, B}(c_{Bac}, c_B) \quad \text{in } Y^i_b,
$$
$$
\partial_t c_{Bac} - \nabla \cdot D_{Bac,b} \nabla c_{Bac} = f_{\text{growth}, B}(c_{O_2}) + f_{\text{decay}, B}(c_{Bac}) + f_{\text{decrease}, B}(c_{Bac}, c_B) \quad \text{in } Y^i_b \cup Y^j_f.
$$

The implementation of different rates into the model is straightforward and are defined as follows: for the biomass growth and decay $f_{\text{growth/decay}}$, we assume a dependence on the availability of the nutrient in the respective cell $Y^i_b$. More precisely, a linear rate (first order kinetics) is chosen for the decay of the biomass and a constant rate (zeroth order kinetics) is chosen for the growth of the biomass.

The increase $f_{\text{increase}, B}$ in the biomass depends on the availability of bacteria diffusing into the bio cell. Depending on the concentration of biomass, between 20% and 80% of the available bacteria are consumed. At the same time, the bacteria concentration decreases at the same rate. Finally, a linear rate (first order kinetics) is chosen for the decay of the bacteria and a constant rate (zeroth order kinetics) is chosen for the growth of the bacteria depending on the availability of the nutrient:

$$
(f_{\text{growth/decay}, B})_i(c_B, c_{O_2}) = \begin{cases} 
-k_{d,B} c_B, & \text{if } \int_{Y^i_b} c_{O_2} \, dx \leq \int_{Y^i_b} c_{up,O_2,min,B} \, dx, \\
\text{const,} & \text{if } \int_{Y^i_b} c_{O_2} \, dx > \int_{Y^i_b} c_{up,O_2,min,B} \, dx 
\end{cases} \quad \text{in } Y^i_b,
$$
$$
f_{\text{increase}, B}(c_{Bac}, c_B) = \frac{1}{c_{B,\text{max}} - c_{B,\text{min}}} (0.6c_B + 0.2c_{B,\text{max}} - 0.8c_{B,\text{min}})c_{Bac} \quad \text{in } Y^i_b,
$$
$$
f_{\text{growth}, B}(c_{O_2}) = \begin{cases} 
0, & \text{if } c_{O_2} \leq 0, \\
\text{const,} & \text{if } c_{O_2} > 0 
\end{cases} \quad \text{in } Y^i_b \cup Y^j_f,
$$
$$
f_{\text{decay}, B}(c_{Bac}) = -k_{d,Bac} c_{Bac} \quad \text{in } Y^i_b \cup Y^j_f,
$$
$$
f_{\text{decrease}, B}(c_{Bac}, c_B) = -f_{\text{increase}, B}(c_{Bac}, c_B) \quad \text{in } Y^i_b.
$$

Finally, following the ideas in [4], the concentration $c_\alpha = (c_{\alpha,l,k})_{l,k \in \{1,\ldots, NX^2\}}$ of the sticky agent (called activity in [4]) is defined, which is actually a surface concentration. Since there is no agent present at the fluid–fluid interfaces, for each time step the support is at most $\bigcup_i \partial Y^i_k \cup \bigcup_i \partial Y^i_b$, i.e. all solid–solid, solid–bio, solid–fluid, bio–fluid, and bio–bio interfaces. The concentration of the sticky agent is time-dependent, but section-wise constant in space, i.e. constant along the single cell faces $\partial Y^k \cap \partial Y^i$. It is evaluated via

$$
\partial_t c_\alpha = \begin{cases} 
f_{\text{increase}, \alpha}(c_{O_2}) + f_{\text{decay}, \alpha}(c_\alpha) \quad \text{on } \bigcup_i \partial Y^i_i \cup \bigcup_i \partial Y^i_b, \\
0 \quad \text{else.} 
\end{cases} \quad (5)
$$
Following the same practice as in [4], in our simulations the reaction rates are defined as follows: For the decay we assume first order kinetics. For an increase in the sticky agent’s concentration, we assume a dependence on the availability of the nutrient, i.e. the rate is zero if no nutrient is available or a zeroth order kinetics if the nutrient is available in the neighboring cells, respectively. For this evaluation, note that according to (1), there is no nutrient present in any solid cell \( Y^k \) and that the components \( (f_{\text{increase},\alpha})_k \) of the rate may only be non-zero for non fluid–fluid interfaces, i.e. \( (Y^f \notin Y^i) \cup (Y^k \notin Y^j) \) c.f. Equation (5).

\[
\begin{align*}
    f_{\text{decay},\alpha}(c_\alpha) = & -k_{d,\alpha}c_\alpha & \text{on } \bigcup_i \partial Y^i \cup \bigcup_j \partial Y^j, \\
    (f_{\text{increase},\alpha})_k(c_{O_2}) = & \begin{cases} 
    0, & \text{if } (\int_{Y^k} c_{O_2} \, dx \leq \int_{Y^j} c_{\text{up},O_2,\text{min},\alpha} \, dx) \land (\int_{Y^l} c_{O_2} \, dx \leq \int_{Y^l} c_{\text{up},O_2,\text{min},\alpha} \, dx), \\
    \text{const}, & \text{if } (\int_{Y^k} c_{O_2} \, dx > \int_{Y^j} c_{\text{up},O_2,\text{min},\alpha} \, dx) \land (\int_{Y^l} c_{O_2} \, dx \leq \int_{Y^l} c_{\text{up},O_2,\text{min},\alpha} \, dx), \\
    2\text{const}, & \text{if } (\int_{Y^k} c_{O_2} \, dx > \int_{Y^j} c_{\text{up},O_2,\text{min},\alpha} \, dx) \land (\int_{Y^l} c_{O_2} \, dx > \int_{Y^l} c_{\text{up},O_2,\text{min},\alpha} \, dx).
\end{cases}
\end{align*}
\]

