Geophysical Research Abstracts
Vol. 12, EGU2010-1653, 2010
EGU General Assembly 2010

3D geometrical modelling of pore space micro-structures to simulate microbial decomposition of organic matter

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Abstract

Up to now, very few works deals with the geometrical modelling of 3D soil micro-structures for simulating biological dynamics. In this paper, we propose to approximate soil pore micro-pore space using generalized cylinders by using as initial data high resolution 3D Computed Tomography images (3-5 μm) of soil samples. Afterwards, we use this composite geometrical representation to simulate microbial decomposition of organic matter.

Our raw data are high resolution (3-5 μm) 3D Computed Tomography images of soil samples. By thresholding, we obtain a set of voxels (cubes) forming poral space which in most cases is a complex volume shape that can not be approximated by simple analytic functions. We propose to represent this complex shape using a compact, stable and robust piece wise analytic approximation by generalized cylinders. This intrinsic shape representation conserves its topological and geometrical properties. Our geometrical modelling algorithm includes three main processing stages. The first stage consists in describing the volume shape by a minimal number of balls included within the shape and whose union recovers shape skeleton. In a second stage, we extract, in an optimal manner, simply connected chains of balls. The last stage deals with the approximation of each simply optimal chain by means of geometrical primitives: circular generalized cylinder, torus, cylinder, troncated cone, balls. Therefore, the final output is an adjacency valuated graph of geometrical primitives forming a composite shape (pore space) representation.

In a second stage, this geometrical representation is used to simulate microbial decomposition of organic matter. Thus, we face the still open problem of modelling dynamic phenomena in a heterogeneous geometry. To achieve this goal, we propose two different approaches : one "algorithmical" relying upon updating valuated graph and another one "mathematical" based on partial differential equations system. The basic principle of the "algorithmical" method is to attach to each node of the graph (pore) information related to microbial and organic matter biomasses. We model the simulation of microbial decomposition by updating the graph regarding biological activities. The "mathematical" method consists in using Partial Differential Equations Systems (PDEs) to simulate more accurately microbial decomposition of organic matter in 3D pore space. Recent Free finite elements solver Freefem3d is used to solve PDE system.

We apply our algorithms to several data set of real 3D volume Computed Tomography soil samples. We show that our geometrical representation approximates well poral space. We also stress its compacity and robustness regarding changes of initial data and also its coherence with the intuitive notion of pores. We also demonstrate the pertinence and the coherence of the simulation resuts provided by either "algorithmical" method or "mathematical" method. The experimental results show clearly the influence of 3D soil structure on biological processes.

Keywords Biological dynamics simulation ; Partial Differential Equations (PDE) ; microbial decomposition of organic matter ; 3D Computed Tomography (CT) image ; soil structure ; pore space ; numerical simulation ; reaction diffusion equations ; Freefem3d PDE solve ; generalized cylinders ; computational geometry ; geometrical modelling.

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