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

Achla Jha[1], Sara Bonetti[2], A. Peyton Smith[1], Rodolfo Souza[1], and Salvatore Calabrese[1]

[1]Texas A&M University
[2]École Polytechnique Fédérale de Lausanne

January 20, 2023

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 soil carbon substrate 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.

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

Achla Jha[1], Sara Bonetti[2], A. Peyton Smith[3], Rodolfo Souza[1], Salvatore Calabrese[1]

[1]Department of Biological and Agricultural Engineering, Texas A&M University, College Station, TX, USA

[2]School of Architecture, Civil and Environmental Engineering, Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

[3]Department of Soil and Crop Sciences, Texas A&M University, College Station, TX, USA

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.

Corresponding author: Salvatore Calabrese, `salvatore.calabrese@ag.tamu.edu`

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 soil carbon substrate and O_2 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(Lal, 1993, 2012; Brady & Weil, 2008; Borrelli et al., 2020). 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 (Young et al., 1998; Lipper et al., 2014). Nevertheless, little information about soil structure dynamics, factors that affect it, and its link to soil biogeochemical cycles is included in current ecohydrological models (Pelak & Porporato, 2019; Meurer et al., 2020), making it difficult to predict the short- and long-term impact of soil structure alteration on ecosystem water and C 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; Young et al., 1998; Lal, 2004). 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 (Zurmühl & Durner, 1996; Beven & Germann, 2013; Bonetti et al., 2021). Aggregation also controls microbial activity by affecting the accessibility of the organic substrate by microbes and the diffusivity of gases (e.g., O_2, CO_2) within the soil matrix (Moyano et al., 2013; Yan et al., 2018; Meurer et al., 2020). These inter-linkages between soil organic C dynamics, soil hydrology, and microbial activity 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 macroposity on soil hydrology are well-known, measures of soil structure that can inform about its dynamics are missing (Beven & Germann, 1982; Dexter, 1988; Larson et al., 1989; Kutílek, 2004). Macroporosity often gives rise to a bi-model pore size distribution, which is visible in water retention and hydraulic conductivity curves (Durner, 1994; B. P. Mohanty, 1999; Tuller & Or, 2001). Measuring these curves, however, provides information at a specific location and cannot be easily generalizable, e.g., to large scales relevant for Land Surface Models applications or 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 metrices (e.g., Gross Primary Productivity (GPP), aboveground vegetation biomass, Leaf Area Index (LAI)) as surrogates for soil structure modifications of 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

100 can be readily affected by rapid environmental changes as well as management practices

101 in agricultural fields (e.g., tillage) (Cagnarini et al., 2019; Or et al., 2021; Fatichi et al.,

102 2020; Bonetti et al., 2021). Additionally, while vegetation may predominantly influence

103 soil hydrology on large scales, e.g., field to regional, soil aggregates are the primary drivers

104 of soil hydraulic properties and biogeochemical cycles on the pedon scale (Kutílek, 2004;

105 Ebrahimi & Or, 2018; Franklin et al., 2021; Jungkunst et al., 2022). This highlights the

106 necessity of introducing additional measures of soil structure, beyond the vegetation in-

107 dexes, that are more closely related to soil aggregation and different soil management

108 practices in agricultural soils.

109 Recent developments in soil C modeling may help address this gap. In particular,

110 the novel Millennial Model (R. Abramoff et al., 2018; R. Z. Abramoff et al., 2022) ex-

111 plicitly considers the dynamics of "measurable" C pools, representing a major advance-

112 ment from traditional C models based on the CENTURY framework, such as the DAY-

113 CENT (Parton et al., 1998) and the DeNitrification-DeComposition (DNDC) models (Powlson

114 et al., 1996), which conceptualize the soil organic C in different C pools with presumed

115 turnover times. Measurable pools include the C in the microbial biomass, the particu-

116 late organic matter (e.g., leaves, roots), the fraction of dissolved organic C (DOC) ad-

117 sorbed on mineral surfaces ("mineral associated organic matter"), the DOC obtained from

118 root and microbial exudates, and the C trapped into soil aggregates. Since organic C is

119 an essential component of soil aggregates, the aggregated C may serve as a good proxy

120 for soil structure. The "Millennial Model" approach also provides a process-based rep-

121 resentation of the biological, chemical, and physical processes that affect the C occluded

122 within the soil aggregates (such as formation and breakdown of aggregates), thus offer-

123 ing an opportunity to link soil hydraulic parameterization (i.e. soil hydraulic conduc-

124 tivity) to the temporal evolution of soil structure. This linkage may pave the way for quan-

125 tifying how structure affects microbial dynamics, if appropriate microbial growth laws

126 considering soil structural features are adopted (e.g., Yan et al. (2018)).

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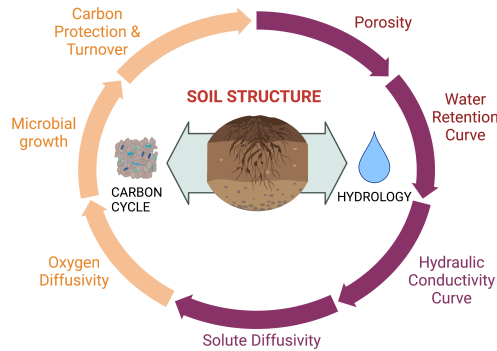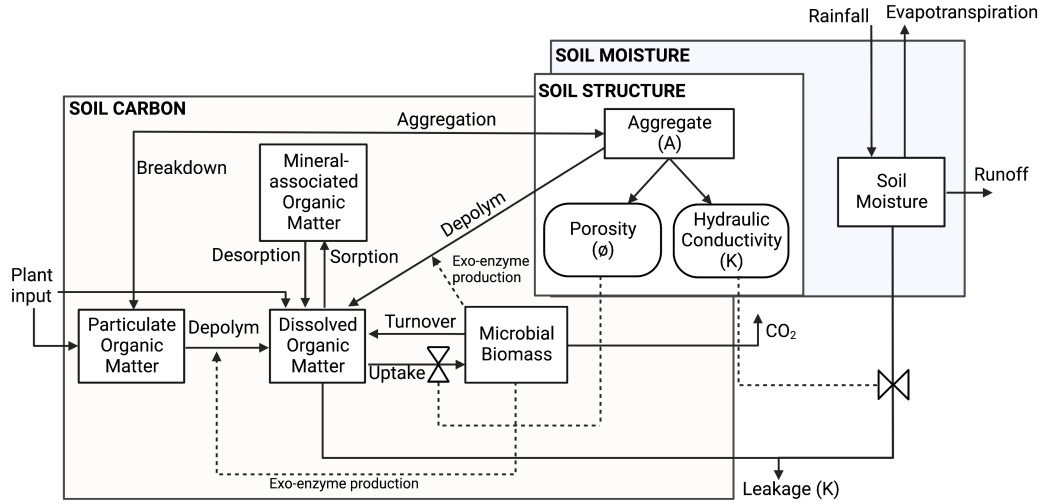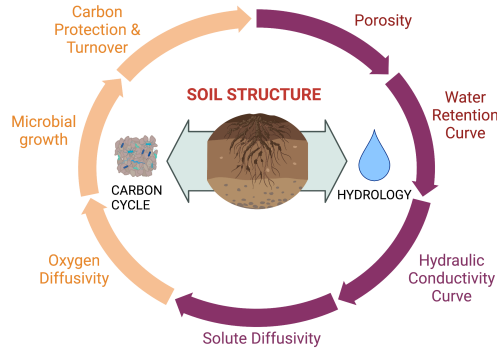

Figure 1. Schematic representing the linkage of soil structure dynamics with soil hydraulic properties, soil microbial activity and soil C cycle in the proposed framework.

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 (R. Abramoff et al., 2018; R. Z. Abramoff et al., 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 the aggregated
C. Such a framework provides an ideal starting point to investigate how land manage-
ment practices and climate change modify soil structure, in turn affecting microbial ac-
tivity and C sequestration and soil hydrologic processes.
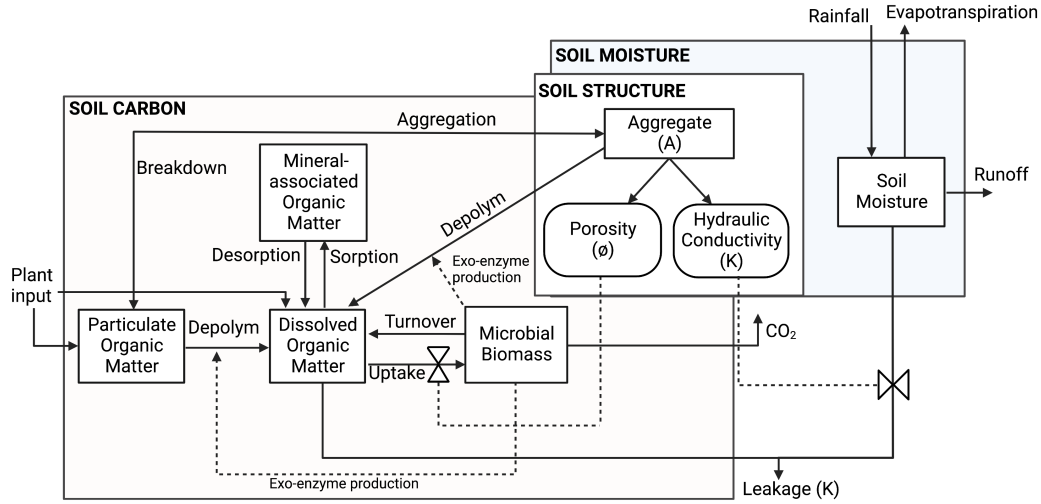
Figure 2.   Conceptual diagram of the theoretical framework linking a soil C module, soil
moisture module, and a soil structure module. The link is established through the aggregated C,
a soil C pool, which regulates the variability in soil hydraulic conductivity and porosity, hence
affecting the soil 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 Millennial model introduces a novel representation of soil C cycling based on
"measurable C pools" (R. Abramoff et al., 2018; R. Z. Abramoff et al., 2022), namely
the particulate organic matter (P), dissolved organic C (DOC), aggregate C (A), min-
eral associated C (M) and microbial biomass (B). Unlike traditional C models, which rely
on C pools defined by the chemical recalcitrant 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 depoly-
merization 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 dynam-

158 ics of the five C pools (namely P, DOC, A, M, and B) and describing the main inter-

159 actions between them, as illustrated in (Fig. 2). We briefly describe the model in the

160 Appendix, including some modifications from the original formulation that we introduced,

161 but we refer to R. Z. Abramoff et al. (2022) for more details. Below, we describe how

162 the Millennial model can be extended to account for the effects of soil structure on mi-

163 crobial activity and soil hydraulic properties.

3 Effect of soil structure on microbial activity

165 Changes in soil structural features affect the diffusion of C substrate and oxygen

166 to the soil microsites, hence impacting the activity of soil microbial communities. A pos-

167 sible approach to account for this is to adopt microbial growth laws that reflect the ac-

168 tual availability of substrate and oxygen in microsites, which in turn are controlled by

169 their ability to diffuse from the bulk soil (Moyano et al., 2013; Davidson et al., 2014).

170 Using the Michaelis-Menten kinetics, the microbial uptake (U) of DOC can be expressed

171 as (Moyano et al., 2013; Davidson et al., 2014)

$$U = U_{max} \frac{DOC_A}{DOC_A + K_{DOC}} \frac{O_{2_A}}{O_{2_A} + K_{O_2}} \tag{1}$$

172 where U_{max} is a maximum uptake rate, DOC_A and O_{2_A} are the concentrations of avail-

173 able DOC and O_2 in soil microsites, and K_{DOC} and K_{O_2} are half-saturation constants

174 for DOC and O_2, respectively. The availability of DOC and O_2 in the microsites is then

175 controlled by their diffusivities, which in turn depend on the soil pore structure includ-

176 ing the water-filled and air-filled pore networks and their connectivity at different wa-

177 ter saturation conditions. Following Yan et al. (2018), the DOC diffusivity, D_{DOC} nor-

178 malized to the diffusivity of pure water, $D_{0,DOC}$, can be expressed as

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

179 where ϕ is the soil porosity, m_s and n_s are cementation and saturation exponents (as-

180 suming values of 1.5 and 2 for structured soils, respectively) accounting for the effects

181 of the pore structure and water connectivity on DOC diffusion, θ is the moisture con-

182 tent, and p is a SOC-microorganisms collocation factor varying between 0 and 1. The

183 cementation exponent represents the pore connectivity and tortuosity while the satura-

184 tion exponent describes the effect of water saturation depending on the pore size distri-

185 bution of the soil. The collocation factor represents the degree of collocation between

186 the SOC and the microorganisms. The expression for the O_2 diffusivity takes a similar

187 form (Yan et al., 2018),

$$\frac{D_{O_2}}{D_{0,O_2}} = \phi^{(m_g - n_g)}(\theta - \phi)^{n_g} \tag{3}$$

188 where m_g and n_g are cementation and saturation exponents accounting for the effects

189 of the pore structure and water connectivity on O_2 diffusion, and D_{0,O_2} is the diffusiv-

190 ity in free air.

191 The concentrations, DOC_A and O_{2_A}, can then be expressed as proportional to the

192 bulk concentrations (DOC_b and O_b) through their respective diffusivity coefficients (Moyano

193 et al., 2013; Davidson et al., 2014), e.g., $DOC_A = DOC_b(D_{DOC}/D_{0,DOC}) = DOC_b\phi^{p(m_s - n_s)}\theta^{pn_s}$,

194 and substituting back in Eq. (1), the microbial uptake of the DOC can be expressed in

195 terms of soil porosity(ϕ) and water content(θ) as

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

196 The microbial uptake law, Eq. 4, accounts for how both soil structure (i.e., through

197 the cementation and saturation exponents and the soil porosity) and soil water content

198 control the availability of the C substrate and oxygen, hence regulating microbial activ-

199 ity (Fig. 3(a)).