Since the biomass, the bacteria, and also the sticky agent consume the nutrient, the nutrient concentration must be updated as follows:

\[
\partial_t c_{O_2} - \nabla \cdot D_{O_2,b/f} \nabla c_{O_2} = -f_{\text{up},O_2,a}(c_{O_2}) - f_{\text{up},O_2,B}(c_{O_2}) - f_{\text{up},O_2,Bac}(c_{O_2}) \quad \text{in } Y_b \cup Y_f,
\]

\[
\begin{align*}
    (f_{\text{up},O_2,a})_k(c_{O_2}) = & \begin{cases} 
    0, & \text{if } \int_{Y^k} c_{O_2} \, dx \leq \int_{Y^j} c_{\text{up},O_2,\text{min},\alpha} \, dx, \\
    \text{const}, & \text{if } \int_{Y^k} c_{O_2} \, dx > \int_{Y^j} c_{\text{up},O_2,\text{min},\alpha} \, dx.
\end{cases} & \quad \text{in } Y^k, \\
    (f_{\text{up},O_2,a})_l(c_{O_2}) = & \begin{cases} 
    0, & \text{if } \int_{Y^l} c_{O_2} \, dx \leq \int_{Y^l} c_{\text{up},O_2,\text{min},\alpha} \, dx, \\
    \text{const}, & \text{if } \int_{Y^l} c_{O_2} \, dx > \int_{Y^l} c_{\text{up},O_2,\text{min},\alpha} \, dx.
\end{cases} & \quad \text{in } Y^l, \\
    (f_{\text{up},O_2,B})_i(c_{O_2}) = & \begin{cases} 
    0, & \text{if } \int_{Y^i} c_{O_2} \, dx \leq \int_{Y^i} c_{\text{up},O_2,B} \, dx, \\
    \text{const}, & \text{if } \int_{Y^i} c_{O_2} \, dx > \int_{Y^i} c_{\text{up},O_2,B} \, dx.
\end{cases} & \quad \text{in } Y^i, \\
    f_{\text{up},O_2,Bac}(c_{O_2}) = & \begin{cases} 
    0, & \text{if } c_{O_2} \leq 0, \\
    \text{const}, & \text{if } c_{O_2} > 0.
\end{cases} & \quad \text{in } Y_b \cup Y_f.
\end{align*}
\]

Note that “const” in all rates as related to the nutrient consumption must not necessarily be identical.

Furthermore, note that the agent is a surface-related quantity and the nutrient concentration is a volume-related quantity. Consequently, the respective quantities “const” in the rates for the agent must be scaled with the specific surface. The sticky agent glues together discrete solid or biomass cells and consequently finally contributes to the change of the solid/biomass structure, see Section 2.3.2 and Section 2.3.1 for the corresponding jumping rules.

### 2.3 Cellular automaton

A redistribution of solid and biomass is defined according to jumping/spreading rules as defined below and the fluid cells are defined as remainder.
2.3.1 Biomass spreading rule

We implemented a biomass spreading rule similar to the CAM CA-3 described in [11] and to the CAM as outlined in [13]. In summary, we proceed as follows: In each time step the biomass cells $Y_{i}^{b}$ are identified whenever the mean biomass concentration exceeds its threshold value $\int_{Y_{i}} c_{B,max} \, dx$. Simultaneously, for all these cells (center cells), the neighboring non-solid cells are tested whether they may take up a certain amount of excess biomass. In doing so a shortest path strategy is applied. More precisely, the cells belonging to the stencil consisting of four direct neighbors in 2D is investigated first, c.f. Figure 2. If necessary, thereafter, a stencil consisting of 12 neighboring cells in 2D is taken into account, c.f. Figure 2. If these stencils are not sufficient (which rarely occurs in practice) the length of the path to all cells that are non-solid and have a mean biomass concentration below $\int_{Y_{i}} c_{B,max} \, dx$ is calculated. Hereby the length of the path is defined by the $\| \cdot \|_1$-distance between the centers of two cells, c.f. Figure 2. Of these potential target cells, the closest one is incrementally chosen. If several of the closest candidates are available, the one with the highest capacity is chosen. If more than one such target cell is identified, one is randomly chosen.

Note that pushing forward any further as described in [11] is, however, not necessary since we consider only one biomass species and mixing is consequently no issue. If the selected target cell may not take the complete amount of excess biomass the procedure described above is applied repeatedly. This results in the fact that the excess amount of biomass is potentially distributed to several target cells, each taking a certain part of the overall excess amount of biomass. This may cause a conflict if the same target cell is selected for different center cells exceeding their threshold value. To resolve such conflicts only one center cell may distribute its excess biomass to the target cell (randomly chosen). The distribution of the excess biomass of the remaining cells is postponed to subsequent iterations of the above scheme (all within the same time step). Finally, if no additional target cell may be found the amount of biomass is altered in the center cell to its maximum value and the rest is discarded.

