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Modeling the effect of soil meso- and macropores topology on the biodegradation of a soluble carbon substrate

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ABSTRACT

Soil structure and interactions between biotic and abiotic processes are increasingly recognized as important for explaining the large uncertainties in the outputs of macroscopic SOM decomposition models. We present a numerical analysis to assess the role of meso- and macropore topology on the biodegradation of a soluble carbon substrate in variably water saturated and pure diffusion conditions . Our analysis was built as a complete factorial design and used a new 3D pore-scale model, LBioS, that couples a diffusion lattice-Boltzmann model and a compartmental biodegradation model. The scenarios combined contrasted modalities of four factors: meso- and macropore space geometry, water saturation, bacterial distribution and physiology. A global sensitivity analysis of these factors highlighted the role of physical factors in the biodegradation kinetics of our scenarios. Bacteria location explained 28% of the total variance in substrate concentration in all scenarios, while the interactions among location, saturation and geometry explained up to 51% of it.

1. Introduction

Soil is the most complex and heterogeneous material on earth due to its complicated architecture and the high diversity of organisms that it hosts. It is also one of the biggest carbon storage pools containing more than twice the amount of carbon present in the atmosphere. Soil Organic Matter (SOM) decomposition, even if it is evaluated to a relative loss of carbon of less than a percent [1], is thus a key process regarding CO_2 emissions.

Experimental observations at the millimeter scale have shown that the distribution of bacteria is characterized by the presence of hot-spots [2–5]. The heterogeneity of the arrangement of soil particles (inter-aggregate vs intra-aggregate porosity) and the variation of water saturation conditions contribute to maintain gradients in abiotic conditions (nutrients, pH and redox conditions) and therefore locally promote or not the growth of micro-organisms [6]. The patchy distribution patterns of bacteria in soils can result in spatial disconnection between organic residues and decomposers and thereby influence the kinetics of decomposition of organic compounds, as has been shown experimentally by [7,8]. The sinuous water diffusion pathways in the soil pore space through which nutrients can be transported can thus play a major role in these situations [9,10] although this can be mitigated by cells migration mechanisms allowing the microorganisms to reach distant resources [11–14].

The complex interactions between the biotic and abiotic components of soil that occur at the scale of the microhabitats of soil decomposers has been identified as being a major regulator of the C and N cycles [15–17].

Despite these considerations, SOM decomposition models are dominated by macroscopic models in which soil structure is not explicitely represented and the role of physical environmental conditions – especially hydration statuses – is described by non-robust empirical macroscopic functions [18,19]. Indeed, since microscale

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heterogeneities are hidden within these macroscale functions, they may appear to cause large uncertainties in model outputs [20,21].

The combination of non invasive X-ray tomographic tools to describe the 3D structure of soil [22,23] and the development of pore-scale models [24] can now be used to test hypotheses on the role of soil structure. An increasing number of modeling studies have begun to account for pore-scale spatial heterogeneity when simulating biodegradation kinetics (e.g. [25–30]) but they have been restricted to relatively simple artificial media. Few attempts to model biological activity using 3D tomographic images of soil have pointed out that the combination of different soil pore space geometries and hydration status can affect organic matter decomposition [31] and/or the growth and colonization of soil by fungi [32]. However, a global sensitivity analysis to assess the influence of pore space topology, hydration status, spatial arrangement of organic substrates and decomposers, and the intrinsic physiology of the microorganisms on the decomposition of SOM has yet to be tackled.

The aim of this paper was to quantify the relative influence of physical and biological drivers both as separate and interacting factors on the biodegradation kinetics of a soluble substrate. We performed a modeling exercise describing a simplified picture of the 3D soil pore space retaining only the meso- and macroporal space but combining different diffusion pathways in variably saturated conditions and with patchy distributions of bacteria.

We simulated bacterial dynamics in 3D meso- and macropore topologies obtained from X-Ray computed tomography images of undisturbed soil samples at a resolution of 68 μm. Following the approach found in Chau et al. [33], we first numerically computed explicit air-water interfaces in the pore space using the two-phase two-relaxation-time lattice Boltzmann model (TRT-LBM) [34]. We then simulated the diffusion and biodegradation of a non-sorbing soluble substrate at different water saturation levels under pure diffusive conditions (no water flow due to precipitation). To do so, the advection-diffusion TRT-LBM [35] was coupled to a compartmental model dedicated to bacteria-driven biodegradation, forming the new LBioS model (Lattice-Boltzmann model for biodegradation affected by soil structure). We built a complete factorial design, in which physical factors (the geometry of the meso- and macropores, water saturation, bacteria spatialization) and a physiological factor were varied in combination. A global sensitivity analysis was applied to the outputs of 54 generated scenarios. For this exploratory work, our objectives were twofold: (i) to assess our modeling approach as a tool for investigating the effect of spatial heterogeneity on biodegradation processes and, (ii) to quantify the effect of physical and biological factors on biodegradation kinetics. The simplifications made in this work are presented in details throughout the paper and discussed through their consequences on the obtained results.