4 Linking soil hydraulic properties to C cycling

4.1 Hydraulic properties of structured soils

202 In addition to affecting the diffusivities of the C substrate and O_2, soil structure

203 also introduces a bimodality in the soil pore size distribution, which affects both the wa-

204 ter 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 distribu-

tion (and water retention curve) the unsaturated hydraulic conductivity K can be es-

timated from the Mualem model (Mualem, 1976).

However, the Mualem model is based on the assumption that the pore system con-

sists 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,

$$\mathrm{K_{total}} = \mathrm{K_{s,tex}K_{r,tex}} + \mathrm{K_{s,str}K_{r,str}} \tag{5}$$

where $\mathrm{K_{s,tex}}$ and $\mathrm{K_{r,tex}}$ are the saturated and relative hydraulic conductivity, respectively,

for the textural pore spaces, and $\mathrm{K_{s,str}}$ and $\mathrm{K_{r,str}}$ are the saturated and relative hydraulic

conductivity, respectively, for the structural ones. Being independent, $\mathrm{K_{r,tex}}$ and $\mathrm{K_{r,str}}$

can be individually computed from the Mualem model.

Additionally, water in bimodal soils 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 (Fig. 3(b)). There-

fore, using for example the van Genuchten-Mualem model, K can be expressed as (Smettem

& Kirkby, 1990; B. Mohanty et al., 1997, 1998)

$$\mathrm{K_{total}} = \begin{cases} \mathrm{K_{s,tex}S_{e,tex}^{0.5}}[1 - (1 - \mathrm{S_{e,tex}^{1/a_{tex}}})^{a_{tex}}]^2, & \theta < \theta_m \\ \mathrm{K_{s,tex}} + \mathrm{K_{s,str}S_{e,str}^{0.5}}[1 - (1 - \mathrm{S_{e,str}^{1/a_{str}}})^{a_{str}}]^2, & \theta > \theta_m \end{cases} \tag{6}$$

where K_s is the saturated hydraulic conductivity, $\mathrm{a_{tex}}$ is the shape parameter of the hy-

draulic conductivity curve of the textural pore space, and $\mathrm{a_{str}}$ is the corresponding shape

parameter of the structure-modified hydraulic conductivity curve. Note that the effec-

tive saturation of the soil in the micropore ($\mathrm{S_{e,tex}}$) and the macropore systems ($\mathrm{S_{e,str}}$)

are relative to the corresponding porosities, $\mathrm{S_{e,tex}} = (\theta - \theta_r)/(\theta_m - \theta_r)$ and $\mathrm{S_{e,str}} = (\theta -$

$\theta_m)/(\theta_s - \theta_m)$, where θ_r is the residual water content, θ_s is the water content at satu-

ration (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}).

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, $K_{s,str}/K_{s,tex}$, is assumed to vary between 1 for low GPP to 1000 for high GPP (typical of tropical rain forests), and the ratio a_{str}/a_{tex} (see Eq. 6) was then estimated as a function of $K_{s,str}/K_{s,tex}$, varying from 0 for low $K_{s,str}/K_{s,tex}$ to 30 for high $K_{s,str}/K_{s,tex}$ values.

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 vary 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

255   can extend this approach to link the changes in soil hydraulic properties to the evolu-

256   tion of soil structure using the aggregated C (A, in the Millennial model) as a measure

257   of soil structure. The structural saturated hydraulic conductivity could be computed as

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

258   where $K_{s,tot}$ and $K_{s,tex}$ represent the maximum saturated hydraulic conductivity of a soil

259   with fully developed structure, which can be estimated from equation 9, and saturated

260   hydraulic conductivity of an unstructured/texture-only soil, respectively, and α and β

261   are shape parameters (Fig. 3(c)).

262   While the parameterization of Bonetti et al. (2021) focused on the hydraulic con-

263   ductivity, the generality of the adopted mathematical expressions is such that a similar

264   parameterization likely applies to porosity. Accordingly, the structural porosity may be
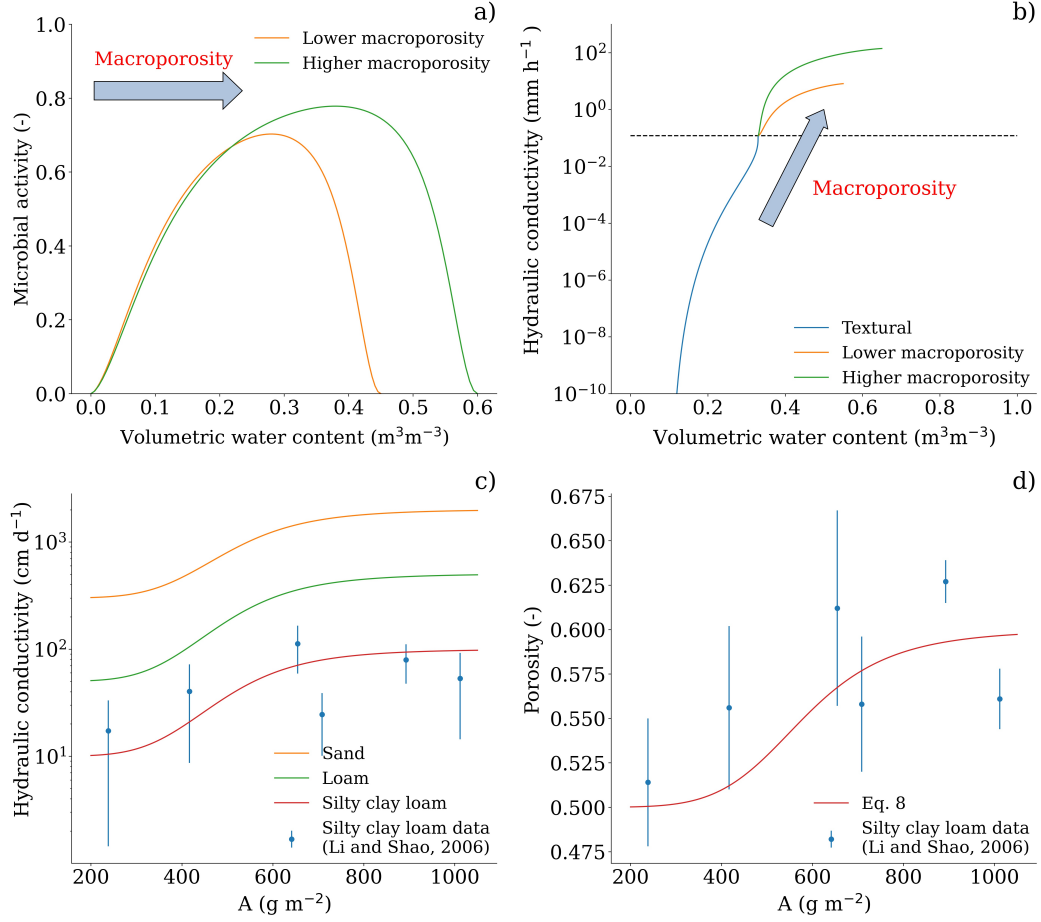
265   linked to A via

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

266   where ϕ_{tot} and ϕ_{tex} represent the maximum porosity of a soil with fully developed struc-

267   ture, and porosity of an unstructured/texture-only soil, respectively, and α and β are

268   shape parameters (Fig. 3(d)). Our case study below also suggests that a single set of α

269   and β may be needed for Eqs. 7 and 8.

270   Based on empirical evidence, Bonetti et al. (2021) expressed the $K_{s,tot}/K_{s,tex}$ ra-

271   tio as a function of the sand fraction,

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

272   where Sa is the sand fraction % in the soil. Linking the hydraulic parameterization by

273   Bonetti et al. (2021) to the Millennial model allows explicitly modeling the dynamics of

274   soil hydraulic properties as the soil structure evolves in response to environmental changes.

275   In particular, coupling the soil C cycling to the soil water balance (e.g., Laio et al. (2001b);

276   Pelak and Porporato (2019)) through the dynamics of soil structure and hydraulic prop-

277   erties, as introduced here, may be a significant step towards modeling more holistically

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 computed using Eqs. (7) and (9) with $\alpha = 580$ and $\beta = 6$ for various soil textural types: sand from Bonetti et al. (2021) (85% sand, $K_{s,tex} = 300$ cm d^{-1}, $K_{s,tot} = 2016.66$ cm d^{-1}), loam from Bonetti et al. (2021) (50% sand, $K_{s,tex} = 50$ cm d^{-1}, $K_{s,tot} = 506.54$ cm d^{-1}), silty clay loam from Li and Shao (2006) ($K_{s,tex} = 10$ cm d^{-1}, $K_{s,tot} = 100$ cm d^{-1}). d) Relation between porosity and aggregated C, computed using Eq. 8. Data from Li and Shao (2006).

278   soil processes as part of an integrated biochemical and physical system controlled by cli-
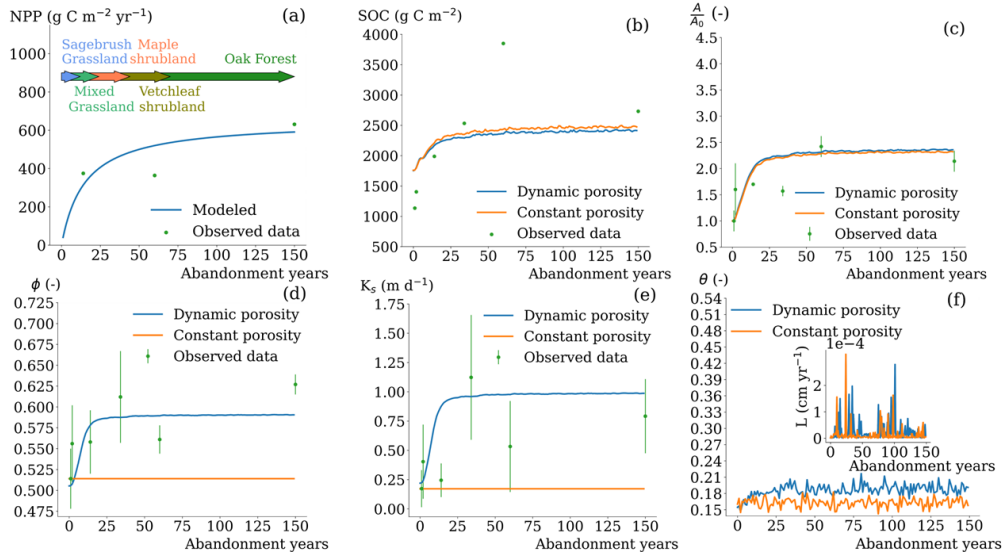
matic changes (such as rainfall, temperature, etc.) as well as human activities (e.g., land

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 used the mean weight diameter of soil aggregates as a proxy for aggregated C and represented it as a relative change ratio (A/A_0) with A_0 being the mean weight diameter at one year after abandonment. Soils were silty clay loam across the sites. We refer to Li & 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 (Fig. 4(a)). 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 statistics ob-

tained from Funk et al. (2015). Parameters related to the soil water balance were taken

from Laio et al. (2001a), except for measured porosity and hydraulic conductivity, while

parameters for the C module were taken from R. Abramoff et al. (2018) and R. Z. Abramoff

et al. (2022). These parameters were adjusted to capture observations from the site and

are provided in Table 1 of the supplementary information. After an initial spin up of 2000

years, we ran the model for 150 years with an hourly timestep and then aggregated the

results to yearly values for illustrative purposes.

Figure 4. Change in soil biophysical properties during the ecological succession from an abandoned cropland to forest: (a) Net primary productivity (NPP) for different vegetation recovery stages; (b) Soil organic C (SOC); (c) Relative aggregates ($\frac{A}{A_0}$) with A_0 corresponding to aggregate at one 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 the supplementary information.

As evident from the observations (Fig. 4), following abandonment, the soil under-
goes important biophysical changes, especially over the first twenty-five years. The in-
crease in vegetation productivity over the years provided larger inputs of organic mat-
ter (root exudates and litterfall) to the soil (Fig. 4(b)), which led to the formation of ag-
gregates (Fig. 4(c)) and mineral-associated organic matter (not shown here). As aggre-
gates form, the development of macroporosity can be seen from the increase in total poros-
ity and saturated hydraulic conductivity (Fig. 4(d) and (e)). 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) (Fig. 4(f)). A comparison with a simulation run using constant soil physi-
cal 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 pro-
cesses. In particular, the development of macroporosity increased the soil water content
on average but also accelerated the hydrologic cycle by increasing the percolation. How-
ever, 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 un-
der constant porosity conditions. 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 micro-
bial 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 chal-

341 lenge. Here, we built upon recent advances in soil C modeling and soil hydraulic param-

342 eterization to present an integrated modeling framework that can account for the effects

343 of soil structure on hydrologic and C cycling processes using the amount of aggregated

344 C as a proxy. In particular, aggregated C is here linked to the formation of macropores

345 with consequent increase in saturated hydraulic conductivity and changes in oxygen and

346 substrate diffusivity that affect microbial activity. The application to an abandoned crop-

347 land in the Loess Plateau of China showed the ability of the new framework to capture

348 soil regeneration following vegetation succession from cropland, to grassland, shrubland,

349 and ultimately forest and, overall, its potential to predict temporal changes in soil bio-

350 physical properties. The modeling framework can be particularly advantageous for ap-

351 plications involving land management practices and land-use changes.

352   Beyond making predictions, an advantage of using a modeling framework based on

353 measurable properties is that it can provide more physical, chemical, and biological-based

354 insights into system dynamics, especially given the fact that observations are not always

355 available. A model can identify drivers of changes in the soil organic C or explain dif-

356 ferences in C turnover times across different biomes, climates, and management factors.