The redistribution of biomass is repeated until no biomass cell exceeds its threshold value or all cells have reached the maximum amount of biomass.

Figure 2: Center cell (red); stencil consisting of four neighbors (orange) and 12 neighbors (yellow); shortest path: $\|OA\|_1 = 5$ and $\|OB\|_1 = 4$. 
2.3.2 Solid jumping rules

The jumping rules for the solid cells are inspired by [4]. However in [4] the stability of “particle clusters” is calculated by “summing over the affinities of particle-particle bonds”. Afterwards the 1% of weakest clusters is selected and one cell per cluster is redistributed, whereas we proceed as follows: In each time step, “single” solid cells are identified, i.e. cells that are not glued by the sticky agent to neither biomass nor other solid cells. More precisely, a “single” solid block potentially has certain solid or biomass neighbor cells as long as no sticky agent is present between them. Moreover, it may have a sticky agent on its solid–fluid interfaces.

The “stickiness” $A_i$ measures the potential of the $i$-th fluid cell to attract a solid cell. It is evaluated in the fluid cells within a stencil consisting of 12 neighboring cells (possible target cells) and for the ”single” cell (center cell) itself in 2D, c.f. Figure 2:

$$A_i = \gamma \left( \sum_{\text{neighbors } Y^j \text{ of } Y^i_f} c_{\alpha,ij} \right) + \text{number of solid neighbors of } Y^i_f \text{ in } Y^i_f,$$

with proportional constant $\gamma$ and $i$ denoting the index of a cell contained in the stencil around the center cell c.f. Figure 2.

Then the target grid cell $Y^j_f$ with the largest $A_i$ is selected. If more than one such target cell is identified, one is randomly chosen and the jumping is carried out. Note that this entails the exchange of a solid and fluid cell including all its properties such as nutrient and bacterial concentration within the grid cell.

A conflict may occur if the same target cell is selected by different solid center cells. To resolve such conflicts one solid cell is randomly chosen to jump to the respective target cell for each of the conflicts. The possible jumping of the remaining solid cells is postponed to subsequent time steps.

Likewise, “double” solid grid blocks are identified and the same procedure is applied as before. The same could also be used for larger agglomerates.

2.4 Upscaling rules

Finally, we attempt to evaluate the effect of the aforementioned mechanisms on characteristic properties of the porous medium such as porosity and effective diffusion tensor. Hereby, we focus on the role of the solid’s restructuring and geometrical changes induced by biomass growth.

In order to evaluate the porosity $\theta$ and the reduced porosity $\theta_{\text{red}}$, we calculate the time-dependent volume of the fluid domain $Y^i_f$ and fluid-bio domain $Y^i_f \cup Y^i_b$ with respect to the total volume of the reference element $Y$:

$$\theta_{\text{red}} = \frac{|Y^i_f|}{|Y|},$$

$$\theta = \frac{|Y^i_f \cup Y^i_b|}{|Y|}.$$ (8)

Further, we hypothesize that the diffusion tensor for any species may be determined via

$$D_{ij} := \frac{1}{|Y|} \int_{Y^i_f \cup Y^i_b} D_{O_2/Bac,b/f}(\partial_y \zeta_i + \delta_{ij}) \, dy.$$ (9)
\[ t_0 = 0 \]

\textbf{While} \( t_n < T \)

\textbf{While} \( t^n_n < t_n \)

Continuum model component: Solve PDEs for bacteria and nutrient in current geometry (LDG for transport part of Equation (1) and (2)).

Continuum model component: Solve ODEs for sticky agent and thus for consumption of nutrient (implicit Euler for reactive part of Equation (1) and (2)).

Continuum model component: Solve ODEs for generation of biomass by bacteria and nutrient and thus for decrease in bacteria and consumption of nutrient, i.e. update geometric structure (implicit Euler for reactive part of Equation (1) and (2)).

Continuum model component: Solve ODEs for concentration of bacteria and thus for consumption of nutrient (implicit Euler for reactive part of Equation (1) and (2)).

\[ t^{k+1}_n = t^k_n + \tau^k_n \]

Discrete model component: CAM for biomass spreading, i.e. update geometric structure.

Discrete model component: CAM for solid, i.e. update geometric structure.

Possibly compute characteristic properties in current geometry (LDG).

\[ t_{n+1} = t_n + \tau_n \]

Table 2: Algorithm for discrete–continuum model.

with supplementary cell problems in \( \zeta_j, j = 1, \ldots, n \)

\begin{align}
- \nabla_y \cdot (\nabla_y \zeta_j + e_j) &= 0 \quad \text{in} \ Y_f \cup Y_b, & \text{(10a)} \\
(\nabla_y \zeta_j + e_j) \cdot \nu &= 0 \quad \text{on} \ \partial Y_s, & \text{(10b)} \\
\zeta_j \text{ periodic in} \ y \ \text{and} \ \langle \zeta_j, 1 \rangle_{L^2} &= 0. & \text{(10c)}
\end{align}

Hereby, \( \nu \) denotes the unit outer normal and \( e_j \) the unit vector in direction \( j \). This result is well known in periodic settings and may be derived in such situations by means of asymptotic expansion [2] or two-scale convergence in standard homogenization theory [1].

