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To what extent do uncertainty and sensitivity analyses help unravel the influence of microscale physical and biological drivers in soil carbon dynamics models?

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ABSTRACT

Soil respiration causes the second largest C flux between ecosystems and the atmosphere. Emerging soil carbon dynamics models consider the complex interplay of microscale interactions between the physical and biological drivers of soil organic matter decomposition occurring in the 3D soil architecture. They are expected to provide a way to upscale results to the macroscopic level and as such appear as an alternative modelling approach to the traditional "black-box" macroscopic models. However, these models still need to be tested under a broader range of their parameters values and structures than has been the case to date. We thus conducted uncertainty and global sensitivity analyses to test the robustness of previous predictions on dissolved organic carbon biodegradation obtained by one of these microscopic carbon dynamics models, LBioS. Six parameters of the carbon dynamics module of LBioS, associated with bacterial metabolism and three microscopic 3D descriptors of soil architecture were considered as uncertain inputs. We built two complete factorial designs in which the minimum and maximum of uncertainty intervals are considered. Each factorial design is assigned to a particular structure of the model, one including dormancy of bacteria and the other considering optimal bacterial activity. The scenarios took place in 3D computed tomography images of an undisturbed cultivated soil. The sensitivity indices at different simulations dates were computed with an ANOVA procedure taking into account main effects and interactions among factors. The uncertainty analysis shows that only in the limiting case of low accessibility of resources to bacteria the different microbial metabolisms tested can modify to a small extent the system responses, and uncertainty linked to parameters describing soil architecture becomes preponderant. In the case of optimal accessibility output variability is due predominantly to uncertainty of the microbial metabolism parameters. The sensitivity analysis suggests that whatever the structure of the model, the role of soil architecture in the microbial activity can be evidenced using either *DOC* or CO_2 as proxy measures. Beyond these results, we stress that results of uncertainty and sensitivity analyses of soil carbon models need to be interpreted with caution, dependent as they are on the status of the model itself, as well as on the particular scenarios used in the uncertainty and sensitivity analyses.

1. Introduction

With globally 68 to 120 Pg C year^{-1}, soil respiration represents the second largest C flux between ecosystems and the atmosphere. Among the hundreds of computer models that describe the dynamics of soil carbon under a range of soil and environmental conditions (Manzoni and Porporato, 2009), many adhere to a traditional, macroscopic perspective, in which the soil organic matter is divided into a number of connected pools, but no detail is included on the spatial distribution of organic matter in the pore space, nor on the biodiversity and activity of the biomass. In contrast to this traditional approach, a number of researchers have attempted to describe in detail the complex interplay of microscale processes that determine the fate of organic matter (Monga et al., 2008; Falconer et al., 2012; Ebrahimi and Or, 2015; Vogel et al., 2015), the anticipation being that if a proper description of these processes can be achieved, and one can find a way to upscale the result to the macroscopic scale, the description of emergent processes will be far better than what traditional black-box models produce.

Even though measurements techniques able to provide quantitative data on microscopic parameters of soils have experienced tremendous technological advances in the recent decade, many of the microscopic processes these models involve are still little more than assumptions at

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this point (Kovarova-Kovar and Egli, 1998; Gignoux et al., 2001), or their descriptions are gross simplification of what we suspect is really occurring. Nevertheless, even under these conditions, as various authors have argued (Gras et al., 2010, 2011; Folse and Allison, 2012; Manzoni et al., 2014), microscale models of soil processes can be very useful guides for further research, as long as they are supplemented by thorough uncertainty and sensitivity analyses. Uncertainty analysis aims at characterizing the distribution of global output variables resulting from the probability distribution of several uncertain input factors (Saltelli et al., 2009; Wallach et al., 2013). The purpose of sensitivity analysis is to evaluate the extent to which each model parameter is responsible for the observed outcome uncertainty (Saltelli et al., 2009). Whereas the latter analysis has been often used solely to identify the sensitive parameters of a given model, in order to point out the ones whose measurement or independent estimation should deserve particular attention (e.g. Neff and Asner, 2001; Cazelles et al., 2013; Pagel et al., 2014; Dwivedi et al., 2017), uncertainty analysis has seldom been used in the context of soil carbon dynamic modelling. Only a few articles have carried out both types of analyses (Boulange et al., 2012; Wang et al., 2013, 2005; Xenakis et al., 2008).

Among the recent articles that have combined the development of a microscale computer model with a detailed sensitivity analysis of it, Vogel et al. (2015) try to assess the role of meso- and macropore topology on the biodegradation of a soluble carbon substrate in a soil, under variably water saturated and pure diffusion conditions. In order to do this, they describe a 3D pore-scale model, LBioS that couples a diffusion lattice-Boltzmann model and a compartmental biodegradation model. With LBioS, they simulate a number of hypothetical scenarios in which four factors are systematically varied: meso- and macropore space geometry, water saturation, bacterial distribution, and physiology. A global sensitivity analysis of these factors highlights the influence of physical factors, related to soil architecture, on biodegradation kinetics. The location of bacterial cells explains 28% of the total variance in substrate concentration in all scenarios, while the interactions among location, saturation, and geometry explain up to 51% of it. However, this result is obtained by using only one set of parameters describing microbial metabolism, and no uncertainty analysis is carried out.