357 For example, it can help assess when, based on climate and other soil factors, changes

358 in soil organic C are driven by physical protection/release of C within aggregates (e.g.,

359 due to no till/till), by sorption/desorption of microbial necromass in mineral surfaces (e.g.,

360 shifts in hydrologic regime), or a combination of the two. Interestingly, such a model could

361 be used to estimate soil organic C sequestration potentials across the globe, based on

362 both natural and anthropogenic drivers. The latter, however, would need to be explic-

363 itly incorporated as forcing in the model, for which more work is needed. Another im-

364 portant aspect, relevant to ecosystem ecology and water resources, is that the coupling

365 between C dynamics and hydraulic properties further allows to interpret and quantify

366 changes in soil hydrology over time, especially in response to land use changes. The case

367 study explored here is a good example in which soil recovery leads to increase water re-

tention within microporosity, but also more leakage due to macroporosity—an effect that cannot be quantitatively captured without the inclusion of soil structural effects.

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; Vezzani et al., 2018; Lucas et al., 2019), 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 (Moyano et al., 2013; Davidson et al., 2014; 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 soil organic C 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 (e.g., (Allison et al., 2010; Todd-Brown et al., 2012; Allison, 2014; Wieder et al., 2015; Sihi et al., 2016; Ballantyne IV & Billings, 2018; Sulman et al., 2018; Calabrese et al., 2022)). 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 (Prosser, 2015; Overy et al., 2021) into our proposed modeling framework might pave the way for a more holistic understanding of en-

vironmental changes and land use impacts on the soil system, in terms of structure (i.e.,

physical properties, heterogeneity), biological activity (i.e., microbial community com-

position, traits, C cycling), and their interaction (Kallenbach et al., 2019; Fatichi et al.,

2020; Bonetti et al., 2021; Sullivan et al., 2022).

7 Data Availability Statement

The Python codes for the modeling framework and the plots are available at

https://doi.org/10.4211/hs.6e4f08d8380a49f99314bae8a7ac41e2.

Appendix A Soil C model description

The novel Millennial model for soil C dynamics (R. Abramoff et al., 2018; R. Z. Abramoff

et al., 2022) is based on a system of equations of C transfer between five C pools: par-

ticulate organic matter (P), dissolved organic C (DOC), aggregate C (A), mineral-associated

organic matter (M) and microbial biomass (B) as shown in the conceptual diagram (Fig.

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,

$$\frac{d\mathrm{P}}{dt} = p_i F_i + F_a - F_{pa} - F_{pl}^p, \tag{A1}$$

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,

$$\frac{d\mathrm{A}}{dt} = F_{pa} - F_a - F_{pl}^a, \tag{A2}$$

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 aggrega-

tion.

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

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

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,

$$\frac{d\text{M}}{dt} = F_{lm} - F_{ld}, \qquad (A4)$$

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 (R. Z. Abramoff et al., 2021).

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

$$\frac{d\text{B}}{dt} = CUE \cdot U - F_{bm}, \qquad (A5)$$

where CUE is the C use efficiency, the microbial uptake of DOC (U), as described in (Eq.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 (R. Z. 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 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 two order of magnitude lower rate.

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. (2001b); Rodríguez-Iturbe and Porporato (2004), the soil moisture dynamics was modeled at the daily time scale by solving stochastic water balance differential equation:

$$Z_r \frac{d\phi_{\text{tot}} s}{dt} = R - I - Q - ET - L \tag{A6}$$

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

$$F_l = L\text{DOC}/(\phi Z_r s). \tag{A7}$$

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

Acknowledgments

References

Abramoff, R., Xu, X., Hartman, M., O'Brien, S., Feng, W., Davidson, E., ... Mayes, M. A. (2018, January). The Millennial model: in search of measurable pools and transformations for modeling soil carbon in the new century. *Biogeochemistry*, *137*(1), 51–71. Retrieved 2021-10-17, from https://doi.org/10.1007/s10533-017-0409-7 doi: 10.1007/s10533-017-0409-7

Abramoff, R. Z., Georgiou, K., Guenet, B., Torn, M. S., Huang, Y., Zhang, H., ... others (2021). How much carbon can be added to soil by sorption? *Biogeochemistry*, *152*(2), 127–142.

Abramoff, R. Z., Guenet, B., Zhang, H., Georgiou, K., Xu, X., Viscarra Rossel, R. A., ... Ciais, P. (2022, January). Improved global-scale predictions of soil carbon stocks with Millennial Version 2. *Soil Biology and Biochemistry*, *164*, 108466. Retrieved 2022-02-02, from https://www.sciencedirect.com/science/article/pii/S0038071721003400 doi: 10.1016/j.soilbio.2021.108466

Allison, S. D. (2014). Modeling adaptation of carbon use efficiency in microbial communities. *Frontiers in Microbiology*, *5*, 571.

Allison, S. D., Wallenstein, M. D., & Bradford, M. A. (2010). Soil-carbon response to warming dependent on microbial physiology. *Nature Geoscience*, *3*(5), 336–340.

Angers, D. A., & Caron, J. (1998, August). Plant-induced Changes in Soil Structure: Processes and Feedbacks. *Biogeochemistry*, *42*(1), 55–72. Retrieved 2022-06-14, from https://doi.org/10.1023/A:1005944025343 doi: 10.1023/A:1005944025343

Ballantyne IV, F., & Billings, S. A. (2018). Model formulation of microbial co2 production and efficiency can significantly influence short and long term soil c projections. *The ISME journal*, *12*(6), 1395–1403.

Beven, K., & Germann, P. (1982). Macropores and water flow in soils. *Wa-*

ter Resources Research, *18*(5), 1311–1325. Retrieved 2022-06-10, from https://onlinelibrary.wiley.com/doi/abs/10.1029/WR018i005p01311 (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/WR018i005p01311) doi: 10.1029/WR018i005p01311

Beven, K., & Germann, P. (2013). Macropores and water flow in soils revisited. *Water Resources Research*, *49*(6), 3071–3092. Retrieved 2022-06-10, from https://onlinelibrary.wiley.com/doi/abs/10.1002/wrcr.20156 (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/wrcr.20156) doi: 10.1002/wrcr.20156

Bodner, G., Mentler, A., & Keiblinger, K. (2021). Plant Roots for Sustainable Soil Structure Management in Cropping Systems. In *The Root Systems in Sustainable Agricultural Intensification* (pp. 45–90). John Wiley & Sons, Ltd. Retrieved 2022-06-14, from https://onlinelibrary.wiley.com/doi/abs/10.1002/9781119525417.ch3 (Section: 3 _eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/9781119525417.ch3) doi: 10.1002/9781119525417.ch3

Bonetti, S., Wei, Z., & Or, D. (2021, December). A framework for quantifying hydrologic effects of soil structure across scales. *Communications Earth & Environment*, *2*(1), 107. Retrieved 2021-10-17, from http://www.nature.com/articles/s43247-021-00180-0 doi: 10.1038/s43247-021-00180-0

Borrelli, P., Robinson, D. A., Panagos, P., Lugato, E., Yang, J. E., Alewell, C., . . . Ballabio, C. (2020, September). Land use and climate change impacts on global soil erosion by water (2015-2070). *Proceedings of the National Academy of Sciences*, *117*(36), 21994–22001. Retrieved 2021-10-18, from http://www.pnas.org/lookup/doi/10.1073/pnas.2001403117 doi: 10.1073/pnas.2001403117

Brady, N. C., & Weil, R. R. (2008). *The nature and properties of soils* (Vol. 13). Prentice Hall Upper Saddle River, NJ.

Bronick, C. J., & Lal, R.   (2005, January).   Soil structure and management: a review.   *Geoderma*, *124*(1), 3–22.   Retrieved 2021-10-18, from `https://www.sciencedirect.com/science/article/pii/S0016706104000898`   doi: 10.1016/j.geoderma.2004.03.005

Cagnarini, C., Blyth, E., Emmett, B. A., Evans, C. D., Griffiths, R. I., Keith, A., . . . Cosby, B. J.   (2019).   Zones of influence for soil organic matter dynamics: A conceptual framework for data and models.   *Global Change Biology*, *25*(12), 3996–4007.   Retrieved 2022-08-08, from `https://onlinelibrary.wiley.com/doi/abs/10.1111/gcb.14787`   (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/gcb.14787)   doi: 10.1111/gcb.14787

Calabrese, S., Mohanty, B. P., & Malik, A. A.   (2022).   Soil microorganisms regulate extracellular enzyme production to maximize their growth rate.   *Biogeochemistry*, *158*(3), 303–312.

Chakrawal, A., Herrmann, A. M., Koestel, J., Jarsjö, J., Nunan, N., Kätterer, T., & Manzoni, S.   (2020).   Dynamic upscaling of decomposition kinetics for carbon cycling models.   *Geoscientific Model Development*, *13*(3), 1399–1429.

Chandrasekhar, P., Kreiselmeier, J., Schwen, A., Weninger, T., Julich, S., Feger, K.-H., & Schwärzel, K.   (2018, December).   Why We Should Include Soil Structural Dynamics of Agricultural Soils in Hydrological Models.   *Water*, *10*(12), 1862.   Retrieved 2022-06-13, from `https://www.mdpi.com/2073-4441/10/12/1862`   (Number: 12 Publisher: Multidisciplinary Digital Publishing Institute)   doi: 10.3390/w10121862

Conant, R. T., Ryan, M. G., Ågren, G. I., Birge, H. E., Davidson, E. A., Eliasson, P. E., . . . others   (2011).   Temperature and soil organic matter decomposition rates–synthesis of current knowledge and a way forward.   *Global Change Biology*, *17*(11), 3392–3404.

Davidson, E. A., Savage, K. E., & Finzi, A. C.   (2014).   A big-microsite framework

for soil carbon modeling. *Global Change Biology*, *20*(12), 3610–3620. Retrieved 2021-09-26, from `https://onlinelibrary.wiley.com/doi/abs/10.1111/gcb` `.12718` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/gcb.12718) doi: 10.1111/gcb.12718

Dexter, A. R. (1988, June). Advances in characterization of soil structure. *Soil and Tillage Research*, *11*(3), 199–238. Retrieved 2022-06-09, from `https://` `www.sciencedirect.com/science/article/pii/0167198788900025` doi: 10 .1016/0167-1987(88)90002-5

Durner, W. (1994). Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resources Research*, *30*(2), 211–223. Retrieved 2021-10-18, from `https://onlinelibrary.wiley.com/doi/abs/10.1029/93WR02676` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/93WR02676) doi: 10.1029/93WR02676

Ebrahimi, A., & Or, D. (2018). On Upscaling of Soil Microbial Processes and Biogeochemical Fluxes From Aggregates to Landscapes. *Journal of Geophysical Research: Biogeosciences*, *123*(5), 1526–1547. Retrieved 2022-08-08, from `https://onlinelibrary.wiley.com/doi/abs/10.1029/2017JG004347` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/2017JG004347) doi: 10.1029/2017JG004347

Fatichi, S., Or, D., Walko, R., Vereecken, H., Young, M. H., Ghezzehei, T. A., . . . Avissar, R. (2020, January). Soil structure is an important omission in Earth System Models. *Nature Communications*, *11*(1), 522. Retrieved 2021-07-26, from `https://www.nature.com/articles/s41467-020-14411-z` (Bandiera_abtest: a Cc_license_type: cc_by Cg_type: Nature Research Journals Number: 1 Primary_atype: Research Publisher: Nature Publishing Group Subject_term: Climate sciences;Hydrology Subject_term_id: climate-sciences;hydrology) doi: 10.1038/s41467-020-14411-z

Franklin, S. M., Kravchenko, A. N., Vargas, R., Vasilas, B., Fuhrmann, J. J., &

Jin, Y.   (2021, October).   The unexplored role of preferential flow in soil carbon dynamics.   *Soil Biology and Biochemistry*, *161*, 108398.   Retrieved 2022-08-08, from `https://www.sciencedirect.com/science/article/pii/S0038071721002728`   doi: 10.1016/j.soilbio.2021.108398

Funk, C., Peterson, P., Landsfeld, M., Pedreros, D., Verdin, J., Shukla, S., . . . others   (2015).   The climate hazards infrared precipitation with stations—a new environmental record for monitoring extremes. *Scientific data*, *2*(1), 1–21.

Golchin, A., Oades, J. M., Skjemstad, J. O., & Clarke, P. (1994). Soil structure and carbon cycling.   *Soil Research*, *32*(5), 1043–1068.   Retrieved 2022-06-14, from `https://www.publish.csiro.au/sr/sr9941043`   (Publisher: CSIRO PUBLISHING) doi: 10.1071/sr9941043

Hirmas, D. R., Giménez, D., Nemes, A., Kerry, R., Brunsell, N. A., & Wilson, C. J.   (2018, September).   Climate-induced changes in continental-scale soil macroporosity may intensify water cycle.   *Nature*, *561*(7721), 100–103.   Retrieved 2022-06-16, from `https://www.nature.com/articles/s41586-018-0463-x`   (Number: 7721 Publisher: Nature Publishing Group) doi: 10.1038/s41586-018-0463-x

Jungkunst, H. F., Göpel, J., Horvath, T., Ott, S., & Brunn, M.   (2022).   Global soil organic carbon–climate interactions: Why scales matter.   *WIREs Climate Change*, *13*(4), e780.   Retrieved 2022-08-08, from `https://onlinelibrary.wiley.com/doi/abs/10.1002/wcc.780`   (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/wcc.780)   doi: 10.1002/wcc.780

Kallenbach, C. M., Wallenstein, M. D., Schipanksi, M. E., & Grandy, A. S.   (2019). Managing agroecosystems for soil microbial carbon use efficiency: ecological unknowns, potential outcomes, and a path forward. *Frontiers in Microbiology*, *10*, 1146.

Kutílek, M.   (2004, December).   Soil hydraulic properties as related to soil

655 structure. *Soil and Tillage Research*, *79*(2), 175–184. Retrieved 2022-

656 06-10, from https://www.sciencedirect.com/science/article/pii/

657 S0167198704001436 doi: 10.1016/j.still.2004.07.006

658 Laio, F., Porporato, A., Ridolfi, L., & Rodriguez-Iturbe, I. (2001a). Plants in

659 water-controlled ecosystems: active role in hydrologic processes and response

660 to water stress: Ii. probabilistic soil moisture dynamics. *Advances in Water*

661 *Resources*, *24*(7), 707–723.