### 2.5 Algorithm and implementation

The structure of the overall algorithm is depicted in Table 2. In each global time step \( t_n \) the continuum and also the discrete components of the model are processed. The frequency of updates of the geometric structure (defining \( \tau_n \)) has an important impact on the evolution of the domain and thus has to be related with realistic time intervals in a non-artificial simulation. In [13] twice a day was chosen. A sub-time stepping with local time step \( t^n_n \) is introduced for the continuum model components, due to technical reasons (discontinuous reaction rates). The choice of both time steps defines the temporal discretization for the implicit Euler/LDG method.

An operator splitting algorithm is applied to decouple transport and reaction terms since the reaction rates are discontinuous (see Section 2.2) and also depend on the underlying geometry of the computational domain.

The transport part in the splitting scheme is discretized using a special version of the local discontinuous Galerkin (LDG) method first introduced by Cockburn and Shu for
convection-diffusion systems in [3] while the time-discretization is done by an implicit Euler scheme. In doing so, a mixed setting is applied to discretize second order terms and mass is conserved locally. The precise formulation of the LDG scheme can be found in [6], but here we use a rectangular grid and the diffusion coefficient is allowed to be a matrix and not (only) a scalar. Moreover, the polynomial ansatz-space is \( Q_1 := \text{span}(1, x, y, xy) \) for the primary unknown and for both components of the flux unknowns. Additionally, the reactive part in the splitting scheme consisting of ordinary differential equations (ODEs) for the concentration of the sticky agent, the transformation of bacteria into biomass, the growth of bacteria, and the consumption of the nutrient by biomass, sticky agent, and bacteria is solved consecutively using an implicit Euler scheme.

Within the discrete model component – which is solved for all global time steps – the main factors relates to structural changes, apart from the generation of biomass from bacteria, are investigated, namely the biomass spreading and the solid restructuring. Thereafter, characteristic time-dependent properties such as porosity and effective diffusion tensor are possibly evaluated.

The simulation software was implemented in MATLAB 2016a\(^1\) and M++ [17]. Note that the evaluation of the stencils from Section 2.3.1 and Section 2.3.2 is done simultaneously as well as for all cells exceeding the threshold value \( c_{B, \text{max}} \). The evaluation of the shortest path is computationally much more expensive since it must be done for all cells individually (and long loops are very inefficient in MATLAB implementations). Hence, we use vectorized operations whenever possible.

### 3 Simulation scenarios and model evaluation

To the best of our knowledge, our research combines for the first time geometric changes resulting from biomass development and solid restructuring within a sophisticated numerical discretization. Likewise, bridging scales in this context has rarely been been done in other research and is another focus of our work.

Furthermore, different simulation and upscaling scenarios are evaluated. At first, the structural changes originating from biomass growth and decay, or from the restructuring of the solid, are illustrated separately, see Section 3.1 and Section 3.2, respectively. Particular attention is paid to the impact of the underlying structure on the effective diffusion tensor as defined in (9). In summary it can be said that altering the pore space leads to a significant change in the medium’s characteristic properties.

Thereafter, in Section 3.3 and Section 3.4, comprehensive simulation scenarios illustrating the capability of the overall model as described in Section 2 are given. In detail the combination of moving solid particles and biomass growth and decay are shown. First, an artificial, but illustrating scenario is given. Additionally, we investigate a scenario with random initial geometry. For this setting, we compute the related (time-dependent) diffusion tensors. Moreover, in Section 3.5 the computational method is analyzed systematically. For all simulation scenarios, periodic conditions are prescribed on the square’s boundary \( \partial Y \). Moreover, we assume that there are no external sources of nutrient, biomass, solid, or bacteria within the domain.

Finally, in Section 3.6 the previously derived time-dependent effective diffusion tensors are used to demonstrate the influence the pore-scale geometry has on the behavior of a

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problem defined on a larger scale. To this end, a weakly coupled multiscale problem is set up and different scenarios, i.e. assuming differently prescribed effective diffusion tensors, are evaluated.

3.1 Illustration of the biomass development and its impact on the effective diffusion tensor

![Image](image)

Figure 3: Evolution of biomass concentration \( \frac{c_B}{\bar{c}_B} \) and normalized diffusion tensor \( \bar{D}/D_{O2,f} \) at \( t_0, t_5 \) and \( t_{10} \) (from left to right).

In this subsection, we illustrate the impact of the biomass development on the effective diffusion tensor defined in (9).

As illustrated in Figure 3 the square \( Y \) consisting of \( 16 \times 16 \) cells is considered. Throughout the simulation no solid is present. Initially, the nutrient distribution in the fluid has a parabolic profile in the horizontal direction and is constant in the vertical direction, i.e.

\[
\frac{c_{O2}(x, y, 0)}{\bar{c}_{O2}} = \frac{100}{NX^2} \cdot x \cdot (NX - x), \quad x, y \in (0, NX),
\]

where \( NX^2 = 16^2 \) equals the number of cells of size 1 within our domain and \( \bar{c}_{O2} \) denotes a characteristic concentration of nutrient.

