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Key Points:

- A framework linking soil structure, carbon, and hydrology is needed for holistic predictions under environmental and land use changes
- The novel Millennial model for soil carbon cycling is linked to a recent soil hydraulic parameterization
- Aggregated carbon is used as a proxy for soil macroporosity to simultaneously model the changes in soil properties and microbial activity

Supporting Information:

Supporting Information may be found in the online version of this article.

Correspondence to:

S. Calabrese,
salvatore.calabrese@ag.tamu.edu

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Author Contributions:

Conceptualization: Achla Jha, Salvatore Calabrese

Funding acquisition: Salvatore Calabrese

Investigation: Achla Jha, Sara Bonetti, A. Peyton Smith, Rodolfo Souza, Salvatore Calabrese

Methodology: Achla Jha, Sara Bonetti, A. Peyton Smith, Rodolfo Souza, Salvatore Calabrese

Software: Achla Jha, Rodolfo Souza



Supervision: Salvatore Calabrese

Visualization: Achla Jha, Sara Bonetti

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Linking Soil Structure, Hydraulic Properties, and Organic Carbon Dynamics: A Holistic Framework to Study the Impact of Climate Change and Land Management

Achla Jha¹ , Sara Bonetti², A. Peyton Smith³, Rodolfo Souza¹, and Salvatore Calabrese¹ 

¹Department of Biological and Agricultural Engineering, Texas A&M University, College Station, TX, USA, ²School of Architecture, Civil and Environmental Engineering, Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland, ³Department of Soil and Crop Sciences, Texas A&M University, College Station, TX, USA

Abstract Climate change and unsustainable land management practices have resulted in extensive soil degradation, including alteration of soil structure (i.e., aggregate and pore size distributions), loss of soil organic carbon, and reduction of water and nutrient holding capacities. Although soil structure, hydrologic processes, and biogeochemical fluxes are tightly linked, their interaction is often unaccounted for in current ecohydrological, hydrological and terrestrial biosphere models. For more holistic predictions of soil hydrological and biogeochemical cycles, models need to incorporate soil structure and macroporosity dynamics, whether in a natural or agricultural ecosystem. Here, we present a theoretical framework that couples soil hydrologic processes and soil microbial activity to soil organic carbon dynamics through the dynamics of soil structure. In particular, we link the Millennial model for soil carbon dynamics, which explicitly models the formation and breakdown of soil aggregates, to a recent parameterization of the soil water retention and hydraulic conductivity curves and to solute and O₂ diffusivities to soil microsites based on soil macroporosity. To illustrate the significance of incorporating the dynamics of soil structure, we apply the framework to a case study in which soil and vegetation recover over time from agricultural practices. The new framework enables more holistic predictions of the effects of climate change and land management practices on coupled soil hydrological and biogeochemical cycles.

Plain Language Summary Soil degradation due to climate change and unsustainable land management practices is a global phenomenon that threatens food security and Earth livability at large. While soil degradation involves modifications of both physical and biological properties of soils, mathematical models to predict these changes have focused independently on these two aspects, limiting our ability to holistically assess climate and human drivers of soil degradation. Here, we connected recent advances in modeling physical and biological soil processes to develop a unified framework that can account more holistically for potential changes in soil properties over time. The potential of this framework to predict soil changes is illustrated through an analysis of a case study of soil and vegetation recovery from agricultural practices. This work may represent an important step toward predicting the effects of land use and climate changes on soil degradation, hence enabling the design of more sustainable land management strategies.

1. Introduction

Climate change and intense land management practices continue to alter and degrade soils globally, with detrimental implications for multiple ecosystem services, ranging from food production to sustaining biodiversity, mitigation of greenhouse gas emissions, and conservation of water quantity and quality (Borrelli et al., 2020; Brady & Weil, 2008; Lal, 1993, 2012). An important aspect of soil degradation is the alteration of soil structure (i.e., size, shape, and arrangement of soil pore spaces and aggregates/peds) (Bronick & Lal, 2005; Meurer et al., 2020; Or et al., 2021). Changes in soil structure impact the retention and cycling of water, nutrients, and carbon (C), in turn affecting above and below ground ecosystem processes (Or & Ghezzehei, 2002; Rabot et al., 2018; Romero-Ruiz et al., 2018). Thus, determining how soil structure evolves is key for quantifying the effects of climate change and land management practices on ecosystem processes and services (Lipper et al., 2014; Young et al., 1998). Nevertheless, little information about soil structure dynamics, factors that affect it, and its link to soil biogeochemical cycles is included in current ecohydrological models (Meurer et al., 2020; Pelak & Porporato, 2019), making it difficult to predict the short- and long-term impact of soil structure alteration on ecosystem water and C

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fluxes under changing environmental conditions (Hirmas et al., 2018; Sullivan et al., 2022). This paper illustrates how combining recent advances in soil C modeling with novel parameterization of soil hydraulic properties and microbial activity may allow integration of soil structure dynamics into ecohydrological models without increasing model complexity.

Soil structure derives from the accumulation of organic matter and formation of soil aggregates due to plant roots, fungal hyphae, and biological activity (Golchin et al., 1994; Lal, 2004; Young et al., 1998). This aggregation in turn gives rise to structural macroporosity that may increase soil hydraulic conductivity by multiple orders of magnitude, especially in fine-textured soils where micropores are intrinsically abundant (Beven & Germann, 2013; Bonetti et al., 2021; Zurmühl & Durner, 1996). Aggregation also controls microbial activity by affecting the accessibility of the organic substrate by microbes and the diffusivity of gases (e.g., O₂, CO₂) within the soil matrix (Meurer et al., 2020; Moyano et al., 2013; Yan et al., 2018). These interactions between soil organic C (SOC) dynamics, soil hydrology, and microbial activity, which are particularly dynamic within the soil rooting zone depth, demonstrate the need to develop novel quantitative approaches that explicitly account for soil structure and how this is affected by climate and land-use.