662 Laio, F., Porporato, A., Ridolfi, L., & Rodriguez-Iturbe, I. (2001b, July). Plants

663 in water-controlled ecosystems: active role in hydrologic processes and re-

664 sponse to water stress: II. Probabilistic soil moisture dynamics. *Advances*

665 *in Water Resources*, *24*(7), 707–723. Retrieved 2021-10-17, from https://

666 www.sciencedirect.com/science/article/pii/S0309170801000057 doi:

667 10.1016/S0309-1708(01)00005-7

668 Lal, R. (1993, October). Tillage effects on soil degradation, soil resilience, soil

669 quality, and sustainability. *Soil and Tillage Research*, *27*(1), 1–8. Retrieved

670 2021-10-18, from https://www.sciencedirect.com/science/article/pii/

671 016719879390059X doi: 10.1016/0167-1987(93)90059-X

672 Lal, R. (2004, November). Soil carbon sequestration to mitigate climate

673 change. *Geoderma*, *123*(1), 1–22. Retrieved 2021-10-18, from https://

674 www.sciencedirect.com/science/article/pii/S0016706104000266 doi:

675 10.1016/j.geoderma.2004.01.032

676 Lal, R. (2012, September). Climate Change and Soil Degradation Mitigation by

677 Sustainable Management of Soils and Other Natural Resources. *Agricultural*

678 *Research*, *1*(3), 199–212. Retrieved 2021-10-18, from http://link.springer

679 .com/10.1007/s40003-012-0031-9 doi: 10.1007/s40003-012-0031-9

680 Larson, W. E., Blake, G. R., Allmaras, R. R., Voorhees, W. B., & Gupta, S. C.

681 (Eds.). (1989). *Mechanics and Related Processes in Structured Agri-*

682 *cultural Soils*. Dordrecht: Springer Netherlands. Retrieved 2022-06-10,

683   from `http://link.springer.com/10.1007/978-94-009-2421-5`   doi:

684   10.1007/978-94-009-2421-5

685   Lehmann, J., & Kleber, M.   (2015).   The contentious nature of soil organic matter.

686   *Nature*, *528*(7580), 60–68.

687   Li, Y. Y., & Shao, M. A. (2006, January). Change of soil physical properties under

688   long-term natural vegetation restoration in the Loess Plateau of China.   *Jour-*

689   *nal of Arid Environments*, *64*(1), 77–96. Retrieved 2021-12-10, from `https://`

690   `www.sciencedirect.com/science/article/pii/S0140196305001072` doi: 10

691   .1016/j.jaridenv.2005.04.005

692   Liang, C., Schimel, J. P., & Jastrow, J. D.   (2017).   The importance of anabolism in

693   microbial control over soil carbon storage. *Nature microbiology*, *2*(8), 1–6.

694   Lipper, L., Thornton, P., Campbell, B. M., Baedeker, T., Braimoh, A., Bwalya, M.,

695   . . . others (2014). Climate-smart agriculture for food security. *Nature climate*

696   *change*, *4*(12), 1068–1072.

697   Lucas, M., Schlüter, S., Vogel, H.-J., & Vetterlein, D.   (2019, November).   Roots

698   compact the surrounding soil depending on the structures they encounter. *Sci-*

699   *entific Reports*, *9*(1), 16236. Retrieved 2022-06-14, from `https://www.nature`

700   `.com/articles/s41598-019-52665-w` (Number: 1 Publisher: Nature Publish-

701   ing Group) doi: 10.1038/s41598-019-52665-w

702   Manzoni, S., & Porporato, A. (2009, July). Soil carbon and nitrogen mineralization:

703   Theory and models across scales.   *Soil Biology and Biochemistry*, *41*(7), 1355–

704   1379. Retrieved 2022-06-15, from `https://www.sciencedirect.com/science/`

705   `article/pii/S0038071709000765` doi: 10.1016/j.soilbio.2009.02.031

706   Meurer, K., Barron, J., Chenu, C., Coucheney, E., Fielding, M., Hallett, P., . . .

707   Jarvis, N. (2020). A framework for modelling soil structure dynamics induced

708   by biological activity.   *Global Change Biology*, *26*(10), 5382–5403.   Retrieved

709   2021-10-18, from `https://onlinelibrary.wiley.com/doi/abs/10.1111/gcb`

710   `.15289`   (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/gcb.15289)

711   doi: 10.1111/gcb.15289

712 Mohanty, B., Bowman, R., Hendrickx, J., & Van Genuchten, M. T.   (1997).   New

713   piecewise-continuous hydraulic functions for modeling preferential flow in an

714   intermittent-flood-irrigated field.   *Water Resources Research*, *33*(9), 2049–

715   2063.

716 Mohanty, B., Skaggs, T., & Van Genuchten, M. T.   (1998).   Impact of saturated

717   hydraulic conductivity on the prediction of tile flow.   *Soil Science Society of*

718   *America Journal*, *62*(6), 1522–1529.

719 Mohanty, B. P.   (1999).   Scaling hydraulic properties of a macroporous soil.   *Wa-*

720   *ter Resources Research*, *35*(6), 1927–1931.   Retrieved 2021-10-18, from

721   https://onlinelibrary.wiley.com/doi/abs/10.1029/1999WR900050

722   (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/1999WR900050)

723   doi: 10.1029/1999WR900050

724 Moyano, F. E., Manzoni, S., & Chenu, C.   (2013, April).   Responses of soil het-

725   erotrophic respiration to moisture availability: An exploration of processes

726   and models.   *Soil Biology and Biochemistry*, *59*, 72–85.   Retrieved 2021-

727   08-25, from https://www.sciencedirect.com/science/article/pii/

728   S0038071713000138 doi: 10.1016/j.soilbio.2013.01.002

729 Mualem, Y.   (1976).   A new model for predicting the hydraulic conduc-

730   tivity of unsaturated porous media.   *Water Resources Research*,

731   *12*(3), 513–522.   Retrieved 2021-09-13, from https://onlinelibrary

732   .wiley.com/doi/abs/10.1029/WR012i003p00513   (_eprint:

733   https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/WR012i003p00513)

734   doi: 10.1029/WR012i003p00513

735 Or, D., & Ghezzehei, T. A.   (2002, February).   Modeling post-tillage soil struc-

736   tural dynamics: a review.   *Soil and Tillage Research*, *64*(1), 41–59.   Retrieved

737   2022-06-09, from https://www.sciencedirect.com/science/article/pii/

738   S0167198701002562 doi: 10.1016/S0167-1987(01)00256-2

Or, D., Keller, T., & Schlesinger, W. H. (2021, April). Natural and managed soil structure: On the fragile scaffolding for soil functioning. *Soil and Tillage Research*, *208*, 104912. Retrieved 2021-10-18, from `https://www.sciencedirect.com/science/article/pii/S0167198720306942` doi: 10.1016/j.still.2020.104912

Overy, D. P., Bell, M. A., Habtewold, J., Helgason, B. L., & Gregorich, E. G. (2021). "omics" technologies for the study of soil carbon stabilization: A review. *Frontiers in Environmental Science*, *9*, 617952.

Parton, W. J., Hartman, M., Ojima, D., & Schimel, D. (1998, December). DAYCENT and its land surface submodel: description and testing. *Global and Planetary Change*, *19*(1), 35–48. Retrieved 2021-10-18, from `https://www.sciencedirect.com/science/article/pii/S092181819800040X` doi: 10.1016/S0921-8181(98)00040-X

Pelak, N., & Porporato, A. (2019). Dynamic evolution of the soil pore size distribution and its connection to soil management and biogeochemical processes. *Advances in Water Resources*, *131*. doi: 10.1016/j.advwatres.2019.103384

Porporato, A., Feng, X., Manzoni, S., Mau, Y., Parolari, A. J., & Vico, G. (2015). Ecohydrological modeling in agroecosystems: Examples and challenges. *Water Resources Research*, *51*(7), 5081–5099.

Powlson, D. S., Smith, P., & Smith, J. U. (Eds.). (1996). *Evaluation of Soil Organic Matter Models: Using Existing Long-Term Datasets.* Berlin, Heidelberg: Springer Berlin Heidelberg. Retrieved 2021-10-19, from `http://link.springer.com/10.1007/978-3-642-61094-3` doi: 10.1007/978-3-642-61094-3

Prosser, J. I. (2015). Dispersing misconceptions and identifying opportunities for the use of 'omics' in soil microbial ecology. *Nature Reviews Microbiology*, *13*(7), 439–446.

Rabot, E., Wiesmeier, M., Schlüter, S., & Vogel, H. J. (2018, March). Soil structure

as an indicator of soil functions: A review. *Geoderma*, *314*, 122–137. Retrieved 2022-03-03, from `https://www.sciencedirect.com/science/article/pii/` `S0016706117310273` doi: 10.1016/j.geoderma.2017.11.009

Robertson, A. D., Paustian, K., Ogle, S., Wallenstein, M. D., Lugato, E., & Cotrufo, M. F. (2019, March). Unifying soil organic matter formation and persistence frameworks: the MEMS model. *Biogeosciences*, *16*(6), 1225–1248. Retrieved 2022-06-15, from `https://bg.copernicus.org/articles/16/1225/2019/` (Publisher: Copernicus GmbH) doi: 10.5194/bg-16-1225-2019

Rodríguez-Iturbe, I., & Porporato, A. (2004). *Ecohydrology of water-controlled ecosystems: soil moisture and plant dynamics.* Cambridge University Press.

Romero-Ruiz, A., Linde, N., Keller, T., & Or, D. (2018). A Review of Geophysical Methods for Soil Structure Characterization. *Reviews of Geophysics*, *56*(4), 672–697. Retrieved 2022-06-09, from `https://` `onlinelibrary.wiley.com/doi/abs/10.1029/2018RG000611` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/2018RG000611) doi: 10.1029/2018RG000611

Schlüter, S., Leuther, F., Albrecht, L., Hoeschen, C., Kilian, R., Surey, R., . . . Vogel, H.-J. (2022). Microscale carbon distribution around pores and particulate organic matter varies with soil moisture regime. *Nature communications*, *13*(1), 1–14.

Shi, A., Chakrawal, A., Manzoni, S., Fischer, B. M., Nunan, N., & Herrmann, A. M. (2021). Substrate spatial heterogeneity reduces soil microbial activity. *Soil Biology and Biochemistry*, *152*, 108068.

Sihi, D., Gerber, S., Inglett, P. W., & Inglett, K. S. (2016, March). Comparing models of microbial–substrate interactions and their response to warming. *Biogeosciences*, *13*(6), 1733–1752. Retrieved 2021-08-27, from `https://bg.copernicus.org/articles/13/1733/2016/` (Publisher: Copernicus GmbH) doi: 10.5194/bg-13-1733-2016

Smettem, K. R. J., & Kirkby, C. (1990, September). Measuring the hydraulic properties of a stable aggregated soil. *Journal of Hydrology*, *117*(1), 1–13. Retrieved 2021-10-17, from `https://www.sciencedirect.com/science/article/pii/002216949090084B` doi: 10.1016/0022-1694(90)90084-B

Sullivan, P., Billings, S., Hirmas, D., Li, L., Zhang, X., Ziegler, S., . . . others (2022). Embracing the dynamic nature of soil structure: A paradigm illuminating the role of life in critical zones of the anthropocene. *Earth-Science Reviews*, *225*, 103873.

Sulman, B. N., Moore, J. A., Abramoff, R., Averill, C., Kivlin, S., Georgiou, K., . . . others (2018). Multiple models and experiments underscore large uncertainty in soil carbon dynamics. *Biogeochemistry*, *141*(2), 109–123.

Todd-Brown, K. E. O., Hopkins, F. M., Kivlin, S. N., Talbot, J. M., & Allison, S. D. (2012, July). A framework for representing microbial decomposition in coupled climate models. *Biogeochemistry*, *109*(1), 19–33. Retrieved 2021-10-19, from `https://doi.org/10.1007/s10533-011-9635-6` doi: 10.1007/s10533-011-9635-6

Tuller, M., & Or, D. (2001). Hydraulic conductivity of variably saturated porous media: Film and corner flow in angular pore space. *Water Resources Research*, *37*(5), 1257–1276. Retrieved 2021-10-18, from `https://onlinelibrary.wiley.com/doi/abs/10.1029/2000WR900328` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/2000WR900328) doi: 10.1029/2000WR900328

Vezzani, F. M., Anderson, C., Meenken, E., Gillespie, R., Peterson, M., & Beare, M. H. (2018, January). The importance of plants to development and maintenance of soil structure, microbial communities and ecosystem functions. *Soil and Tillage Research*, *175*, 139–149. Retrieved 2022-06-14, from `https://www.sciencedirect.com/science/article/pii/S0167198717301691` doi: 10.1016/j.still.2017.09.002

Weynants, M., Vereecken, H., & Javaux, M. (2009). Revisiting vereecken pedotransfer functions: Introducing a closed-form hydraulic model. *Vadose Zone Journal*, *8*(1), 86–95.

Wieder, W. R., Allison, S. D., Davidson, E. A., Georgiou, K., Hararuk, O., He, Y., ... others (2015). Explicitly representing soil microbial processes in earth system models. *Global Biogeochemical Cycles*, *29*(10), 1782–1800.

Wilson, C. H., & Gerber, S. (2021). Theoretical insights from upscaling michaelis–menten microbial dynamics in biogeochemical models: a dimensionless approach. *Biogeosciences*, *18*(20), 5669–5679.

Xie, B., Qin, Z., Wang, Y., & Chang, Q. (2014, January). Spatial and temporal variation in terrestrial net primary productivity on Chinese Loess Plateau and its influential factors. *Transactions of the Chinese Society of Agricultural Engineering*, *30*(11), 244–253.