In the middle of the domain \( Y \) a considerably high concentration of bacteria \( c_{Bac}/\bar{c}_{Bac} = 20 \) (particularly above the threshold value \( c_{Bac,\text{max}}/\bar{c}_{Bac} = 10 \)) covering \( 4 \times 4 \) cells is prescribed. Here, and in the following \( c_{B,\text{min}}/\bar{c}_B = 0 \) and \( c_{B,\text{max}}/\bar{c}_B = 100 \).

The picture and effective diffusion tensor on the left in Figure 3 indicate that biomass is initially absent within the whole domain and that the diffusion tensor is equal to the identity, which naturally represents free diffusion.

According to Equation (3) and the CAM described in Section 2.3.1, a biomass is developing from bacteria and grows, as seen in the middle picture in Figure 3. The porosity values as defined in (7) develop as follows: The porosity \( \theta_{\text{red}} \) for the fluid decreases drastically from \( \theta_{\text{red}} = 1 \) to \( \theta_{\text{red}} = 0.710 \) and then to \( \theta_{\text{red}} = 0 \) whereas the porosity \( \theta \) for the bio cells and fluid must remain constant (\( \theta = 1 \)) throughout the simulation. Moreover, the eigenvalues
of the effective diffusion tensor reasonably decrease, see the tensors in Figure 3. This is due to the fact that diffusion is significantly lower (reduced by 80%) in the bio cells compared to the fluid.

Finally, as depicted in the picture on the right in Figure 3, the biomass has grown substantially and covers the whole domain. As expected the eigenvalues of the diffusion tensor are equal to $0.2D_{O_2,f}$. It is remarkable that this value is independent of the biomass concentration and only depends on its occurrence, potentially in relation to the occurrence of a fluid or solid.

As oxygen is the main driving force and completely consumed on the long run, the initial state equals the final stationary state (not depicted here).

### 3.2 Illustration of solid particle agglomeration and its impact on the effective diffusion tensor

![Figure 4](image)

Figure 4: Evolution of solid and normalized diffusion tensor ($D/D_{O_2,f}$); concentration of nutrient $c_{O_2}/\bar{c}_{O_2}$ (blue/low to red/high), solids are dark blue; at $t_0$, $t_5$, and $t_{50}$ (from left to right).

As a second example, we evaluate the reorganization of the solid cells due to the jumping rules as described in Section 2.3.2, and their impact on the effective diffusion tensor as defined in (9).

As illustrated in Figure 4 the square $Y$ consisting of $16 \times 16$ cells is considered. The initial distribution of solid cells and its remainder — the fluid — are randomly chosen. The initial nutrient distribution obeys (11), except for the domain of the solid, see picture on the left in Figure 4. Note that neither bacteria nor bio cells are present in this scenario. Throughout the simulation scenario equations (1) and (5) are solved. Moreover, the solid jumping rules as described in Section 2.3.2 are applied. This results in a redistribution of the solid cells due to the sticky agent consuming the nutrient and thereby growth of the sticky agent, but also due to the lack of the nutrient and the degradation of the sticky agent as time proceeds. In Figure 4, the structural changes of the solid are depicted. After the first global time steps the nutrient has diffused and been consumed within the pore space, which has been altered due to the jumping rules and the evaluation of (6), see picture in the middle of Figure 4. In addition to the movement of single cells, it is evident from Figure 4 that double-blocks have rearranged.
Due to the absence of growing or decaying biomass, the porosity of the sample has the fixed value 0.6914. The diffusion tensor alters due to the alteration of the pore space and is computed according to Equation (9), c.f. Figure 4.

As we have no sources for the nutrient in this scenario, the nutrient is diffusing and being consumed in the long run, and consequently also the movement of the solid particles tends to a quasi stationary state where still some solid cells may jump to an equally favorable position.

Interestingly, the size (or number) of the particles in our domain $Y$ seems to have no significant effect on the effective diffusion tensor or its eigenvalues. This is further demonstrated by simulations prescribing the same porosity and consisting of $10 \times 10$, $20 \times 20$, $50 \times 50$, or $100 \times 100$ cells in our domain $Y$. Figure 5 shows the quasi stationary states, diffusion tensors and eigenvalues at $t_{end} = t_{200}$ for these four different configurations. The solid always coalesces in (several) not necessarily rectangular bigger blocks in the quasi stationary limit. This coalescence is due to the fact that the second term in (6) (number of neighbors) dominates the impact of the degrading sticky agent. However, the bigger aggregates may not coalesce further in this setting due to the definition of the stencil, compare Section 2.

3.3 Comprehensive model and physical entrapment

In the following, we analyze the capability of the overall model as described in Section 2. In particular, the interaction between different simultaneously occurring processes is highlighted, e.g. the physical protection of the solid by the bio cells. Moreover, the fundamental role or lack of the nutrient, potentially resulting in the agglomeration or destabilization of the solid structure, is discussed.