While the effects of soil structure and macroporosity on soil hydrology are well-known, measures of soil structure that can inform about its dynamics are missing (Beven & Germann, 1982; Dexter, 1988; Kutválek, 2004; Larson et al., 1989). Macroporosity often gives rise to a bi-modal pore size distribution, which is visible in water retention and hydraulic conductivity curves (Durner, 1994; Mohanty, 1999; Tuller & Or, 2001). Measuring these curves, however, provides information at a specific location and cannot be easily generalizable, for example, to large scale relevant to land surface models applications or to areas with limited soil data. To address this limitation, the work by Fatichi et al. (2020) and Bonetti et al. (2021) proposed the use of vegetation metrics (e.g., Gross Primary Productivity (GPP), aboveground vegetation biomass, Leaf Area Index (LAI)) as surrogates for soil structure modifications and soil hydraulic properties. These works refined the representation of soil hydrological processes in land surface models by allowing a two-way interaction between natural vegetation and soil hydraulic properties. However, these frameworks are mostly applicable to unmanaged soils, where plant rooting systems, and therefore vegetation cover, primarily control the development of soil structure. They do not consider the effects of macroporosity due to formation of soil aggregates, which can be readily affected by rapid environmental changes as well as management practices in agricultural fields (e.g., tillage) (Bonetti et al., 2021; Cagnarini et al., 2019; Fatichi et al., 2020; Or et al., 2021). Additionally, while vegetation may predominantly influence soil hydrology on large scales (e.g., field to regional), soil aggregates may be the primary drivers of soil hydraulic properties and biogeochemical cycles on the pedon scale (Ebrahimi & Or, 2018; Franklin et al., 2021; Jungkunst et al., 2022; Kutválek, 2004). This highlights the necessity of introducing additional measures of soil structure, beyond vegetation indices, that are more closely related to soil aggregation and different soil management practices in agricultural soils.

Recent developments in soil C modeling may help address this gap. In particular, the novel Millennial Model (Abramoff et al., 2018, 2022) explicitly considers the dynamics of “measurable” C pools, representing a major advancement from traditional C models based on the CENTURY framework, such as the DAYCENT (Parton et al., 1998) and the DeNitrification-DeComposition models (Powlson et al., 1996), which conceptualize the SOC in different C pools with presumed turnover times. Measurable pools include the C in the microbial biomass, the particulate organic matter (e.g., leaves, roots), the fraction of dissolved organic C (DOC) adsorbed on mineral surfaces (“mineral associated organic matter”), the DOC obtained from root and microbial exudates, and the C trapped into soil aggregates. Since organic C is an essential component of soil aggregates, aggregated C may serve as a good proxy for soil structure. In addition, the “Millennial Model” provides a process-based representation of the biological, chemical, and physical processes that affect the C occluded within the soil aggregates (such as formation and breakdown of aggregates), thus offering an opportunity to link soil hydraulic parameterization (i.e., soil hydraulic conductivity) to the temporal evolution of soil structure. This linkage may pave the way for quantifying how structure affects microbial dynamics, if appropriate microbial growth laws considering soil structural features are adopted (e.g., Yan et al., 2018).

Here we provide a framework for the integrated study of soil structure, hydrology, and C dynamics in response to natural and human-induced environmental changes across time scales (Figure 1). Considering the rooting zone depth, our framework couples the parameterization of soil hydraulic properties for soil water balance models to the Millennial model (Abramoff et al., 2018, 2022; Bonetti et al., 2021; Fatichi et al., 2020) for soil C cycling. We

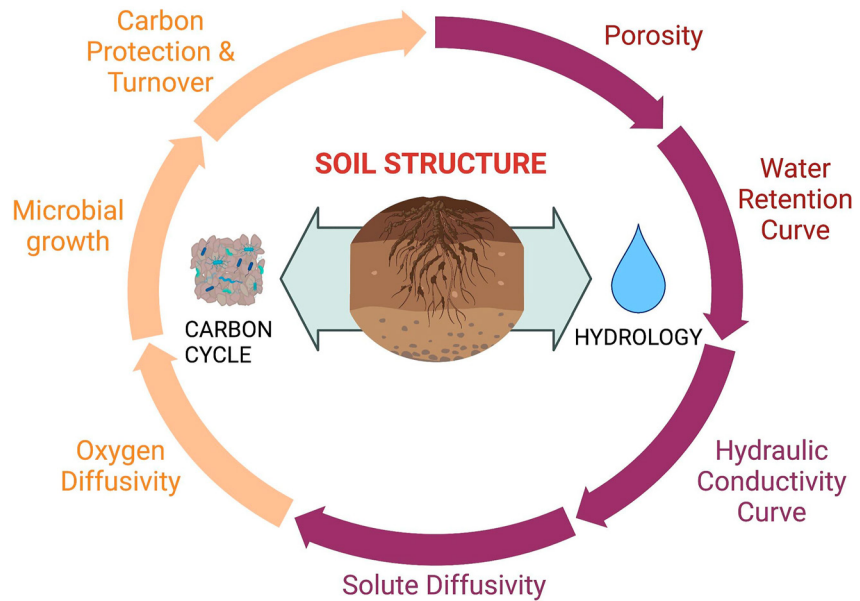


Figure 1. Schematic representing the linkage of soil structure dynamics with soil hydraulic properties, soil microbial activity, and soil C cycle in the proposed framework.

then demonstrate the potential of this integrated framework by applying it to a case study of natural recovery of soils in an abandoned farmland. We conclude by highlighting critical aspects that require further investigation as well as opportunities for future research.

2. The Millennial Model Approach for Soil Structure Dynamics

While traditional ecohydrological models consider soils as a rigid element with constant soil properties (Manzoni & Porporato, 2009; Robertson et al., 2019), land use changes and management practices such as tillage, reforestation, crop rotation, and land use conversions can alter soil structural features (pore and aggregate size distribution) over different time scales (Chandrasekhar et al., 2018). To extend ecohydrologic models and account for these effects, soil structural features need to be included as prognostic variables. The Millennial model approach (Abramoff et al., 2018, 2022) is particularly useful, as it explicitly simulates different C pools and processes that are good indicators of soil structure, such as the formation and breakdown of aggregated C. Such a framework provides an ideal starting point to investigate how land management practices and climate change modify soil structure, in turn affecting microbial activity, C sequestration, and hydrologic processes.

The Millennial model introduces a novel representation of soil C cycling based on “measurable C pools” (Abramoff et al., 2018, 2022), namely the particulate organic matter (*P*), DOC, aggregate C (*A*), mineral associated C (*M*) and microbial biomass (*B*). Unlike traditional C models, which rely on C pools defined by the chemical recalcitrance of the organic C, the Millennial model aims to emphasize the important roles that C aggregation and interaction with mineral surfaces and microbial processes (e.g., production of extracellular enzymes and depolymerization of high molecular weight C compounds) play on soil C cycling. The model is framed as a system of five mass balance differential equations governing the dynamics of the five C pools (namely *P*, DOC, *A*, *M*, and *B*) and describing the main interactions between them, as illustrated in (Figure 2). We briefly describe the model in the Appendix, including some modifications from the original formulation that we introduced, but we refer to Abramoff et al. (2022) for more details. Below, we describe how the Millennial model can be extended to account for the effects of soil structure on microbial activity and soil hydraulic properties.