Yan, Z., Bond-Lamberty, B., Todd-Brown, K. E., Bailey, V. L., Li, S., Liu, C., & Liu, C. (2018, July). A moisture function of soil heterotrophic respiration that incorporates microscale processes. *Nature Communications*, *9*(1), 2562. Retrieved 2021-08-25, from `https://www.nature.com/articles/s41467-018-04971-6` (Bandiera_abtest: a Cc_license_type: cc_by Cg_type: Nature Research Journals Number: 1 Primary_atype: Research Publisher: Nature Publishing Group Subject_term: Carbon cycle Subject_term_id: carbon-cycle) doi: 10.1038/s41467-018-04971-6

Young, I. M., Blanchart, E., Chenu, C., Dangerfield, M., Fragoso, C., Grimaldi, M., ... Monrozier, L. J. (1998). The interaction of soil biota and soil structure under global change. *Global Change Biology*, *4*(7), 703–712. Retrieved 2022-06-10, from `https://onlinelibrary.wiley.com/doi/abs/10.1046/j.1365-2486.1998.00194.x` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1046/j.1365-2486.1998.00194.x) doi: 10.1046/j.1365-2486.1998.00194.x

851   Zurmühl, T., & Durner, W. (1996). Modeling Transient Water

852   and Solute Transport in a Biporous Soil. *Water Resources Re-*

853   *search*, *32*(4), 819–829. Retrieved 2021-09-13, from `https://`

854   `onlinelibrary.wiley.com/doi/abs/10.1029/95WR01678` (_eprint:

855   https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/95WR01678) doi:

856   10.1029/95WR01678

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

Achla Jha[1], Sara Bonetti[2], A. Peyton Smith[3], Rodolfo Souza[1], Salvatore Calabrese[1]

[1]Department of Biological and Agricultural Engineering, Texas A&M University, College Station, TX, USA

[2]School of Architecture, Civil and Environmental Engineering, Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

[3]Department of Soil and Crop Sciences, Texas A&M University, College Station, TX, USA

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.

Corresponding author: Salvatore Calabrese, `salvatore.calabrese@ag.tamu.edu`

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 soil carbon substrate and O_2 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(Lal, 1993, 2012; Brady & Weil, 2008; Borrelli et al., 2020). 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 (Young et al., 1998; Lipper et al., 2014). Nevertheless, little information about soil structure dynamics, factors that affect it, and its link to soil biogeochemical cycles is included in current ecohydrological models (Pelak & Porporato, 2019; Meurer et al., 2020), making it difficult to predict the short- and long-term impact of soil structure alteration on ecosystem water and C 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.

72   Soil structure derives from the accumulation of organic matter and formation of

73 soil aggregates due to plant roots, fungal hyphae, and biological activity (Golchin et al.,

74 1994; Young et al., 1998; Lal, 2004). This aggregation in turn gives rise to structural macro-

75 porosity that may increase soil hydraulic conductivity by multiple orders of magnitude,

76 especially in fine-textured soils where micropores are intrinsically abundant (Zurmühl

77 & Durner, 1996; Beven & Germann, 2013; Bonetti et al., 2021). Aggregation also con-

78 trols microbial activity by affecting the accessibility of the organic substrate by microbes

79 and the diffusivity of gases (e.g., O_2, CO_2) within the soil matrix (Moyano et al., 2013;

80 Yan et al., 2018; Meurer et al., 2020). These inter-linkages between soil organic C dy-

81 namics, soil hydrology, and microbial activity demonstrate the need to develop novel quan-

82 titative approaches that explicitly account for soil structure and how this is affected by

83 climate and land-use.

84   While the effects of soil structure and macroposity on soil hydrology are well-known,

85 measures of soil structure that can inform about its dynamics are missing (Beven & Ger-

86 mann, 1982; Dexter, 1988; Larson et al., 1989; Kutílek, 2004). Macroporosity often gives

87 rise to a bi-model pore size distribution, which is visible in water retention and hydraulic

88 conductivity curves (Durner, 1994; B. P. Mohanty, 1999; Tuller & Or, 2001). Measur-

89 ing these curves, however, provides information at a specific location and cannot be eas-

90 ily generalizable, e.g., to large scales relevant for Land Surface Models applications or

91 areas with limited soil data. To address this limitation, the work by Fatichi et al.(2020)

92 and Bonetti et al.(2021) proposed the use of vegetation metrices (e.g., Gross Primary

93 Productivity (GPP), aboveground vegetation biomass, Leaf Area Index (LAI)) as sur-

94 rogates for soil structure modifications of soil hydraulic properties. These works refined

95 the representation of soil hydrological processes in Land Surface models by allowing a

96 two-way interaction between natural vegetation and soil hydraulic properties. However,

97 these frameworks are mostly applicable to unmanaged soils, where plant rooting systems,

98 and therefore vegetation cover, primarily control the development of soil structure. They

99 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) (Cagnarini et al., 2019; Or et al., 2021; Fatichi et al.,

2020; Bonetti et al., 2021). Additionally, while vegetation may predominantly influence

soil hydrology on large scales, e.g., field to regional, soil aggregates are the primary drivers

of soil hydraulic properties and biogeochemical cycles on the pedon scale (Kutílek, 2004;

Ebrahimi & Or, 2018; Franklin et al., 2021; Jungkunst et al., 2022). This highlights the

necessity of introducing additional measures of soil structure, beyond the vegetation in-

dexes, 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 (R. Abramoff et al., 2018; R. Z. Abramoff et al., 2022) ex-

plicitly considers the dynamics of "measurable" C pools, representing a major advance-

ment from traditional C models based on the CENTURY framework, such as the DAY-

CENT (Parton et al., 1998) and the DeNitrification-DeComposition (DNDC) models (Powlson

et al., 1996), which conceptualize the soil organic C in different C pools with presumed

turnover times. Measurable pools include the C in the microbial biomass, the particu-

late organic matter (e.g., leaves, roots), the fraction of dissolved organic C (DOC) ad-

sorbed 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, the aggregated C may serve as a good proxy

for soil structure. The "Millennial Model" approach also provides a process-based rep-

resentation of the biological, chemical, and physical processes that affect the C occluded

within the soil aggregates (such as formation and breakdown of aggregates), thus offer-

ing an opportunity to link soil hydraulic parameterization (i.e. soil hydraulic conduc-

tivity) to the temporal evolution of soil structure. This linkage may pave the way for quan-

tifying how structure affects microbial dynamics, if appropriate microbial growth laws

considering soil structural features are adopted (e.g., Yan et al. (2018)).

127   Here we provide a framework for the integrated study of soil structure and hydrol-

128 ogy, with microbial and C dynamics in response to natural and human-induced environ-

129 mental changes across time scales. Our framework couples the parameterization of soil

130 hydraulic properties for soil water balance models to the Millennial model (R. Abramoff

131 et al., 2018; R. Z. Abramoff et al., 2022)(Fatichi et al., 2020; Bonetti et al., 2021) for soil

132 C cycling. We then demonstrate the potential of this integrated framework by apply-

133 ing it to a case study of natural recovery of soils in an abandoned farmland. We conclude

134 by highlighting critical aspects that require further investigation as well as opportuni-

135 ties for future research.

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.

2 The Millennial model approach for soil structure dynamics

137   While traditional ecohydrological models consider soils as a rigid element with con-

138 stant soil properties (Manzoni & Porporato, 2009; Robertson et al., 2019), land use changes

139 and management practices such as tillage, reforestation, crop rotation, and land use con-

140 versions can alter soil structural features (pore and aggregate size distribution) over dif-

141 ferent time scales (Chandrasekhar et al., 2018). To extend ecohydrologic models and ac-

142 count for these effects, soil structural features need to be included as prognostic variables.

143 The Millennial model approach (R. Abramoff et al., 2018; R. Z. Abramoff et al., 2022)

144 is particularly useful, as it explicitly simulates different C pools and processes that are

145 good indicators of soil structure, such as the formation and breakdown of the aggregated

146 C. Such a framework provides an ideal starting point to investigate how land manage-

147 ment practices and climate change modify soil structure, in turn affecting microbial ac-

148 tivity and C sequestration and soil hydrologic processes.

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.

149 The Millennial model introduces a novel representation of soil C cycling based on

150 "measurable C pools" (R. Abramoff et al., 2018; R. Z. Abramoff et al., 2022), namely

151 the particulate organic matter (P), dissolved organic C (DOC), aggregate C (A), min-

152 eral associated C (M) and microbial biomass (B). Unlike traditional C models, which rely

153 on C pools defined by the chemical recalcitrant of the organic C, the Millennial model

154 aims to emphasize the important roles that C aggregation and interaction with mineral

155 surfaces and microbial processes (e.g., production of extracellular enzymes and depoly-

156 merization of high molecular weight C compounds) play on soil C cycling. The model

157 is framed as a system of five mass balance differential equations governing the dynam-

158 ics of the five C pools (namely P, DOC, A, M, and B) and describing the main inter-

159 actions between them, as illustrated in (Fig. 2). We briefly describe the model in the

160 Appendix, including some modifications from the original formulation that we introduced,

161 but we refer to R. Z. Abramoff et al. (2022) for more details. Below, we describe how

162 the Millennial model can be extended to account for the effects of soil structure on mi-

163 crobial activity and soil hydraulic properties.

3 Effect of soil structure on microbial activity

165 Changes in soil structural features affect the diffusion of C substrate and oxygen

166 to the soil microsites, hence impacting the activity of soil microbial communities. A pos-

167 sible approach to account for this is to adopt microbial growth laws that reflect the ac-

168 tual availability of substrate and oxygen in microsites, which in turn are controlled by

169 their ability to diffuse from the bulk soil (Moyano et al., 2013; Davidson et al., 2014).

170 Using the Michaelis-Menten kinetics, the microbial uptake (U) of DOC can be expressed

171 as (Moyano et al., 2013; Davidson et al., 2014)

$$U = U_{\max} \frac{DOC_A}{DOC_A + K_{DOC}} \frac{O_{2_A}}{O_{2_A} + K_{O_2}} \tag{1}$$

172 where $U_{\max}$ is a maximum uptake rate, DOC_A and O_{2_A} are the concentrations of avail-

173 able DOC and O_2 in soil microsites, and K_{DOC} and K_{O_2} are half-saturation constants

174 for DOC and O_2, respectively. The availability of DOC and O_2 in the microsites is then

175 controlled by their diffusivities, which in turn depend on the soil pore structure includ-

176 ing the water-filled and air-filled pore networks and their connectivity at different wa-

177 ter saturation conditions. Following Yan et al. (2018), the DOC diffusivity, D_{DOC} nor-

178 malized to the diffusivity of pure water, $D_{0,DOC}$, can be expressed as

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

179 where ϕ is the soil porosity, m_s and n_s are cementation and saturation exponents (as-

180 suming values of 1.5 and 2 for structured soils, respectively) accounting for the effects

181 of the pore structure and water connectivity on DOC diffusion, θ is the moisture con-

182 tent, and p is a SOC-microorganisms collocation factor varying between 0 and 1. The

183 cementation exponent represents the pore connectivity and tortuosity while the satura-

184 tion exponent describes the effect of water saturation depending on the pore size distri-

185 bution of the soil. The collocation factor represents the degree of collocation between

186 the SOC and the microorganisms. The expression for the O_2 diffusivity takes a similar

187 form (Yan et al., 2018),

$$\frac{D_{O_2}}{D_{0,O_2}} = \phi^{(m_g - n_g)}(\theta - \phi)^{n_g} \tag{3}$$

188 where m_g and n_g are cementation and saturation exponents accounting for the effects

189 of the pore structure and water connectivity on O_2 diffusion, and D_{0,O_2} is the diffusiv-

190 ity in free air.

191 The concentrations, DOC_A and O_{2_A}, can then be expressed as proportional to the

192 bulk concentrations (DOC_b and O_b) through their respective diffusivity coefficients (Moyano

193 et al., 2013; Davidson et al., 2014), e.g., $DOC_A = DOC_b(D_{DOC}/D_{0,DOC}) = DOC_b\phi^{p(m_s - n_s)}\theta^{pn_s}$,

194 and substituting back in Eq. (1), the microbial uptake of the DOC can be expressed in

195 terms of soil porosity(ϕ) and water content(θ) as

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

196 The microbial uptake law, Eq. 4, accounts for how both soil structure (i.e., through

197 the cementation and saturation exponents and the soil porosity) and soil water content

198 control the availability of the C substrate and oxygen, hence regulating microbial activ-

199 ity (Fig. 3(a)).

4 Linking soil hydraulic properties to C cycling

4.1 Hydraulic properties of structured soils

202 In addition to affecting the diffusivities of the C substrate and O_2, soil structure

203 also introduces a bimodality in the soil pore size distribution, which affects both the wa-

204 ter retention and hydraulic conductivity curves. The lower mode (i.e., microporosity)

205 derives from the textural component of the soil matrix, whereas the higher mode (i.e.,

206 macroporosity) derives from the structural one. Generally, from the pore size distribu-

207 tion (and water retention curve) the unsaturated hydraulic conductivity K can be es-

208 timated from the Mualem model (Mualem, 1976).

209 However, the Mualem model is based on the assumption that the pore system con-

210 sists of fully interacting pores (Mualem, 1976), an assumption which may not be true

211 for structured soils, in which macropores may develop as an independent pore system.

212 In this case, one can express the total unsaturated hydraulic conductivity as the sum of

213 the conductivities of textural and structural components of the soil matrix,

$$\mathrm{K_{total} = K_{s,tex}K_{r,tex} + K_{s,str}K_{r,str}} \tag{5}$$

214 where $\mathrm{K_{s,tex}}$ and $\mathrm{K_{r,tex}}$ are the saturated and relative hydraulic conductivity, respectively,

215 for the textural pore spaces, and $\mathrm{K_{s,str}}$ and $\mathrm{K_{r,str}}$ are the saturated and relative hydraulic

216 conductivity, respectively, for the structural ones. Being independent, $\mathrm{K_{r,tex}}$ and $\mathrm{K_{r,str}}$

217 can be individually computed from the Mualem model.