We consider the square $Y$ of $64 \times 64$ cells which initially contains solid cells arranged as a centered cross while the rest of the square contains the fluid (see left column in Figure 6). Initially a block of nutrient is located vertically symmetric at the lower half of the square, i.e. 

$$c_{O_2}(x,y,0) = \left(\frac{2}{NX} \cdot x \cdot (NX - x) \cdot y \cdot (NX/2 - y)\right)_+ + 5, \; x, y \in (0,NX).$$

The bacteria concentration has a parabolic profile in the horizontal direction and is constant in the
As can be deduced from the second column from the left in Figure 6, bacteria have been transformed into biomass wherever the concentration of bacteria exceed the threshold value $c_{\text{Bac, max}}/c_{\text{Bac}} = 10$, c.f. (3). Moreover, the remaining bacteria have diffused within the fluid. Likewise, the nutrient has diffused and has been consumed by the sticky agent, which is located at solid-solid, solid-bio, solid-fluid, bio-fluid, and bio-bio interphases. As a result the solid blocks remain glued together. Their immobility is further enhanced since they are now physically entrapped by biomass.

From the middle column in Figure 6 it is evident that nearly the entire nutrient has been consumed. As a consequence, the biomass has diminished considerably. This applies in particular to those parts of the domain in which less nutrient was present. The occurrence of biomass in the upper middle of the picture is not an artifact, but rather a result of the applied periodic boundary conditions on $\partial Y$. As can be expected, the bacteria have re-diffused into the domain that was previously occupied by biomass. It is remarkable that bacteria that have also diffused into the biomass are integrated into the biomass as described by $f_{\text{decrease,Bac}} = -f_{\text{increase,B}}$ in Section 2.2.

The fourth column from the left in Figure 6 illustrates that the bacteria’s diffusion further alters the concentration of bacteria in the regions that have previously been occupied by
biomass. As a consequence of the nutrient being unavailable the biomass in the upper half of the domain has disappeared. The same holds true for the sticky agent which is, however, not depicted in Figure 6. Hence, the upper half of the cross has started to redistribute. Conversely, the lower half of the cross is still immobile. This is due to the fact that it is physically entrapped by biomass and may be further enhanced by the presence of the sticky agent.

Finally, the column on the right in Figure 6 shows a state in which bacteria and biomass have completely vanished due to the lack of a nutrient. Subsequently, the solid, consisting of a cross initially, has also been redistributed in its lower half.

3.4 Comprehensive model and effective diffusion tensors

As a fourth example, we evaluate a scenario similar to the one above, but focus on the impact the structural changes have on the effective diffusion tensor as defined in (9).

As illustrated in Figure 7 the square $Y$ consisting of $16 \times 16$ cells is considered. The initial distribution of solid cells is randomly chosen. Initially no biomass is present. The initial bacteria and also the nutrient concentrations obey (11) see pictures on the left in Figure 7. The distribution of the solid results in an effective diffusion tensor that has zero as an eigenvalue. This indicates that diffusion is possible from top to bottom, but is not possible from left to right (note that we applied periodic boundary conditions to $\partial Y$).

After the first global time steps, no solid blocks have moved, as biomass has nearly filled the complete pore space and inhibits their movement, compare Section 3.3 and the second pictures from left in Figure 7. Moreover, due to the availability of the nutrient the solid cells are additionally held together by the sticky agent.

The computation of the effective diffusion tensor shows the behavior that is expected for such a setting: the eigenvectors (principle directions of diffusion) and the eigenvalue equal to zero remain fixed, since the solid has not changed its structure and biomass has filled the complete pore space. Yet the other normalized eigenvalue ($\lambda_i/D_{O_2,f}$) decreases significantly from 0.3240 to 0.0749 $\approx$ 20% $\cdot$ 0.3240 due to the fact that the diffusion is significantly lower (reduced by 80%) in the biomass compared to the fluid, compare Section 3.1. This indicates that diffusion is still dominant from top to bottom, and is not possible from left to right.

As can be seen in the pictures on the right in Figure 7, after 50 time steps the biomass has decayed completely again due to the lack of oxygen. This enables the restructuring of the solids and as in Section 3.2 larger solid blocks have formed. As can be deduced from the corresponding diffusion tensor in Figure 7, diffusion is now also possible from left to right.

3.5 Evaluation of the model

3.5.1 Degeneration of homogenized tensors

The homogenization problem has proven to potentially be ill posed for certain time steps, i.e. when the system matrix is close to singular. This is due to the fact that insulated fluid or biomass cells appear (e.g. one single fluid cell and a pair of fluid cells in the center of the computational domain as depicted in Figure 8). In such a situation the pore space is no longer connected and the underlying mathematical problems (10) are not uniquely solvable. Such situations become more pronounced as the porosity $\theta$ decreases. However,
Figure 7: Evolution of bacteria (top), biomass (middle), nutrient and solid (bottom); at $t_0$, $t_3$, and $t_{50}$ (from left to right).
restructuring of the solid and coalescing into bigger solid blocks may in turn lead to a connected pore space for which the diffusion tensors are again well defined.

### 3.5.2 Influence of coincidence on the homogenized tensors

As a next step, we investigate the influence coincidence has on the calculated diffusion tensors. In doing so, we consider the square $Y$ of $16 \times 16$ cells in which initially a U-shaped solid as shown in the picture on the left of Figure 9 is prescribed. Moreover, initially
Figure 11: Large eigenvalue (red cross) and small eigenvalue (blue circle) for different executions of a random scenario with the same porosity $\theta = 1 - 40/256$ as for the “U” scenario.