3. Effect of Soil Structure on Microbial Activity

Changes in soil structural features affect the diffusion of C substrate and oxygen to soil microsites, hence impacting the activity of soil microbial communities. A possible approach to account for this is to adopt microbial growth

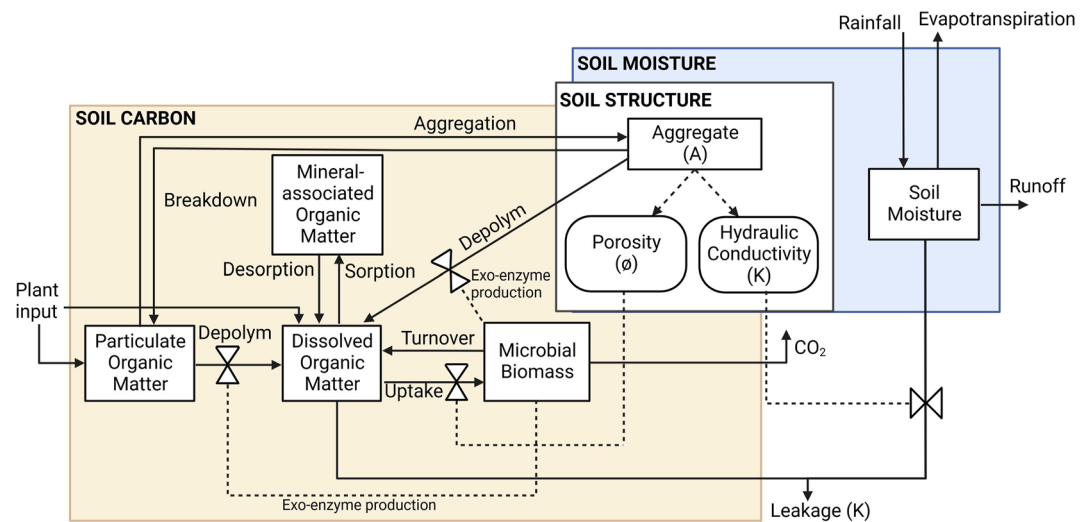


Figure 2. Conceptual diagram of the theoretical framework linking a soil C module, soil moisture module, and a soil structure module. The link is established through the aggregated C, a soil C pool, which regulates the variability in soil hydraulic conductivity and porosity, hence affecting the soil moisture dynamics. The soil moisture dynamics in turn affects the aggregated C, as soil moisture exerts an important control on multiple soil C fluxes. The solid lines represent fluxes. The dashed lines represent control with a collate symbol to indicate a direct control on a specific flux. The dashed arrows indicate that K and ϕ are functions of A .

laws that reflect the actual availability of substrate and oxygen in microsites, which in turn are controlled by their ability to diffuse from the bulk soil (Davidson et al., 2014; Moyano et al., 2013). Using the Michaelis-Menten kinetics, the microbial uptake (U) of DOC can be expressed as (Davidson et al., 2014; Moyano et al., 2013)

$$U = U_{\max} \frac{\text{DOC}_A}{\text{DOC}_A + K_{\text{DOC}}} \frac{\text{O}_{2A}}{\text{O}_{2A} + K_{\text{O}_2}}, \quad (1)$$

where U_{\max} is a maximum uptake rate, DOC_A and O_{2A} are the concentrations of available DOC and O_2 in soil microsites, and K_{DOC} and K_{O_2} are half-saturation constants for DOC and O_2 , respectively. The availability of DOC and O_2 in the microsites is then controlled by their diffusivities, which in turn depend on the soil pore structure including the water-filled and air-filled pore networks and their connectivity at different water saturation conditions. Following Yan et al. (2018), the DOC diffusivity, D_{DOC} normalized to the diffusivity of pure water, $D_{0,\text{DOC}}$, can be expressed as

$$\frac{D_{\text{DOC}}}{D_{0,\text{DOC}}} = \phi^{p(m_s - n_s)} \theta^{n_s}, \quad (2)$$

where ϕ is the soil porosity, m_s and n_s are cementation and saturation exponents accounting for the effects of the pore structure and water connectivity on DOC diffusion, θ is the moisture content, and p is a SOC-microorganisms collocation factor varying between 0 and 1. The cementation exponent represents the pore connectivity and tortuosity, while the saturation exponent describes the effect of water saturation depending on the pore size distribution of the soil. The collocation factor represents the degree of collocation between the SOC and the microorganisms. The expression for the O_2 diffusivity takes a similar form (Yan et al., 2018),

$$\frac{D_{\text{O}_2}}{D_{0,\text{O}_2}} = \phi^{(m_g - n_g)} (\theta - \phi)^{n_g}, \quad (3)$$

where m_g and n_g are cementation and saturation exponents accounting for the effects of the pore structure and water connectivity on O_2 diffusion, and D_{0,O_2} is the diffusivity in free air.

The concentrations, DOC_A and O_{2A} , can then be expressed as proportional to the bulk concentrations (DOC_b and O_b) through their respective diffusivity coefficients (Davidson et al., 2014; Moyano et al., 2013), for example, $\text{DOC}_A = \text{DOC}_b (D_{\text{DOC}}/D_{0,\text{DOC}}) = \text{DOC}_b \phi^{p(m_s - n_s)} \theta^{n_s}$, and substituting back in Equation 1, the microbial uptake of the DOC can be expressed in terms of soil porosity (ϕ) and water content (θ) as