218 Additionally, water in bimodal soils may flow only within the textural pore spaces

219 at low soil water content and may begin flowing also within the structural pore spaces

220 only when the water content crosses a given water content threshold (Fig. 3(b)). There-

221 fore, using for example the van Genuchten-Mualem model, K can be expressed as (Smettem

222 & Kirkby, 1990; B. Mohanty et al., 1997, 1998)

$$\mathrm{K_{total}} = \begin{cases} \mathrm{K_{s,tex}S_{e,tex}^{0.5}[1 - (1 - S_{e,tex}^{1/a_{tex}})^{a_{tex}}]^2,} & \theta < \theta_m \\ \mathrm{K_{s,tex} + K_{s,str}S_{e,str}^{0.5}[1 - (1 - S_{e,str}^{1/a_{str}})^{a_{str}}]^2,} & \theta > \theta_m \end{cases} \tag{6}$$

223 where K_s is the saturated hydraulic conductivity, $\mathrm{a_{tex}}$ is the shape parameter of the hy-

224 draulic conductivity curve of the textural pore space, and $\mathrm{a_{str}}$ is the corresponding shape

225 parameter of the structure-modified hydraulic conductivity curve. Note that the effec-

226 tive saturation of the soil in the micropore ($\mathrm{S_{e,tex}}$) and the macropore systems ($\mathrm{S_{e,str}}$)

227 are relative to the corresponding porosities, $\mathrm{S_{e,tex}} = (\theta - \theta_r)/(\theta_m - \theta_r)$ and $\mathrm{S_{e,str}} = (\theta -$

228 $\theta_m)/(\theta_s - \theta_m)$, where θ_r is the residual water content, θ_s is the water content at satu-

ration (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}).

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, $K_{\text{s,str}}/K_{\text{s,tex}}$, is assumed to vary between 1 for low GPP to 1000 for high GPP (typical of tropical rain forests), and the ratio $a_{\text{str}}/a_{\text{tex}}$ (see Eq. 6) was then estimated as a function of $K_{\text{s,str}}/K_{\text{s,tex}}$, varying from 0 for low $K_{\text{s,str}}/K_{\text{s,tex}}$ to 30 for high $K_{\text{s,str}}/K_{\text{s,tex}}$ values.

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 vary 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

255 can extend this approach to link the changes in soil hydraulic properties to the evolu-

256 tion of soil structure using the aggregated C (A, in the Millennial model) as a measure

257 of soil structure. The structural saturated hydraulic conductivity could be computed as

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

258 where $K_{s,tot}$ and $K_{s,tex}$ represent the maximum saturated hydraulic conductivity of a soil

259 with fully developed structure, which can be estimated from equation 9, and saturated

260 hydraulic conductivity of an unstructured/texture-only soil, respectively, and α and β

261 are shape parameters (Fig. 3(c)).

262 While the parameterization of Bonetti et al. (2021) focused on the hydraulic con-

263 ductivity, the generality of the adopted mathematical expressions is such that a similar

264 parameterization likely applies to porosity. Accordingly, the structural porosity may be
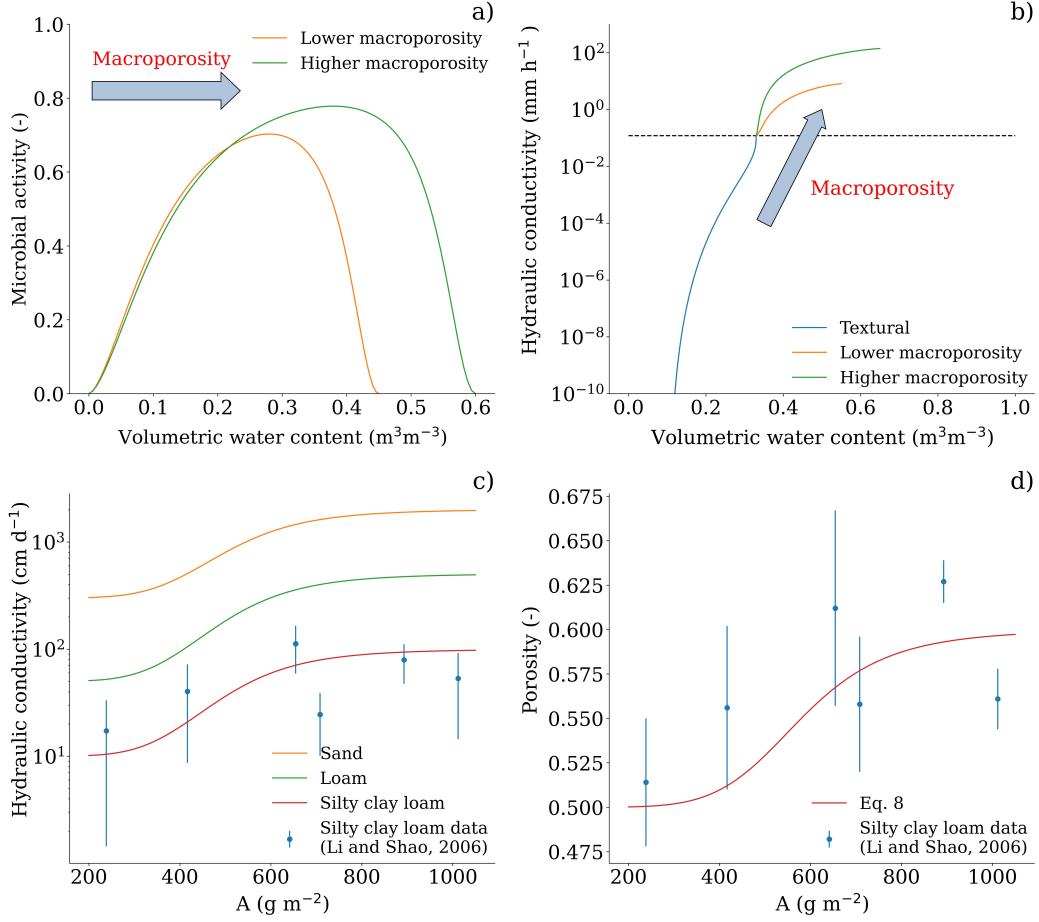
265 linked to A via

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

266 where ϕ_{tot} and ϕ_{tex} represent the maximum porosity of a soil with fully developed struc-

267 ture, and porosity of an unstructured/texture-only soil, respectively, and α and β are

268 shape parameters (Fig. 3(d)). Our case study below also suggests that a single set of α

269 and β may be needed for Eqs. 7 and 8.

270 Based on empirical evidence, Bonetti et al. (2021) expressed the $K_{s,tot}/K_{s,tex}$ ra-

271 tio as a function of the sand fraction,

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

272 where Sa is the sand fraction % in the soil. Linking the hydraulic parameterization by

273 Bonetti et al. (2021) to the Millennial model allows explicitly modeling the dynamics of

274 soil hydraulic properties as the soil structure evolves in response to environmental changes.

275 In particular, coupling the soil C cycling to the soil water balance (e.g., Laio et al. (2001b);

276 Pelak and Porporato (2019)) through the dynamics of soil structure and hydraulic prop-

277 erties, as introduced here, may be a significant step towards modeling more holistically

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 computed using Eqs. (7) and (9) with $\alpha = 580$ and $\beta = 6$ for various soil textural types: sand from Bonetti et al. (2021) (85% sand, $K_{s,tex} = 300$ cm d^{-1}, $K_{s,tot} = 2016.66$ cm d^{-1}), loam from Bonetti et al. (2021) (50% sand, $K_{s,tex} = 50$ cm d^{-1}, $K_{s,tot} = 506.54$ cm d^{-1}), silty clay loam from Li and Shao (2006) ($K_{s,tex} = 10$ cm d^{-1}, $K_{s,tot} = 100$ cm d^{-1}). d) Relation between porosity and aggregated C, computed using Eq. 8. Data from Li and Shao (2006).

278   soil processes as part of an integrated biochemical and physical system controlled by cli-
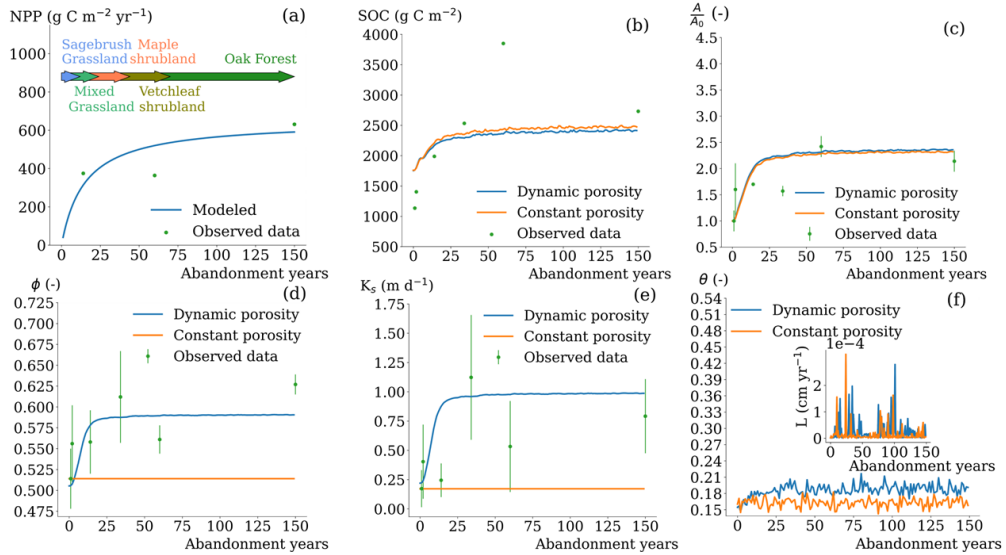
matic changes (such as rainfall, temperature, etc.) as well as human activities (e.g., land use, management) (Porporato et al., 2015).

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 used the mean weight diameter of soil aggregates as a proxy for aggregated C and represented it as a relative change ratio (A/A_0) with A_0 being the mean weight diameter at one year after abandonment. Soils were silty clay loam across the sites. We refer to Li & 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 (Fig. 4(a)). 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 statistics ob-

tained from Funk et al. (2015). Parameters related to the soil water balance were taken

from Laio et al. (2001a), except for measured porosity and hydraulic conductivity, while

parameters for the C module were taken from R. Abramoff et al. (2018) and R. Z. Abramoff

et al. (2022). These parameters were adjusted to capture observations from the site and

are provided in Table 1 of the supplementary information. After an initial spin up of 2000

years, we ran the model for 150 years with an hourly timestep and then aggregated the

results to yearly values for illustrative purposes.

Figure 4. Change in soil biophysical properties during the ecological succession from an abandoned cropland to forest: (a) Net primary productivity (NPP) for different vegetation recovery stages; (b) Soil organic C (SOC); (c) Relative aggregates ($\frac{A}{A_0}$) with A_0 corresponding to aggregate at one 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 the supplementary information.

As evident from the observations (Fig. 4), following abandonment, the soil undergoes important biophysical changes, especially over the first twenty-five years. The increase in vegetation productivity over the years provided larger inputs of organic matter (root exudates and litterfall) to the soil (Fig. 4(b)), which led to the formation of aggregates (Fig. 4(c)) 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 (Fig. 4(d) and (e)). 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) (Fig. 4(f)). 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. 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 chal-

341 lenge. Here, we built upon recent advances in soil C modeling and soil hydraulic param-

342 eterization to present an integrated modeling framework that can account for the effects

343 of soil structure on hydrologic and C cycling processes using the amount of aggregated

344 C as a proxy. In particular, aggregated C is here linked to the formation of macropores

345 with consequent increase in saturated hydraulic conductivity and changes in oxygen and

346 substrate diffusivity that affect microbial activity. The application to an abandoned crop-

347 land in the Loess Plateau of China showed the ability of the new framework to capture

348 soil regeneration following vegetation succession from cropland, to grassland, shrubland,

349 and ultimately forest and, overall, its potential to predict temporal changes in soil bio-

350 physical properties. The modeling framework can be particularly advantageous for ap-

351 plications involving land management practices and land-use changes.

352   Beyond making predictions, an advantage of using a modeling framework based on

353 measurable properties is that it can provide more physical, chemical, and biological-based

354 insights into system dynamics, especially given the fact that observations are not always

355 available. A model can identify drivers of changes in the soil organic C or explain dif-

356 ferences in C turnover times across different biomes, climates, and management factors.

357 For example, it can help assess when, based on climate and other soil factors, changes

358 in soil organic C are driven by physical protection/release of C within aggregates (e.g.,

359 due to no till/till), by sorption/desorption of microbial necromass in mineral surfaces (e.g.,

360 shifts in hydrologic regime), or a combination of the two. Interestingly, such a model could

361 be used to estimate soil organic C sequestration potentials across the globe, based on

362 both natural and anthropogenic drivers. The latter, however, would need to be explic-

363 itly incorporated as forcing in the model, for which more work is needed. Another im-

364 portant aspect, relevant to ecosystem ecology and water resources, is that the coupling

365 between C dynamics and hydraulic properties further allows to interpret and quantify

366 changes in soil hydrology over time, especially in response to land use changes. The case

367 study explored here is a good example in which soil recovery leads to increase water re-

tention within microporosity, but also more leakage due to macroporosity—an effect that cannot be quantitatively captured without the inclusion of soil structural effects.