Figure 11: Large eigenvalue (red cross) and small eigenvalue (blue circle) for different executions of a random scenario with the same porosity $\theta = 1 - 40/256$ as for the “U” scenario.

no biomass is present. The initial bacteria and also the nutrient concentration have a parabolic profile in the horizontal direction and are constant in the vertical direction, cf. (11). Since biomass and bacteria have vanished in the quasi stationary state and the focus lies on the development of the diffusion tensor, their development is not illustrated here.

The same simulation was repeated 100 times. Exemplarily, four stationary states are shown in Figure 9. Moreover, the eigenvalues of the 100 simulation runs are depicted in Figure 10. From this Figure it is evident that the eigenvalues do not differ significantly when having started from the same initial configuration. The same holds true for random starting configurations as is illustrated for scenarios with different porosities in Figure 11 ($\theta = 1 - 40/256$), Figure 12 ($\theta = 60\%$), Figure 13 ($\theta = 70\%$), and Figure 14 ($\theta = 80\%$).

3.5.3 Porosity and eigenvalues of homogenized tensors

Pertaining to the influence of the porosity on the eigenvalues of the computed diffusion tensors, we consider the same situation as in Section 3.4 (up to the initially randomly chosen distribution of the solid).

The resulting (time-dependent) diffusion tensors’ eigenvalues are displayed in Figure 15. Here, the eigenvalues at the time of initiation are depicted in red, while the eigenvalues after 50 global time steps are depicted in blue. The dashed and dotted lines represent the smaller and larger eigenvalues, respectively. In summary, the eigenvalues increase as time proceeds due to the consolidation of larger solid blocks, compare Section 3.2. Likewise, the values increase considerably with an increasing porosity and have a peak at $\theta = 1$ representing free flow.

3.5.4 Computational effort

To analyze the computational effort of our computations, we again consider the same situation as in Section 3.4 (up to the initial random distribution of the solid with porosity values between 0.65 and 0.75) and investigate a square of $NX \times NX$ cells with $NX =$
Figure 12: Eigenvalues of different executions for a random scenario; porosity 60%.

Figure 13: Eigenvalues of different executions for a random scenario; porosity 70%.

Figure 14: Eigenvalues of different executions for a random scenario; porosity 80%.
Porosity θ

Figure 15: Normalized eigenvalues of the normalized diffusion tensor for scenarios with different porosity; evolution of small (dashed lines) and large eigenvalue (dotted lines); eigenvalues at initial time (red) and after 50 global time steps (blue).

We found out that the time needed for solving the PDE system is approximately in $O(n^{2.09})$ while the time for solving the CAM is in $O(n^{2.57})$. Additionally in our example and implementation the time that is needed for solving one of the problems once is almost equal, but as the PDE system is solved within the inner loop, i.e. more often, (c.f. Table 2) the total time for solving all PDE problems is higher than the time that is needed for solving all CAMs.

The computations are performed on a Fujitsu P720 with eight Intel® Core™ i7-4790 CPUs @ 3.60GHz. The simulation time for $110 \times 110$ cells is about 800 seconds.

### 3.6 Hybrid multiscale model

We now illustrate the functionality of this model’s approach to take into account the impact of the microscopic on the macroscopic scale. In particular the effect the underlying microstructure’s evolution has on the macroscopic diffusion is investigated in the following weakly coupled multiscale problem: We consider the following diffusion equation for a macroscopic concentration $c(t, x, y)$ in a macroscopic domain $\Omega$ (a square) with time-dependent Dirichlet boundary conditions on $\partial \Omega$ and constant initial concentration:

$$
\partial_t c - \nabla \cdot (\mathbb{D} \nabla c) = 0 \quad (x, y) \in \Omega, t \in (0, T),
$$

$$
\frac{c(x, y, t)}{\bar{c}} = 1 - t/T \quad (x, y) \in \partial \Omega, t \in (0, T),
$$

$$
\frac{c(x, y, 0)}{\bar{c}} = 1 \quad (x, y) \in \Omega.
$$

On the microscale, we refer to the example and diffusion tensors $\mathbb{D}$ calculated in Section 3.4 and depicted in Figure 7.

Now the obtained time-dependent diffusion tensors that strongly depend on the underlying and changing geometry are integrated into the macroscopic diffusion problem. Note that our example is weakly coupled, i.e. backcoupling the macroscopic diffusion equation’s solution onto the cell problems is not incorporated into the overall multiscale model. The macroscopic problem was discretized using P1-FEM and the software tool M++ [17].
Figure 16: Evolution of macroscopic concentration at $t_1$ (left), at $t_{50}$ (middle), and $t_{100}$ (right). The pictures have been generated with initial, constant tensor (top), evolving tensor (middle) and final, constant tensor (bottom).
In Figure 16, the following varying situations are illustrated: First, at the top row of Figure 16, the initial singular diffusion tensor $D_{O_2,f}(\begin{pmatrix} 0.0000 & -0.0000 \\ -0.0000 & 0.3240 \end{pmatrix})$ with first eigenvalue equal to zero from Figure 7 is taken for all times. Second in the middle row of Figure 16 the time-dependent diffusion tensor, i.e. starting with the singular matrix $D_{O_2,f}(\begin{pmatrix} 0.0000 & -0.0000 \\ -0.0000 & 0.3240 \end{pmatrix})$ which becomes a symmetrical positive definite matrix as time proceeds, is taken into account. Third, at the bottom row of Figure 16 the final non-singular diffusion tensor $D_{O_2,f}(\begin{pmatrix} 0.4118 & -0.0651 \\ -0.0651 & 0.3811 \end{pmatrix})$ from Figure 7 is considered for all times.