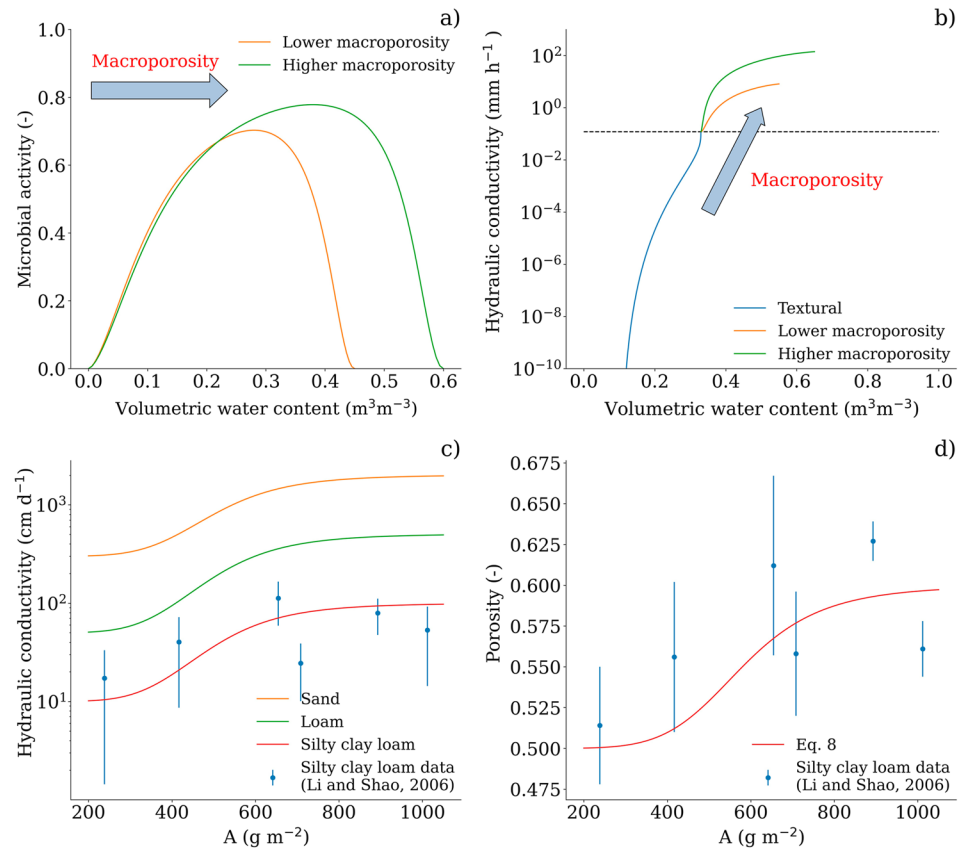


Figure 3. Effect of soil structure on variation of (a) microbial activity with volumetric water content. (b) Hydraulic conductivity with volumetric water content. (c) Relation between hydraulic conductivity and aggregated C ($R^2 = 0.77$; RMSE = 19.89 cm d⁻¹) computed using Equations 7 and 9 with $\alpha = 580$ and $\beta = 6$ for various soil textural types: sand from Bonetti et al. (2021) (85% sand, $K_{s, \text{tex}} = 300$ cm d⁻¹, $K_{s, \text{tot}} = 2,016.66$ cm d⁻¹), loam from Bonetti et al. (2021) (50% sand, $K_{s, \text{tex}} = 50$ cm d⁻¹, $K_{s, \text{tot}} = 506.54$ cm d⁻¹), silty clay loam from Li and Shao (2006) ($K_{s, \text{tex}} = 10$ cm d⁻¹, $K_{s, \text{tot}} = 100$ cm d⁻¹). (d) Relation between porosity and aggregated C ($R^2 = 0.59$; RMSE = 0.05), computed using Equation 8. Data from Li and Shao (2006).

$$U = U_{\max} \frac{\text{DOC}_b \phi^p (m_s - n_s) \theta^{pn_s}}{\text{DOC}_b \phi^p (m_s - n_s) \theta^{pn_s} + K_{\text{DOC}}} \frac{O_b \phi^{(m_g - n_g)} (\theta - \phi)^{n_g}}{O_b \phi^{(m_g - n_g)} (\theta - \phi)^{n_g} + K_{O_2}} \quad (4)$$

The microbial uptake law, Equation 4, accounts for how both soil structure (i.e., through the cementation and saturation exponents and the soil porosity) and soil water content control the availability of the C substrate and oxygen, hence regulating microbial activity (Figure 3a).

4. Linking Soil Hydraulic Properties to C Cycling

4.1. Hydraulic Properties of Structured Soils

In addition to affecting the diffusivities of the C substrate and O₂, soil structure also introduces a bimodality in the soil pore size distribution, which affects both the water retention and hydraulic conductivity curves. The lower mode (i.e., microporosity) derives from the textural component of the soil matrix, whereas the higher mode (i.e., macroporosity) derives from the structural one. Generally, from the pore size distribution (and water retention curve) the unsaturated hydraulic conductivity K can be estimated from the Mualem model (Mualem, 1976). However, the Mualem model is based on the assumption that the pore system consists of fully interacting pores (Mualem, 1976), an assumption which may not be true for structured soils, in which macropores may develop as an independent pore system. In this case, one can express the total unsaturated hydraulic conductivity as the sum of the conductivities of textural and structural components of the soil matrix (Bonetti et al., 2021; Fatichi et al., 2020; Smettem & Kirkby, 1990),

$$K_{\text{total}} = K_{s,\text{tex}}K_{r,\text{tex}} + K_{s,\text{str}}K_{r,\text{str}}, \quad (5)$$

where $K_{s,\text{tex}}$ and $K_{r,\text{tex}}$ are the saturated and relative hydraulic conductivity, respectively, for the textural pore spaces, and $K_{s,\text{str}}$ and $K_{r,\text{str}}$ are the saturated and relative hydraulic conductivity, respectively, for the structural ones. Being independent, $K_{r,\text{tex}}$ and $K_{r,\text{str}}$ can be individually computed from the Mualem model.

Additionally, water in soils with bimodal pore systems may flow only within the textural pore spaces at low soil water content and may begin flowing also within the structural pore spaces only when the water content crosses a given water content threshold (Figure 3b). Therefore, using for example, the van Genuchten-Mualem model, K can be expressed as (Smettem & Kirkby, 1990)

$$K_{\text{total}} = \begin{cases} K_{s,\text{tex}}S_{e,\text{tex}}^l \left[1 - \left(1 - S_{e,\text{tex}}^{1/a_{\text{tex}}} \right)^{a_{\text{tex}}} \right]^2, & \theta < \theta_m \\ K_{s,\text{tex}} + K_{s,\text{str}}S_{e,\text{str}}^l \left[1 - \left(1 - S_{e,\text{str}}^{1/a_{\text{str}}} \right)^{a_{\text{str}}} \right]^2, & \theta > \theta_m \end{cases} \quad (6)$$

where K_s is the saturated hydraulic conductivity, $l = 0.5$ is a parameter accounting for pore connectivity, a_{tex} is the shape parameter of the hydraulic conductivity curve of the textural pore space, and a_{str} is the corresponding shape parameter of the structure-modified hydraulic conductivity curve. Note that the effective saturation of the soil in the micropore ($S_{e,\text{tex}}$) and the macropore systems ($S_{e,\text{str}}$) are relative to the corresponding porosities, $S_{e,\text{tex}} = (\theta - \theta_r)/(\theta_m - \theta_r)$ and $S_{e,\text{str}} = (\theta - \theta_m)/(\theta_s - \theta_m)$, where θ_r is the residual water content, θ_s is the water content at saturation (also equal to total porosity ϕ_{tot}), θ_m is the water content at the boundary between the micro- and macroporosity (namely the textural porosity, ϕ_{tex}). We note that while this framework accounts for flow within macropores originating from aggregation, a multi-domain approach would be needed to account for preferential flow at low antecedent moisture conditions due to for example soil cracking (Aguilar-López et al., 2020; Gerke, 2006; Gerke & van Genuchten, 1993; Mohanty et al., 1997, 1998; Vogel et al., 2000).