In this context, the purpose of the research described in the present article is to assess the robustness of observations made by Vogel et al. (2015), by reproducing the same scenarios but using several sets of parameters describing the microbial metabolism. Our hypothesis is that the strong influence of physical factors related to soil architecture on biodegradation kinetics found by Vogel et al. (2015) in their scenarios may be counterbalanced by the influence of biological factors related to microbial metabolism. With more complete uncertainty- and sensitivity analyses, a different picture may emerge of what the key parameters of the model are and it may suggest to direct our attention to other types of macroscopic measurements than those suggested by Vogel et al. (2015) to test their model.

2. Material and methods

2.1. 3D images of soil micro-environments

Samples of a cultivated soil, a silty loamy (19% clay, 75% silt, 6% sand) Albeluvisol, were obtained by Vogel et al. (2015) and 3D images of the samples were obtained using an X-ray CT scanner at the Simbios center (Dundee). The voxel resolution of the images is 68 μm and the image size is 600^3 voxels. The rather low resolution of the CT images did not permit to visualise the vast majority of the fine particles (clay and silt) of the soil, and therefore neither the smaller-sized pores that are associated with these particles. Therefore, only the meso- and macropores were considered in this study according to classification of Luxmoore (1981). As discussed in Vogel et al. (2015) this resolution was chosen because it could reproduce the millimeter-scale variability of microbial activity found for instance by Vieublé-Gonod et al. (2003).

Table 1
Values of four indicators of the morphology of the pore space of the two sub-images G4 and G6. The Euler-Poincaré characteristic, EPC, is given in lattice units (with 1 lu = 68 μm). τ_g is the average geometrical tortuosity calculated from the different pathways going from the top horizontal plane ($Z = 0$) to the bottom horizontal plane ($Z = 100$) of the sub-image as given in Vogel et al. (2015). SSA is the specific surface area given here as a value normalized by the SSA of a sphere of an equivalent pore volume. ϵ is the porosity of the pore space visible at the 68 μm voxel resolution of the CT scans.

Sub-image	EPC lu^{-3}	τ_g [–]	SSA/SSA_{sphere} [–]	ϵ cm^3cm^{-3}
G4	−2.1	1.08	1.82	0.1125
G6	−105.4	1.73	3.0	0.1882

We selected 2 sub-images (G4 and G6) of 100^3 voxels out of the dataset of Vogel et al. (2015) for their contrasted values of three indicators of the pore space topology. These indicators are the Euler-Poincaré characteristic (EPC), the geometrical tortuosity τ_g, and the specific surface area (SSA). EPC is a measure of the number of non-redundant closed-loop paths in the pore space, τ_g is the ratio of the geodesic distance over the Euclidian distance between two distant points in the pore space, and SSA is the liquid/solid interface area per unit mass (see Vogel et al., 2015 for more details about their calculations). Table 1 gives the values of these indicators for the two sub-images G4 and G6.

The sub-image G4 has a geometrical tortuosity close to one, indicating straight pathways from the top plane to the bottom plane, a specific surface area of about twice that of a sphere of identical pore volume and EPC has a value close to zero, indicating a poorly connected pore network with a low variation in the geometry of the pores. Its pore space is thus considered as topologically homogeneous. The sub-image G6 has a high geometrical tortuosity indicating longer and more tortuous pathways from the top plane to the bottom plane, a specific surface area of about three times that of a sphere of identical pore volume and its EPC has a highly negative value, indicating a continuous well-connected pore space. Its pore space is thus considered as topologically complex. These images correspond to a volume size of about 314 mm^3 and their total macroporosity values are 11.25% and 18.82% for G4 and G6 respectively (Table 1).

Vogel et al. (2015) calculated the 3D water and air distribution for different water saturation indexes (S_w, the proportion of liquid phase on pore phase) in each sub-images, using the model of Genty and Pot (2013). We selected two water and air distributions at the extreme values of the water saturation index: $S_w = 0.25$ and $S_w = 1.00$ (Fig. 1).

We used the incubation experiments reported in Monga et al. (2014) of a single bacteria strain with fructose as sole source of carbon in sand microcosm to define initial substrate and bacteria concentrations in the sub-images: $DOC_0 = 0.62\ mg_C cm^{-3}$ and $B_0 = 1.31\ 10^{-6}\ mg_C cm^{-3}$. The boundary diffusion conditions were fixed to zero flow to mimick the pure diffusion conditions of the incubation experiments. In the simulations, fructose is applied as a pulse on the top horizontal plane of the images. Ten spots representing micro-colonies of the bacteria strain are placed in ten voxels containing water. In Vogel et al. (2015) three types of distribution are tested, the ten selected voxels are close to the initial fructose source (the Top localisation), i.e., the ten spots are localised within the 30 first horizontal planes corresponding to an average Euclidian distance of 1 mm from the initial fructose top horizontal plane; they are far from it (the Bottom localisation) i.e., the ten spots are localised within the 30 last horizontal planes corresponding to a minimal Euclidian distance of 4.7 mm from the initial fructose top horizontal plane; or they are regularly spaced (the Distributed localisation, see Vogel et al. (2015)). We selected the most contrasted localisations, Top and Bottom.

We thus constituted a dataset of 8 images of contrasted soil micro-

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