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; Vezzani et al., 2018; Lucas et al., 2019), 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 (Moyano et al., 2013; Davidson et al., 2014; 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 soil organic C 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 (e.g., (Allison et al., 2010; Todd-Brown et al., 2012; Allison, 2014; Wieder et al., 2015; Sihi et al., 2016; Ballantyne IV & Billings, 2018; Sulman et al., 2018; Calabrese et al., 2022)). 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 (Prosser, 2015; Overy et al., 2021) into our proposed modeling framework might pave the way for a more holistic understanding of en-

vironmental changes and land use impacts on the soil system, in terms of structure (i.e.,

physical properties, heterogeneity), biological activity (i.e., microbial community com-

position, traits, C cycling), and their interaction (Kallenbach et al., 2019; Fatichi et al.,

2020; Bonetti et al., 2021; Sullivan et al., 2022).

7 Data Availability Statement

The Python codes for the modeling framework and the plots are available at

https://doi.org/10.4211/hs.6e4f08d8380a49f99314bae8a7ac41e2.

Appendix A Soil C model description

The novel Millennial model for soil C dynamics (R. Abramoff et al., 2018; R. Z. Abramoff

et al., 2022) is based on a system of equations of C transfer between five C pools: par-

ticulate organic matter (P), dissolved organic C (DOC), aggregate C (A), mineral-associated

organic matter (M) and microbial biomass (B) as shown in the conceptual diagram (Fig.

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,

$$\frac{d\mathrm{P}}{dt} = p_i F_i + F_a - F_{pa} - F_{pl}^p, \tag{A1}$$

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,

$$\frac{d\mathrm{A}}{dt} = F_{pa} - F_a - F_{pl}^a, \tag{A2}$$

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, POM and A depolymerization into DOC, mineral adsorption and desorption of DOC, and microbial uptake of DOC (U),

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

where $(1\text{-}p_i)$ 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,

$$\frac{d\text{M}}{dt} = F_{lm} - F_{ld}, \tag{A4}$$

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 (R. Z. Abramoff et al., 2021).

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

$$\frac{d\text{B}}{dt} = CUE \cdot U - F_{bm}, \tag{A5}$$

where CUE is the C use efficiency, the microbial uptake of DOC (U), as described in (Eq.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 (R. Z. 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 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 two order of magnitude lower rate.

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. (2001b); Rodríguez-Iturbe and Porporato (2004), the soil moisture dynamics was modeled at the daily time scale by solving stochastic water balance differential equation:

$$Z_r \frac{d\phi_{\text{tot}} s}{dt} = R - I - Q - ET - L \tag{A6}$$

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

$$F_l = L\text{DOC}/(\phi Z_r s). \tag{A7}$$

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

Acknowledgments

References

Abramoff, R., Xu, X., Hartman, M., O'Brien, S., Feng, W., Davidson, E., ... Mayes, M. A. (2018, January). The Millennial model: in search of measurable pools and transformations for modeling soil carbon in the new century. *Biogeochemistry*, *137*(1), 51–71. Retrieved 2021-10-17, from `https://doi.org/10.1007/s10533-017-0409-7` doi: 10.1007/s10533-017-0409-7

Abramoff, R. Z., Georgiou, K., Guenet, B., Torn, M. S., Huang, Y., Zhang, H., ... others (2021). How much carbon can be added to soil by sorption? *Biogeochemistry*, *152*(2), 127–142.

Abramoff, R. Z., Guenet, B., Zhang, H., Georgiou, K., Xu, X., Viscarra Rossel, R. A., ... Ciais, P. (2022, January). Improved global-scale predictions of soil carbon stocks with Millennial Version 2. *Soil Biology and Biochemistry*, *164*, 108466. Retrieved 2022-02-02, from `https://www.sciencedirect.com/science/article/pii/S0038071721003400` doi: 10.1016/j.soilbio.2021.108466

Allison, S. D. (2014). Modeling adaptation of carbon use efficiency in microbial communities. *Frontiers in Microbiology*, *5*, 571.

Allison, S. D., Wallenstein, M. D., & Bradford, M. A. (2010). Soil-carbon response to warming dependent on microbial physiology. *Nature Geoscience*, *3*(5), 336–340.

Angers, D. A., & Caron, J. (1998, August). Plant-induced Changes in Soil Structure: Processes and Feedbacks. *Biogeochemistry*, *42*(1), 55–72. Retrieved 2022-06-14, from `https://doi.org/10.1023/A:1005944025343` doi: 10.1023/A:1005944025343

Ballantyne IV, F., & Billings, S. A. (2018). Model formulation of microbial co2 production and efficiency can significantly influence short and long term soil c projections. *The ISME journal*, *12*(6), 1395–1403.

Beven, K., & Germann, P. (1982). Macropores and water flow in soils. *Wa-*

ter Resources Research, *18*(5), 1311–1325.   Retrieved 2022-06-10, from

`https://onlinelibrary.wiley.com/doi/abs/10.1029/WR018i005p01311`

(_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/WR018i005p01311)

doi: 10.1029/WR018i005p01311

Beven, K., & Germann, P.   (2013).   Macropores and water flow in soils revisited.   *Water Resources Research*, *49*(6), 3071–3092.   Retrieved 2022-06-10, from `https://onlinelibrary.wiley.com/doi/abs/10.1002/wrcr.20156` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/wrcr.20156)   doi: 10.1002/wrcr.20156

Bodner, G., Mentler, A., & Keiblinger, K.   (2021).   Plant Roots for Sustainable Soil Structure Management in Cropping Systems.   In *The Root Systems in Sustainable Agricultural Intensification* (pp. 45–90).   John Wiley & Sons, Ltd.   Retrieved 2022-06-14, from `https://onlinelibrary.wiley.com/doi/abs/10.1002/9781119525417.ch3`   (Section: 3 _eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/9781119525417.ch3)   doi: 10.1002/9781119525417.ch3

Bonetti, S., Wei, Z., & Or, D.   (2021, December).   A framework for quantifying hydrologic effects of soil structure across scales.   *Communications Earth & Environment*, *2*(1), 107. Retrieved 2021-10-17, from `http://www.nature.com/articles/s43247-021-00180-0`   doi: 10.1038/s43247-021-00180-0

Borrelli, P., Robinson, D. A., Panagos, P., Lugato, E., Yang, J. E., Alewell, C., ... Ballabio, C.   (2020, September).   Land use and climate change impacts on global soil erosion by water (2015-2070).   *Proceedings of the National Academy of Sciences*, *117*(36), 21994–22001.   Retrieved 2021-10-18, from `http://www.pnas.org/lookup/doi/10.1073/pnas.2001403117`   doi: 10.1073/pnas.2001403117

Brady, N. C., & Weil, R. R.   (2008).   *The nature and properties of soils* (Vol. 13). Prentice Hall Upper Saddle River, NJ.

Bronick, C. J., & Lal, R. (2005, January). Soil structure and management: a review. *Geoderma*, *124*(1), 3–22. Retrieved 2021-10-18, from `https://www.sciencedirect.com/science/article/pii/S0016706104000898` doi: 10.1016/j.geoderma.2004.03.005

Cagnarini, C., Blyth, E., Emmett, B. A., Evans, C. D., Griffiths, R. I., Keith, A., . . . Cosby, B. J. (2019). Zones of influence for soil organic matter dynamics: A conceptual framework for data and models. *Global Change Biology*, *25*(12), 3996–4007. Retrieved 2022-08-08, from `https://onlinelibrary.wiley.com/doi/abs/10.1111/gcb.14787` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/gcb.14787) doi: 10.1111/gcb.14787

Calabrese, S., Mohanty, B. P., & Malik, A. A. (2022). Soil microorganisms regulate extracellular enzyme production to maximize their growth rate. *Biogeochemistry*, *158*(3), 303–312.

Chakrawal, A., Herrmann, A. M., Koestel, J., Jarsjö, J., Nunan, N., Kätterer, T., & Manzoni, S. (2020). Dynamic upscaling of decomposition kinetics for carbon cycling models. *Geoscientific Model Development*, *13*(3), 1399–1429.

Chandrasekhar, P., Kreiselmeier, J., Schwen, A., Weninger, T., Julich, S., Feger, K.-H., & Schwärzel, K. (2018, December). Why We Should Include Soil Structural Dynamics of Agricultural Soils in Hydrological Models. *Water*, *10*(12), 1862. Retrieved 2022-06-13, from `https://www.mdpi.com/2073-4441/10/12/1862` (Number: 12 Publisher: Multidisciplinary Digital Publishing Institute) doi: 10.3390/w10121862

Conant, R. T., Ryan, M. G., Ågren, G. I., Birge, H. E., Davidson, E. A., Eliasson, P. E., . . . others (2011). Temperature and soil organic matter decomposition rates–synthesis of current knowledge and a way forward. *Global Change Biology*, *17*(11), 3392–3404.

Davidson, E. A., Savage, K. E., & Finzi, A. C. (2014). A big-microsite framework

for soil carbon modeling. *Global Change Biology*, *20*(12), 3610–3620. Retrieved 2021-09-26, from `https://onlinelibrary.wiley.com/doi/abs/10.1111/gcb` `.12718` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/gcb.12718) doi: 10.1111/gcb.12718

Dexter, A. R. (1988, June). Advances in characterization of soil structure. *Soil and Tillage Research*, *11*(3), 199–238. Retrieved 2022-06-09, from `https://` `www.sciencedirect.com/science/article/pii/0167198788900025` doi: 10 .1016/0167-1987(88)90002-5

Durner, W. (1994). Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resources Research*, *30*(2), 211–223. Retrieved 2021-10-18, from `https://onlinelibrary.wiley.com/doi/abs/10.1029/93WR02676` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/93WR02676) doi: 10.1029/93WR02676

Ebrahimi, A., & Or, D. (2018). On Upscaling of Soil Microbial Processes and Biogeochemical Fluxes From Aggregates to Landscapes. *Journal of Geophysical Research: Biogeosciences*, *123*(5), 1526–1547. Retrieved 2022-08-08, from `https://onlinelibrary.wiley.com/doi/abs/10.1029/2017JG004347` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/2017JG004347) doi: 10.1029/2017JG004347

Fatichi, S., Or, D., Walko, R., Vereecken, H., Young, M. H., Ghezzehei, T. A., ... Avissar, R. (2020, January). Soil structure is an important omission in Earth System Models. *Nature Communications*, *11*(1), 522. Retrieved 2021-07-26, from `https://www.nature.com/articles/s41467-020-14411-z` (Bandiera_abtest: a Cc_license_type: cc_by Cg_type: Nature Research Journals Number: 1 Primary_atype: Research Publisher: Nature Publishing Group Subject_term: Climate sciences;Hydrology Subject_term_id: climate-sciences;hydrology) doi: 10.1038/s41467-020-14411-z

Franklin, S. M., Kravchenko, A. N., Vargas, R., Vasilas, B., Fuhrmann, J. J., &

627 Jin, Y. (2021, October). The unexplored role of preferential flow in soil

628 carbon dynamics. *Soil Biology and Biochemistry*, *161*, 108398. Retrieved

629 2022-08-08, from `https://www.sciencedirect.com/science/article/pii/`

630 `S0038071721002728` doi: 10.1016/j.soilbio.2021.108398

631 Funk, C., Peterson, P., Landsfeld, M., Pedreros, D., Verdin, J., Shukla, S., . . . oth-

632 ers (2015). The climate hazards infrared precipitation with stations—a new

633 environmental record for monitoring extremes. *Scientific data*, *2*(1), 1–21.

634 Golchin, A., Oades, J. M., Skjemstad, J. O., & Clarke, P. (1994). Soil structure and

635 carbon cycling. *Soil Research*, *32*(5), 1043–1068. Retrieved 2022-06-14, from

636 `https://www.publish.csiro.au/sr/sr9941043` (Publisher: CSIRO PUB-

637 LISHING) doi: 10.1071/sr9941043

638 Hirmas, D. R., Giménez, D., Nemes, A., Kerry, R., Brunsell, N. A., & Wilson,

639 C. J. (2018, September). Climate-induced changes in continental-scale

640 soil macroporosity may intensify water cycle. *Nature*, *561*(7721), 100–

641 103. Retrieved 2022-06-16, from `https://www.nature.com/articles/`

642 `s41586-018-0463-x` (Number: 7721 Publisher: Nature Publishing Group)

643 doi: 10.1038/s41586-018-0463-x

644 Jungkunst, H. F., Göpel, J., Horvath, T., Ott, S., & Brunn, M. (2022). Global

645 soil organic carbon–climate interactions: Why scales matter. *WIREs*

646 *Climate Change*, *13*(4), e780. Retrieved 2022-08-08, from `https://`

647 `onlinelibrary.wiley.com/doi/abs/10.1002/wcc.780` (_eprint:

648 https://onlinelibrary.wiley.com/doi/pdf/10.1002/wcc.780) doi: 10.1002/

649 wcc.780

650 Kallenbach, C. M., Wallenstein, M. D., Schipanksi, M. E., & Grandy, A. S. (2019).

651 Managing agroecosystems for soil microbial carbon use efficiency: ecological

652 unknowns, potential outcomes, and a path forward. *Frontiers in Microbiology*,

653 *10*, 1146.

654 Kutílek, M. (2004, December). Soil hydraulic properties as related to soil

655   structure. *Soil and Tillage Research*, *79*(2), 175–184. Retrieved 2022-

656   06-10, from `https://www.sciencedirect.com/science/article/pii/`

657   `S0167198704001436` doi: 10.1016/j.still.2004.07.006

658   Laio, F., Porporato, A., Ridolfi, L., & Rodriguez-Iturbe, I. (2001a). Plants in

659   water-controlled ecosystems: active role in hydrologic processes and response

660   to water stress: Ii. probabilistic soil moisture dynamics. *Advances in Water*

661   *Resources*, *24*(7), 707–723.