4.2. Linking Soil Hydraulic Properties to Soil C Cycling

While Equation 6 provides a means to compute the hydraulic conductivity curve of structured soils once the saturated hydraulic conductivities have been empirically determined, these conductivities could be directly coupled to the C cycle through the amount of aggregated C, effectively linking hydraulic properties to soil structure dynamics. Fatichi et al. (2020) made a pivotal step in this direction by introducing a parameterization of the hydraulic parameters based on the assumption that soil structure is tightly coupled to the GPP. In particular, the ratio of saturated hydraulic conductivities, $K_{s,\text{str}}/K_{s,\text{tex}}$, is assumed to vary between 1 for low GPP to 1,000 for high GPP (typical of tropical rain forests). Note that while here we expressed the hydraulic conductivity in terms of effective saturation, one can link it to the matric potential using the water retention curve. In this regard, Fatichi et al. (2020) showed how structural and textural parameters of the van Genuchten water retention curve covary with $K_{s,\text{str}}/K_{s,\text{tex}}$, paving the way for further integration with vegetation and microbial models, where matric potential is more indicative of water stress.

Analyzing globally distributed measurements, Bonetti et al. (2021) recently extended this approach by introducing a sigmoidal function relating the ratio of saturated structural to textural hydraulic conductivities to measures of vegetation biomass, such as the LAI, rather than GPP. Whether using GPP or LAI, these approaches are particularly relevant when applied to large scales, over which preferential flow due to the rooting system may prevail over flow through macro-porosity due to soil aggregates. Bonetti et al. (2021) further considered the fact that modification of soil hydraulic conductivity due to structure correction varies across soil types. For instance, a highly conductive sandy soil would not experience a sensible increase in total hydraulic conductivity due to structure compared to a fine textured soil that is more prone to macroporous flow (Weynants et al., 2009).

Adopting the mathematical expressions introduced by Bonetti et al. (2021) to couple the hydraulic conductivity to vegetation indices through a sigmoidal relationship, one can extend this approach to link the changes in soil hydraulic properties to the evolution of soil structure using the aggregated C (A , in the Millennium model) as a measure of soil structure. The structural saturated hydraulic conductivity could be computed as

$$K_{s,\text{str}} = K_{s,\text{tot}} - \frac{K_{s,\text{tot}} - K_{s,\text{tex}}}{1 + \left(\frac{A}{\alpha}\right)^\beta} - K_{s,\text{tex}}, \quad (7)$$

where $K_{s,tot}$ and $K_{s,tex}$ represent the maximum saturated hydraulic conductivity of a soil with fully developed structure, which can be estimated from Equation 9, and saturated hydraulic conductivity of an unstructured/texture-only soil, respectively, and α and β are shape parameters (Figure 3c).

While the parameterization of Bonetti et al. (2021) focused on the hydraulic conductivity, the generality of the adopted mathematical expressions is such that a similar parameterization likely applies to porosity. Accordingly, the structural porosity may be linked to A via

$$\phi_{str} = \phi_{tot} - \frac{\phi_{tot} - \phi_{tex}}{1 + \left(\frac{A}{\alpha}\right)^\beta} - \phi_{tex}, \quad (8)$$

where ϕ_{tot} and ϕ_{tex} represent the maximum porosity of a soil with fully developed structure, and porosity of an unstructured/texture-only soil, respectively, and α and β are shape parameters (Figure 3d). Our case study below also suggests that a single set of α and β may be needed for Equations 7 and 8.

Based on empirical evidence, Bonetti et al. (2021) expressed the $K_{s,tot}/K_{s,tex}$ ratio as a function of the sand fraction,

$$\log_{10} \frac{K_{s,tot}}{K_{s,tex}} = 3.5 - 1.5Sa^{0.13}, \quad (9)$$

where Sa is the sand fraction % in the soil. Linking the hydraulic parameterization by Bonetti et al. (2021) to the Millennial model allows explicitly modeling the dynamics of soil hydraulic properties as the soil structure evolves in response to environmental changes. In particular, coupling the soil C cycling to the soil water balance (Laio et al., 2001; Pelak & Porporato, 2019) through the dynamics of soil structure and hydraulic properties, as introduced here, may be a significant step toward modeling more holistically soil processes as part of an integrated biochemical and physical system controlled by climatic changes (such as rainfall, temperature, etc.) as well as human activities (e.g., land use, management) (Porporato et al., 2015).

5. Application

To illustrate how the theoretical framework detailed above can capture the coupled soil structure, C, and water dynamics, it is instructive to apply it to a case study where these factors are all evolving in time. Here, we consider a 150-year chronological study of soil and vegetation recovery of an abandoned farmland in the Ziwuling area of Fuxian county located in the central Loess Plateau of China (Li & Shao, 2006). Using a space-for-time approach, five recovery stages were identified with the first succession stages represented by the sagebrush and mixed grasslands corresponding to a land abandonment of 2 and 14 years, respectively. The secondary succession stages are represented by maple and vetchleaf pagoda tree shrublands with the land being abandoned for 34 and 60 years, respectively. The mature forest marked the end of the recovery process with the land being abandoned for 150 years at this stage. Observations for total soil porosity, saturated hydraulic conductivity, the mean weight diameter of soil aggregates (0.25–5 mm), and the total SOC are reported as a function of abandonment years, here represented by five sampling sites corresponding to the different stages of vegetation recovery including grasslands, shrublands, and mature oak forest (Li & Shao, 2006). We assumed that the relative change in the mean weight diameter normalized by its initial value (MWD/MWD_0) is directly proportional to the relative change in aggregated C also normalized by its initial value (A/A_0), where the initial value is taken at 1 year after abandonment. Soils were silty clay loam across the sites. We refer to Li and Shao (2006) for more details on the soil sampling and analysis at various vegetation recovery stages.