For the singular diffusion tensor (at the top row in Figure 16) a reasonably high concentration develops in the middle of the macroscopic domain whereas the concentration diminishes at its top and bottom. This is due to the fact that diffusion is strong in the vertical direction and not possible in the horizontal direction (first eigenvalue equal to zero). Horizontally the concentration distribution is homogeneous, but at the left and right boundaries it must satisfy the time-dependent Dirichlet boundary condition.

Using the evolving diffusion tensors for all 50 time steps unless it is badly scaled, c.f. Section 3.5.1 (middle, Figure 16), we obtain a concentration which behaves similar as before in the beginning. After time proceeds the concentration is high in the center of the domain and decreases considerably in the radial direction since the diffusion tensor turns into a symmetric positive definite matrix, meaning that diffusion is possible vertically and also horizontally.

Turning now to the case that the final non-singular diffusion tensor is considered for all times, it can be deduced from the bottom row in Figure 16 that the diffusion occurs faster than in the previous cases since the diffusion is possible in all directions immediately from the beginning (no eigenvalue equal to zero) with considerably high eigenvalues compared to the evolving diffusion tensor.

4 Discussion and conclusion

In this research, we presented a comprehensive mathematical model for biomass development and solid aggregate restructuring. A novel discrete–continuum approach was taken, combining a model of differential equations for reactive multicomponent transport with a cellular automaton method for the interactive development of the biomass and solid structures. With the help of well-known results from homogenization theory the effect of these structural changes occurring on the microscale in macroscopic transport can be taken into account. Different processes leading to geometrical changes were incorporated and thoroughly illustrated by means of numerical simulations.

The main purpose of the current research was to develop a tool to examine the strong interplay between functional properties and geometrical structure even on larger scales. Although our results have already contributed towards enhancing our understanding of the impact of small scale processes and structures on a medium’s functionality, there are several levels of complexity that may be added to the model.

First, an extension to multi-species biomass and potentially also shrinking biomass as discussed in [11, 13] is possible along the lines of these publications. Second, more sophisticated reactions and different types of nutrients (e.g. oxygen and nitrate) could be integrated into the model. In terms of soil aggregates, however without considering the
spatial structure explicitly, in [15] nonlinear diffusion and reaction rates leading to self-oscillatory behavior were considered in 1D.

Another necessary step in broadening further applications is the integration of fluid flow into our model. A pore-scale model taking into account fluid flow and biofilm detachment by shear stress may be found in [13]. Here, biofilm development is calculated by means of a CAM. Likewise, in the context of upscaling, continuum fluid flow and biofilm models were considered in a thin strip in [14], in a locally periodic setting in [10], and in a geometry being extracted from the imaging data of glass beads inoculated with biomass in [9]. Combining such model extensions with the presented concept of solid restructuring seems to be quite promising for further investigations into the factors that affect soil’s functionality in the future.

Finally, more research is needed to investigate unsaturated flow as was done for non-evolving angular pore networks representing soil aggregates in [5]. Here continuum model approaches were combined with an individual model for microbial community. The superposition of the results weighted with aggregate size distributions made it possible to access scales of practical interest.

Of course this work is just a first step in modeling complex physicochemical processes in soil science, but it shows the way to a promising toolbox with versatile model components and is extendable for further process mechanisms. Those have to be identified and validated with the help of experimental studies. This will be another future challenge.

Notation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Dimension</th>
<th>Definition</th>
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$k_d,\alpha$ 1/s rate constant for sticky agent decay
$k_d,B$ 1/s rate constant for biomass decay
$k_B$ 1/s rate constant for biomass increase
$\nu$ -- outer unit normal
$\Omega$ $m^2$ computational macroscopic domain
$\tau_n$ s global time step
$x_n^k$ s local sub-time step
$\theta_{\text{red}}$ -- porosity w.r.t. fluid
$\theta$ -- porosity w.r.t fluid and bio cells
$Y = \bigcup_i Y^i$ $m^2$ computational pore scale domain
$\partial Y$ $m$ periodic boundary
$Y_b = \bigcup_i Y_b^i$ $m^2$ bio cells
$\partial Y_b$ $m$ interface with bio cells
$Y_f = \bigcup_i Y_f^i$ $m^2$ fluid
$\partial Y_f$ $m$ interface with fluid
$Y_s = \bigcup_i Y_s^i$ $m^2$ solid
$\partial Y_s$ $m$ boundary of solid
$Y^i$ $m^2$ rectangular cell
$Y_b^i$ $m^2$ bio cell
$\partial Y_b^i$ $m$ faces of bio cell
$Y_f^i$ $m^2$ fluid cell
$\partial Y_f^i$ $m$ faces of fluid cell
$Y_s^i$ $m^2$ solid cell
$\partial Y_s^i$ $m$ faces of solid cell

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References


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