2. LBioS model description

2.1. Water physics modeling

We used a lattice Boltzmann approach for simulating water physics processes. In the lattice Boltzmann method, the physical behavior of a fluid emerges from the microscopic movements of small entities of the fluid – named the populations (f_q) – that are distributed at the nodes or sites (r) of a regular grid – the lattice. Sites belong either to the solid matrix (solid sites) or to the pore space (fluid sites) and are arranged in order to recreate the discrete structure of a porous medium. At every site, populations accounting for microscopic masses and momentum are ascribed to velocity vectors ($\vec{c_q}$) defining their direction (q) on the grid ($q = 0$ for resting populations and $1 \le q \le Q-1$ for moving populations, with Q the number of directions on the grid). We used the two-relaxation-time scheme [35] that takes advantage of the symmetry of the lattice, so that populations f_q are decomposed into symmetric and antisymmetric components along their opposite velocities $\vec{c_q} = -\vec{c_{\bar{q}}}$ (Eq. (1)):

$$f_q = f_q^+ + f_q^- \text{ and } f_q^\pm = \frac{1}{2}(f_q^\pm \pm f_{\bar{q}}) \qquad q = 1,\ldots,Q-1 \tag{1}$$

$$f_0 = f_0^+ \qquad f_0^- = 0$$

The distribution evolution at the node from time t to $t+1$ is summed up in the equation of evolution (2).

$$f_q(r+\vec{c_q}, t+1) - f_q(r,t) = \lambda_e\left[f_q^+(r,t) - e_q^+(r,t)\right] + \lambda_o\left[f_q^-(r,t) - e_q^-(r,t)\right] + S_q \tag{2}$$

The evolution equation includes the collision operator (two first terms of right hand side of Eq. (2)), a source term (S_q) and the propagation step (left hand side of Eq. (2)). During the collision step, the relaxation of moments resulting from the populations' distribution at time t towards an equilibrium state ($e_q = e_q^+ + e_q^-$) governs the reorganization of these populations.

During the propagation step, moving populations are translated to their neighboring nodes in the q direction, defining a new distribution at $t+1$. S_q is an external source term adding or removing a fraction of the population at a given site. It can represent an external force such as gravity, fluid-fluid interactions (cohesion) or biodegradation. Boundary conditions of bounce back type are applied at the pore walls: populations leaving a fluid site and hitting a solid site are sent back in the opposite direction.

Macroscopic variables such as fluid density (ρ) or momentum (J) are calculated at each site of the lattice from the populations' distribution (Eqs. (3) and (4)).

$$\rho = \sum_q f_q \tag{3}$$

$$J = \rho\vec{u} = \sum_q f_q\vec{c_q} \tag{4}$$

where $\vec{u}$ is the macroscopic velocity. They are expressed in lattice units, that can be easily converted into physical units.

The equilibrium populations e_0 and $e_q^\pm$ in Eq. (2) are defined in Eqs. (5)–(7) from [36].

$$e_0 = \rho - \sum_{q=1}^{Q-1} e_q^+ \tag{5}$$

$$e_q^+ = t_q^* c_s^2 \rho + g_s . E_q^+(\vec{j},\rho) \qquad E_q^+(\vec{j},\rho) = \frac{3j_q^2 - ||\vec{j}||^2}{2\rho}$$

$$\vec{j} = \vec{J} + \frac{\vec{F}}{2} \qquad j_q = \vec{j}.\vec{c_q} \qquad q = 1,\ldots Q-1 \tag{6}$$

$$e_q^- = t_q^*\,\vec{u}\,\vec{c_q} \qquad q = 1,\ldots Q-1 \tag{7}$$

where $\vec{F}$ is a body force, c_s is a free parameter of the model set to $\frac{1}{3}$ and g_s is a parameter equal to 0 or 1. The values of the weights t_q^*, parameters λ_e and λ_o and non linear term $E_q^+(\vec{j},\rho)$ are specific of the model version (see below).

2.1.1. Two-phase TRT-LBM

We used the two-phase TRT-LBM for the resolution of Stokes flow, as described in detail in [34], to simulate air-water distribution in porous media. For modeling the Stokes equation $g_s = 0$ [36]. The Shan–Chen implementation of multiphase flow was used [37] and the LBM was solved on a D3Q19 lattice (three dimensions, 19 directions). t_q^* in Eqs. (6) and (7) was set to $\frac{1}{6}$ for orthogonal velocities ($||\vec{c_q}|| = 1$) and $\frac{1}{12}$ for diagonal velocities ($||\vec{c_q}|| = \sqrt{2}$).

The parameterization of λ_e and λ_o is of critical importance for model performance and stability. λ_e and λ_o must be comprised between -2 and 0, their stability range. In the two-phase model, λ_e is related to the kinematic viscosity ν along $\nu = -\frac{1}{3}(\frac{1}{2} + \frac{1}{\lambda_e})$ while λ_o is set free. We used $\nu = \frac{1}{6}$ and $\lambda_o = \frac{3}{16}$ [34].