Due to the limited availability of temporal data, a detailed model calibration remains difficult. Our focus is only on illustrating the ability of the model to capture the co-evolution of various soil biophysical properties. Net primary productivity (NPP) for different sampling sites is available (Xie et al., 2014) and was interpolated using a Monod relation to force the C module of the framework (Figure 4a). The C module is coupled to a soil water balance model (Rodríguez-Iturbe & Porporato, 2004), which was forced with a rainfall time series generated using a Marked Poisson process, with rainfall statistics obtained from Funk et al. (2015). Parameters related to the soil water balance were taken from Laio et al. (2001), except for measured porosity and hydraulic conductivity, while parameters for the C module were taken from Abramoff et al. (2018) and Abramoff et al. (2022). These parameters were adjusted to capture observations from the site and are provided in Table S1 of the Supporting

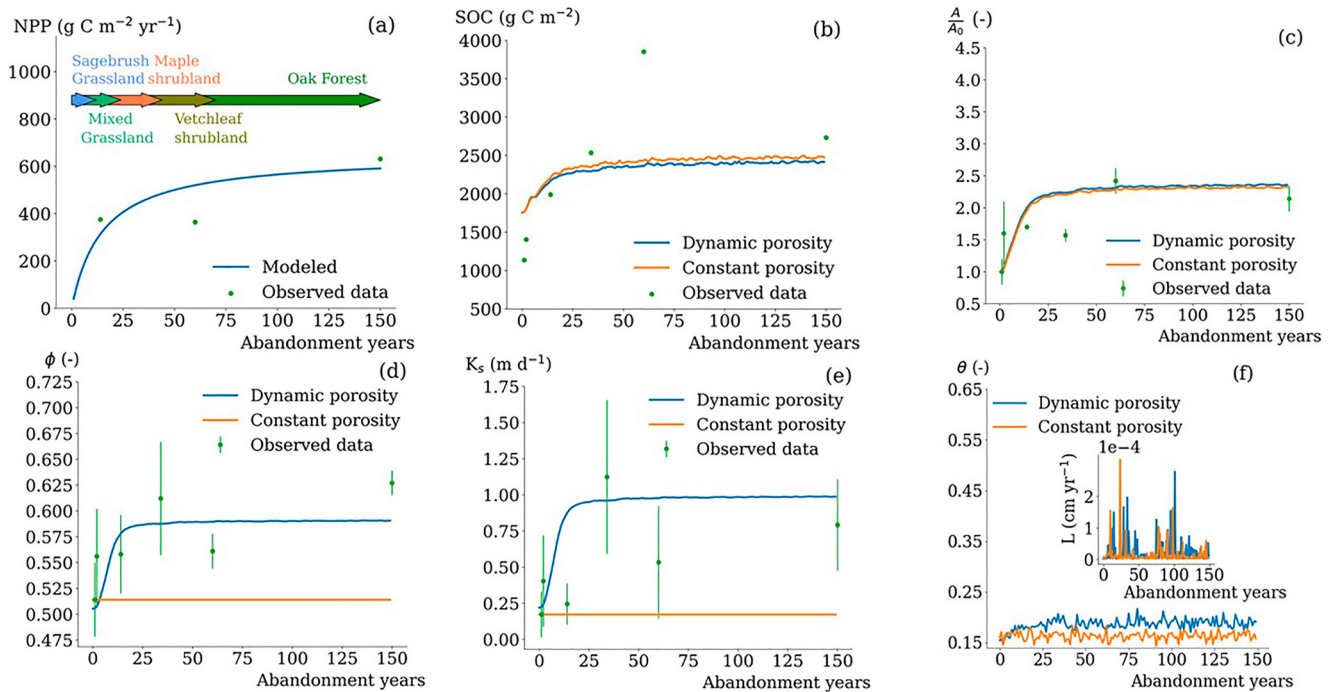


Figure 4. Change in soil biophysical properties during the ecological succession from an abandoned cropland to forest: (a) Net primary productivity for different vegetation recovery stages; (b) Soil organic C; (c) Relative aggregates ($\frac{A}{A_0}$) with A_0 corresponding to aggregate at 1 year after abandonment; (d) Total porosity (ϕ); (e) Total saturated hydraulic conductivity (K_s); (f) Annual volumetric water content (θ), with the inset showing the leakage flux (L) with time. A list of parameters is provided in Supporting Information S1.

Information S1. After an initial spin up of 2,000 years, we ran the model for 150 years with an hourly timestep and then aggregated the results to yearly values for illustrative purposes.

As evident from the observations (Figure 4), following abandonment, the soil undergoes important biophysical changes, especially over the first 25 years. The increase in vegetation productivity over the years provided larger inputs of organic matter (root exudates and litterfall) to the soil (Figure 4b), which led to the formation of aggregates (Figure 4c) and mineral-associated organic matter (not shown here). As aggregates form, the development of macroporosity can be seen from the increase in total porosity and saturated hydraulic conductivity (Figures 4d and 4e). All these aspects are well captured by the model.

Importantly, since the model couples C dynamics and hydraulic properties, the model predicts how soil hydrologic fluxes have changed over time due to an increase in water retention (higher water content) that led to higher drainage (more leaching to deeper soil layers) (Figure 4f). A comparison with a simulation run using constant soil physical properties (equal to soil properties at the cropland stage) reveals the importance of including dynamic soil properties, especially to capture the changes in soil hydrologic processes. In particular, the development of macroporosity increased the soil water content on average, but also accelerated the hydrologic cycle by increasing the percolation. However, it should be noted that the changes in NPP here are fixed in both simulations (with constant and dynamic properties), while vegetation growth might have been different under constant porosity conditions. The absence of large structural pores under constant porosity conditions could have lowered the NPP and impacted the hydraulic properties (e.g., a reduced hydraulic conductivity) in turn affecting the aggregated C. Nevertheless, we would need detailed experiments based on soil evolving with time to validate it. This application shows that a holistic model linking soil structure, hydraulic properties, and C dynamics is needed to predict how the soil system and hydrology, hence ecosystem dynamics, respond to environmental or land use changes.

6. Discussion and Conclusions

Despite the significance of soil structure in controlling soil hydrologic and microbial processes and its linkage to the soil C cycling, the representation of soil structure and its dynamic nature in current process-based

ecohydrological models remains a challenge. Here, we built upon recent advances in soil C modeling and soil hydraulic parameterization to present an integrated modeling framework that can account for the effects of soil structure on hydrologic and C cycling processes using the amount of aggregated C as a proxy. In particular, aggregated C is here linked to the formation of macropores with consequent increase in saturated hydraulic conductivity and changes in oxygen and substrate diffusivity that affect microbial activity. The application to an abandoned cropland in the Loess Plateau of China showed the ability of the new framework to capture soil regeneration following vegetation succession from cropland, to grassland, shrubland, and ultimately forest and, overall, its potential to predict temporal changes in soil biophysical properties. The modeling framework can be particularly advantageous for applications involving land management practices and land-use changes. We stress, however, that simultaneous soil C (in its different forms) and soil hydrology measurements would be required to properly calibrate the model. In this regard, new soil characterization approaches are promising. For instance, X-ray computed tomography has been used to characterize the influence of soil structural changes on carbon losses and hydraulic properties under different land use. In addition, rare earth elements labeling and stable-isotope labeling techniques are used to quantify the rates of aggregate formation and decay across different soils and environmental conditions (Hartmann & Six, 2023; Sullivan et al., 2022). Ideally, long-term experimental studies are needed to capture soil structural changes, which can occur over decades. However, space-for-time substitution studies (like the case study considered here) would still provide useful information.

Beyond making predictions, an advantage of using a modeling framework based on measurable properties is that it can provide more physical, chemical, and biological-based insights into system dynamics, especially given the fact that observations are not always available. A model can identify drivers of changes in the SOC or explain differences in C turnover times across different biomes, climates, and management factors. For example, it can help assess when, based on climate and other soil factors, changes in SOC are driven by physical protection/release of C within aggregates (e.g., due to no till/till), by sorption/desorption of microbial necromass in mineral surfaces (e.g., shifts in hydrologic regime), or a combination of the two. Interestingly, such a model could be used to estimate SOC sequestration potentials across the globe, based on both natural and anthropogenic drivers. The latter, however, would need to be explicitly incorporated as forcing in the model, for which more work is needed. Another important aspect, relevant to ecosystem ecology and water resources, is that the coupling between C dynamics and hydraulic properties further allows interpretation and quantification of changes in soil hydrology over time, especially in response to land use changes. The case study explored here is a good example in which soil recovery leads to increased water retention within microporosity, but also more leakage due to macroporosity—an effect that cannot be quantitatively captured without the inclusion of soil structural effects. Interestingly, since the model estimates water and DOC leaching as the soil evolves, these fluxes could be captured by groundwater data, which could help calibrate the model, especially when interested in large areas.

While here we established a direct link between soil hydrologic and C cycling processes, our objective was also to introduce a framework that offers multiple opportunities to explicitly integrate how different biological factors interact with soil structure. Plants, for instance, affect soil structure both physically and chemically. Large roots physically displace large particles and increase soil macroporosity (Angers & Caron, 1998; Lucas et al., 2019; Vezzani et al., 2018), while smaller, fine roots displace small soil particles and occupy small pores spaces. Plant exudates, released by roots, may also act as a glue favoring aggregation (Bodner et al., 2021). The biogeochemical properties of the rhizosphere “hydraulic network” thus depend on the characteristics of the root system, the relative growth of large or fine roots, and the dynamic release of root exudates. Here, for the sake of simplicity, we included the role of plants only in terms of addition of fresh organic C, either as litterfall or as exudates. This can be expanded by explicitly considering a physically induced macroporosity dependent on the rooting system, as proposed by Bonetti et al. (2021), and a chemically induced one driven by exudates. The latter for example, can be accounted for by introducing a multiplicative factor in the aggregation term that depends on the accumulation of exudates. This however requires systematic experimental approaches across soil and plant types to accurately calibrate such additional factors.

Another key aspect of our modeling framework is that it can account for how changes in soil structure affect microbial growth. We considered the oxygen and substrate availability in soil microsites as dependent on the corresponding concentrations in the bulk soil through the gas and substrate diffusivity, respectively (Davidson et al., 2014; Moyano et al., 2013; Yan et al., 2018). These diffusivities in turn are controlled by soil porosity, which is driven by changes in aggregated C (i.e., proxy for structure) and thus are dynamic. In essence, the microbial growth law changes depending on soil structure. Returning to the example of soil regeneration in the Loess

Plateau, the framework accounts for the fact that the microbial community uptakes substrate and grows differently as the soil accumulates SOC and develops macroporosity. It is, however, possible that two soils that are very different in texture and structure have equal porosity. In this situation, the current substrate uptake law would not be able to distinguish between them, as it does not account for the different forms of heterogeneity that may result.

In this regard, future investigations should explore more in depth how the microbial growth law depends on aggregate or pore size distribution (Or et al., 2021). Analytical scale transition frameworks that derive the pedon scale microbial growth law based on the subscale spatial distributions of microorganisms and substrate quantity and quality are promising approaches to tackle microscale heterogeneity (Chakrawal et al., 2020; Shi et al., 2021; Wilson & Gerber, 2021). However, to avoid increasing model complexity, subscale heterogeneity could be parameterized based on both texture and the amount of aggregated C (i.e., structure), as well as environmental factors that may affect it (e.g., the soil moisture regime) (Schlüter et al., 2022).

Finally, based on the wealth of knowledge gained over the past decades on the pivotal role of microbial processes on soil C cycling (Conant et al., 2011; Lehmann & Kleber, 2015; Liang et al., 2017), there has been an interest in expanding soil C models to explicitly include microbial physiology and processes (Allison, 2014; Allison et al., 2010; Ballantyne IV & Billings, 2018; Calabrese et al., 2022; Huang et al., 2021; Sihi et al., 2016; Sulman et al., 2018; Todd-Brown et al., 2012; Wieder et al., 2015). These models relate microbial growth to intrinsic microbial traits (e.g., maximum substrate uptake rate, mortality rate) and metabolism (e.g., maintenance respiration, C use efficiency), to environmental conditions in the soil (such as moisture, temperature, and availability of C and nutrients), as well as the production of extracellular enzymes to depolymerize high molecular weight C compounds. Integrating such models and emerging omics data on microbial community composition and activity (Overy et al., 2021; Prosser, 2015) into our proposed modeling framework might pave the way for a more holistic understanding of environmental changes and land use impacts on the soil system, in terms of structure (i.e., physical properties, heterogeneity), biological activity (i.e., microbial community composition, traits, C cycling), and their interaction (Bonetti et al., 2021; Fatichi et al., 2020; Hartmann & Six, 2023; Kallenbach et al., 2019; Sullivan et al., 2022).

Appendix A: Soil C Model Description

The novel Millennial model for soil C dynamics (Abramoff et al., 2018, 2022) is based on a system of equations of C transfer between five C pools: particulate organic matter (P), DOC, aggregate C (A), mineral-associated organic matter (M) and microbial biomass (B) as shown in the conceptual diagram (Figure 2). The change in P over time is driven by the balance between plant C input in the form of plant and root litter, aggregated C breakdown, formation of aggregated C from P , and P decomposition into DOC,

$$\frac{dP}{dt} = p_i F_i + F_a - F_{pa} - F_{pl}^p, \quad (\text{A1})$$

where p_i is the proportion of C input in the form of plant and root litter (F_i), F_a is the rate of aggregate C breakdown, F_{pa} is the rate of aggregate C formation from P , and F_{pl}^p is the rate of P depolymerization into DOC.

The time dynamics of aggregated C results from a balance between C aggregates formation, breakdown, and depolymerization,

$$\frac{dA}{dt} = F_{pa} - F_a - F_{pl}^a, \quad (\text{A2})$$

where F_{pa} is the aggregate C formation from P , and F_a is the aggregate C breakdown, whereas F_{pl}^a is the depolymerization of A into DOC. This flux is much smaller than the depolymerization of P to account for the physical protection of C provided by aggregation.

The temporal dynamics of DOC is a function of DOC input from root exudates, DOC leaching loss, P and A depolymerization into DOC, mineral adsorption and desorption of DOC, and microbial uptake of DOC (U),

$$\frac{d\text{DOC}}{dt} = F_i(1 - p_i) + F_{pl} + F_{bm} - U - F_l - F_{lm} + F_{ld}, \quad (\text{A3})$$

where $(1-p_i)$ is the proportion of C released by plants (F_i) as root exudates, F_{bm} is the turnover of microbial biomass, F_{pl} represents the total depolymerization flux (of P and A), U is the uptake of DOC by microbial biomass, F_l is the DOC leaching loss, and F_{lm} and F_{ld} are the adsorption and desorption of DOC on clay mineral surfaces.

The variation of M over time simply depends on the balance between adsorption and desorption of DOC on clay mineral surfaces,

$$\frac{dM}{dt} = F_{lm} - F_{ld}, \quad (\text{A4})$$

where F_{lm} is the rate at which DOC is adsorbed, while F_{ld} is the rate at which M is desorbed. Both these rates depend on the concentrations of DOC and M and the adsorption capacity of the soil as dictated by the amount of clay minerals (Abramoff et al., 2021).

Lastly, the change in microbial biomass with time is regulated by microbial growth and decay according to

$$\frac{dB}{dt} = CUE \cdot U - F_{bm}, \quad (\text{A5})$$

where CUE is the C use efficiency, the microbial uptake of DOC (U), as described in (Equation 4), depends on substrate and O_2 concentrations in soil microsites, which in turn are affected by soil structure.

These equations include modifications that we introduced in the structure of the Millennial model to facilitate the coupling to the daily scale soil water balance and to allow potential extensions to explicitly integrate microbial processes (Allison et al., 2010; Wieder et al., 2015):

1. While the original Millennial model includes a direct exchange of C between the aggregated C and the mineral associated C, we only consider input of C to the mineral associated C pool through adsorption, so that a maximum amount of M can be directly imposed based on estimates of available adsorption sites. As a result, C can be adsorbed only from DOC. Similarly, we do not consider the C flux from mineral associated C to aggregated C. This does not imply that mineral associated C is not present in soil aggregates, but just that the model specifically tracks M independently of the aggregates because of the specific adsorption/desorption mechanisms involved. This is needed to guarantee that for given mineral surface area with specified adsorption capacity, there will be a maximum amount of C that can be adsorbed.
2. We modified the microbial biomass mortality/turnover rate (F_{bm}) and its interaction with DOC and M pools. The Millennial model originally included two separate mortality fluxes, feeding one into DOC and the other directly into M , to explicitly represent adsorption of necromass (Abramoff et al., 2022). Here, we consider a single mortality rate, whereby C is transferred to the DOC pool. Once in the DOC pool, C can then be adsorbed and contribute to the M pool. To include the preferential adsorption of necromass, the latter needs to be defined by its own DOC pool (e.g., DOC_{nec}) with higher affinity for adsorption on mineral surface sites.
3. Since maintenance respiration (rate of C lost via respiration) is accounted for by the C use efficiency CUE (fraction of C taken up allocated to growth), we express the growth rate as a multiplication of CUE and the uptake rate of C (U), so that an additional maintenance term is not needed in the equation. The CUE can be assumed constant or can be derived based on models that account for microbial processes (i.e., their physiology, metabolism, and exo-enzyme production).
4. Although aggregation is an important means of physical protection, aggregated particulate organic matter can still be depolymerized by extracellular enzymes. We thus introduced a depolymerization flux, from A to DOC, similar to the depolymerization of P but with a 10^{-3} factor in front of A to account for lower availability of C in aggregates.
5. Lastly, we coupled the soil C cycling model to a soil water balance, so that percolation and loss of DOC via leaching (F_l) could be computed based on the hydraulic conductivity and soil saturation state. Following Laio et al. (2001) and Rodríguez-Iturbe and Porporato (2004), the soil moisture dynamics were modeled by solving the following stochastic water balance differential equation:

$$Z_r \frac{d\phi_{tot}^s}{dt} = R - I - Q - ET - L, \quad (\text{A6})$$

where ϕ_{tot} is the soil porosity, Z_r is the active soil depth, s is the relative soil water content averaged over the soil depth (given by the soil volumetric water content over the soil porosity), R is the rainfall rate, I is the canopy interception, and Q is the surface runoff (here computed as saturation-excess runoff), ET is the evapotranspiration modeled as a nonlinearly increasing function of s , L is the leakage, which at the daily timescale can be assumed equal to the hydraulic conductivity K . The resulting leaching loss flux in the DOC pool is

$$F_i = LDOC/(\phi Z_{\tau s}). \quad (A7)$$

The system of Equations A1–A5 could also be extended, not shown here, to include explicitly the extracellular enzymes produced by the microbial biomass.

Data Availability Statement

We analyzed the data from experiments by Li and Shao (2006). The code (Jha, 2023) for the model and to execute the analysis in the paper is available at <https://github.com/Achla-Jha/Soil-Structure> (with a DOI of <https://doi.org/10.4211/hs.6e4f08d8380a49f99314bae8a7ac41e2>).

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