662   Laio, F., Porporato, A., Ridolfi, L., & Rodriguez-Iturbe, I. (2001b, July). Plants

663   in water-controlled ecosystems: active role in hydrologic processes and re-

664   sponse to water stress: II. Probabilistic soil moisture dynamics. *Advances*

665   *in Water Resources*, *24*(7), 707–723. Retrieved 2021-10-17, from `https://`

666   `www.sciencedirect.com/science/article/pii/S0309170801000057` doi:

667   10.1016/S0309-1708(01)00005-7

668   Lal, R. (1993, October). Tillage effects on soil degradation, soil resilience, soil

669   quality, and sustainability. *Soil and Tillage Research*, *27*(1), 1–8. Retrieved

670   2021-10-18, from `https://www.sciencedirect.com/science/article/pii/`

671   `016719879390059X` doi: 10.1016/0167-1987(93)90059-X

672   Lal, R. (2004, November). Soil carbon sequestration to mitigate climate

673   change. *Geoderma*, *123*(1), 1–22. Retrieved 2021-10-18, from `https://`

674   `www.sciencedirect.com/science/article/pii/S0016706104000266` doi:

675   10.1016/j.geoderma.2004.01.032

676   Lal, R. (2012, September). Climate Change and Soil Degradation Mitigation by

677   Sustainable Management of Soils and Other Natural Resources. *Agricultural*

678   *Research*, *1*(3), 199–212. Retrieved 2021-10-18, from `http://link.springer`

679   `.com/10.1007/s40003-012-0031-9` doi: 10.1007/s40003-012-0031-9

680   Larson, W. E., Blake, G. R., Allmaras, R. R., Voorhees, W. B., & Gupta, S. C.

681   (Eds.). (1989). *Mechanics and Related Processes in Structured Agri-*

682   *cultural Soils.* Dordrecht: Springer Netherlands. Retrieved 2022-06-10,

from `http://link.springer.com/10.1007/978-94-009-2421-5`   doi: 10.1007/978-94-009-2421-5

Lehmann, J., & Kleber, M. (2015). The contentious nature of soil organic matter. *Nature*, *528*(7580), 60–68.

Li, Y. Y., & Shao, M. A. (2006, January). Change of soil physical properties under long-term natural vegetation restoration in the Loess Plateau of China. *Journal of Arid Environments*, *64*(1), 77–96. Retrieved 2021-12-10, from `https://www.sciencedirect.com/science/article/pii/S0140196305001072` doi: 10.1016/j.jaridenv.2005.04.005

Liang, C., Schimel, J. P., & Jastrow, J. D. (2017). The importance of anabolism in microbial control over soil carbon storage. *Nature microbiology*, *2*(8), 1–6.

Lipper, L., Thornton, P., Campbell, B. M., Baedeker, T., Braimoh, A., Bwalya, M., ... others (2014). Climate-smart agriculture for food security. *Nature climate change*, *4*(12), 1068–1072.

Lucas, M., Schlüter, S., Vogel, H.-J., & Vetterlein, D. (2019, November). Roots compact the surrounding soil depending on the structures they encounter. *Scientific Reports*, *9*(1), 16236. Retrieved 2022-06-14, from `https://www.nature.com/articles/s41598-019-52665-w` (Number: 1 Publisher: Nature Publishing Group) doi: 10.1038/s41598-019-52665-w

Manzoni, S., & Porporato, A. (2009, July). Soil carbon and nitrogen mineralization: Theory and models across scales. *Soil Biology and Biochemistry*, *41*(7), 1355–1379. Retrieved 2022-06-15, from `https://www.sciencedirect.com/science/article/pii/S0038071709000765` doi: 10.1016/j.soilbio.2009.02.031

Meurer, K., Barron, J., Chenu, C., Coucheney, E., Fielding, M., Hallett, P., ... Jarvis, N. (2020). A framework for modelling soil structure dynamics induced by biological activity. *Global Change Biology*, *26*(10), 5382–5403. Retrieved 2021-10-18, from `https://onlinelibrary.wiley.com/doi/abs/10.1111/gcb.15289` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1111/gcb.15289)

711   doi: 10.1111/gcb.15289

712 Mohanty, B., Bowman, R., Hendrickx, J., & Van Genuchten, M. T.   (1997).   New

713   piecewise-continuous hydraulic functions for modeling preferential flow in an

714   intermittent-flood-irrigated field.   *Water Resources Research*, *33*(9), 2049–

715   2063.

716 Mohanty, B., Skaggs, T., & Van Genuchten, M. T.   (1998).   Impact of saturated

717   hydraulic conductivity on the prediction of tile flow.   *Soil Science Society of*

718   *America Journal*, *62*(6), 1522–1529.

719 Mohanty, B. P.   (1999).   Scaling hydraulic properties of a macroporous soil.   *Wa-*

720   *ter Resources Research*, *35*(6), 1927–1931.   Retrieved 2021-10-18, from

721   https://onlinelibrary.wiley.com/doi/abs/10.1029/1999WR900050

722   (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/1999WR900050)

723   doi: 10.1029/1999WR900050

724 Moyano, F. E., Manzoni, S., & Chenu, C.   (2013, April).   Responses of soil het-

725   erotrophic respiration to moisture availability: An exploration of processes

726   and models.   *Soil Biology and Biochemistry*, *59*, 72–85.   Retrieved 2021-

727   08-25, from https://www.sciencedirect.com/science/article/pii/

728   S0038071713000138 doi: 10.1016/j.soilbio.2013.01.002

729 Mualem, Y.   (1976).   A new model for predicting the hydraulic conduc-

730   tivity of unsaturated porous media.   *Water Resources Research*,

731   *12*(3), 513–522.   Retrieved 2021-09-13, from https://onlinelibrary

732   .wiley.com/doi/abs/10.1029/WR012i003p00513   (_eprint:

733   https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/WR012i003p00513)

734   doi: 10.1029/WR012i003p00513

735 Or, D., & Ghezzehei, T. A.   (2002, February).   Modeling post-tillage soil struc-

736   tural dynamics: a review.   *Soil and Tillage Research*, *64*(1), 41–59.   Retrieved

737   2022-06-09, from https://www.sciencedirect.com/science/article/pii/

738   S0167198701002562 doi: 10.1016/S0167-1987(01)00256-2

Or, D., Keller, T., & Schlesinger, W. H. (2021, April). Natural and managed soil structure: On the fragile scaffolding for soil functioning. *Soil and Tillage Research*, *208*, 104912. Retrieved 2021-10-18, from `https://www.sciencedirect.com/science/article/pii/S0167198720306942` doi: 10.1016/j.still.2020.104912

Overy, D. P., Bell, M. A., Habtewold, J., Helgason, B. L., & Gregorich, E. G. (2021). "omics" technologies for the study of soil carbon stabilization: A review. *Frontiers in Environmental Science*, *9*, 617952.

Parton, W. J., Hartman, M., Ojima, D., & Schimel, D. (1998, December). DAYCENT and its land surface submodel: description and testing. *Global and Planetary Change*, *19*(1), 35–48. Retrieved 2021-10-18, from `https://www.sciencedirect.com/science/article/pii/S092181819800040X` doi: 10.1016/S0921-8181(98)00040-X

Pelak, N., & Porporato, A. (2019). Dynamic evolution of the soil pore size distribution and its connection to soil management and biogeochemical processes. *Advances in Water Resources*, *131*. doi: 10.1016/j.advwatres.2019.103384

Porporato, A., Feng, X., Manzoni, S., Mau, Y., Parolari, A. J., & Vico, G. (2015). Ecohydrological modeling in agroecosystems: Examples and challenges. *Water Resources Research*, *51*(7), 5081–5099.

Powlson, D. S., Smith, P., & Smith, J. U. (Eds.). (1996). *Evaluation of Soil Organic Matter Models: Using Existing Long-Term Datasets.* Berlin, Heidelberg: Springer Berlin Heidelberg. Retrieved 2021-10-19, from `http://link.springer.com/10.1007/978-3-642-61094-3` doi: 10.1007/978-3-642-61094-3

Prosser, J. I. (2015). Dispersing misconceptions and identifying opportunities for the use of'omics' in soil microbial ecology. *Nature Reviews Microbiology*, *13*(7), 439–446.

Rabot, E., Wiesmeier, M., Schlüter, S., & Vogel, H. J. (2018, March). Soil structure

as an indicator of soil functions: A review. *Geoderma*, *314*, 122–137. Retrieved 2022-03-03, from `https://www.sciencedirect.com/science/article/pii/` `S0016706117310273` doi: 10.1016/j.geoderma.2017.11.009

Robertson, A. D., Paustian, K., Ogle, S., Wallenstein, M. D., Lugato, E., & Cotrufo, M. F. (2019, March). Unifying soil organic matter formation and persistence frameworks: the MEMS model. *Biogeosciences*, *16*(6), 1225–1248. Retrieved 2022-06-15, from `https://bg.copernicus.org/articles/16/1225/2019/` (Publisher: Copernicus GmbH) doi: 10.5194/bg-16-1225-2019

Rodríguez-Iturbe, I., & Porporato, A. (2004). *Ecohydrology of water-controlled ecosystems: soil moisture and plant dynamics*. Cambridge University Press.

Romero-Ruiz, A., Linde, N., Keller, T., & Or, D. (2018). A Review of Geophysical Methods for Soil Structure Characterization. *Reviews of Geophysics*, *56*(4), 672–697. Retrieved 2022-06-09, from `https://onlinelibrary.wiley.com/doi/abs/10.1029/2018RG000611` (_eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1029/2018RG000611) doi: 10.1029/2018RG000611

Schlüter, S., Leuther, F., Albrecht, L., Hoeschen, C., Kilian, R., Surey, R., ... Vogel, H.-J. (2022). Microscale carbon distribution around pores and particulate organic matter varies with soil moisture regime. *Nature communications*, *13*(1), 1–14.

Shi, A., Chakrawal, A., Manzoni, S., Fischer, B. M., Nunan, N., & Herrmann, A. M. (2021). Substrate spatial heterogeneity reduces soil microbial activity. *Soil Biology and Biochemistry*, *152*, 108068.

Sihi, D., Gerber, S., Inglett, P. W., & Inglett, K. S. (2016, March). Comparing models of microbial–substrate interactions and their response to warming. *Biogeosciences*, *13*(6), 1733–1752. Retrieved 2021-08-27, from `https://bg.copernicus.org/articles/13/1733/2016/` (Publisher: Copernicus GmbH) doi: 10.5194/bg-13-1733-2016

Smettem, K. R. J., & Kirkby, C.   (1990, September).   Measuring the hydraulic

properties of a stable aggregated soil.   *Journal of Hydrology*, *117*(1), 1–13.

Retrieved 2021-10-17, from `https://www.sciencedirect.com/science/`

`article/pii/002216949090084B` doi: 10.1016/0022-1694(90)90084-B

Sullivan, P., Billings, S., Hirmas, D., Li, L., Zhang, X., Ziegler, S., . . . others (2022).

Embracing the dynamic nature of soil structure: A paradigm illuminating the

role of life in critical zones of the anthropocene.   *Earth-Science Reviews*, *225*,

103873.

Sulman, B. N., Moore, J. A., Abramoff, R., Averill, C., Kivlin, S., Georgiou, K., . . .

others (2018).   Multiple models and experiments underscore large uncertainty

in soil carbon dynamics. *Biogeochemistry*, *141*(2), 109–123.

Todd-Brown, K. E. O., Hopkins, F. M., Kivlin, S. N., Talbot, J. M., & Allison,

S. D.   (2012, July).   A framework for representing microbial decomposi-

tion in coupled climate models.   *Biogeochemistry*, *109*(1), 19–33.   Retrieved

2021-10-19, from `https://doi.org/10.1007/s10533-011-9635-6`   doi:

10.1007/s10533-011-9635-6

Tuller, M., & Or, D.   (2001).   Hydraulic conductivity of variably saturated

porous media: Film and corner flow in angular pore space.   *Water Re-

sources Research*, *37*(5), 1257–1276.   Retrieved 2021-10-18, from `https://`

`onlinelibrary.wiley.com/doi/abs/10.1029/2000WR900328`   (_eprint:

https://onlinelibrary.wiley.com/doi/pdf/10.1029/2000WR900328)   doi:

10.1029/2000WR900328

Vezzani, F. M., Anderson, C., Meenken, E., Gillespie, R., Peterson, M., & Beare,

M. H.   (2018, January).   The importance of plants to development and main-

tenance of soil structure, microbial communities and ecosystem functions.   *Soil

and Tillage Research*, *175*, 139–149.   Retrieved 2022-06-14, from `https://`

`www.sciencedirect.com/science/article/pii/S0167198717301691`   doi:

10.1016/j.still.2017.09.002

823   Weynants, M., Vereecken, H., & Javaux, M. (2009). Revisiting vereecken pedotrans-
824   fer functions: Introducing a closed-form hydraulic model. *Vadose Zone Jour-*
825   *nal*, *8*(1), 86–95.

826   Wieder, W. R., Allison, S. D., Davidson, E. A., Georgiou, K., Hararuk, O., He, Y.,
827   . . . others (2015). Explicitly representing soil microbial processes in earth
828   system models. *Global Biogeochemical Cycles*, *29*(10), 1782–1800.

829   Wilson, C. H., & Gerber, S. (2021). Theoretical insights from upscaling michaelis–
830   menten microbial dynamics in biogeochemical models: a dimensionless ap-
831   proach. *Biogeosciences*, *18*(20), 5669–5679.

832   Xie, B., Qin, Z., Wang, Y., & Chang, Q. (2014, January). Spatial and temporal
833   variation in terrestrial net primary productivity on Chinese Loess Plateau
834   and its influential factors. *Transactions of the Chinese Society of Agricultural*
835   *Engineering*, *30*(11), 244–253.

836   Yan, Z., Bond-Lamberty, B., Todd-Brown, K. E., Bailey, V. L., Li, S., Liu, C., &
837   Liu, C. (2018, July). A moisture function of soil heterotrophic respira-
838   tion that incorporates microscale processes. *Nature Communications*, *9*(1),
839   2562. Retrieved 2021-08-25, from https://www.nature.com/articles/
840   s41467-018-04971-6 (Bandiera_abtest: a Cc_license_type: cc_by Cg_type:
841   Nature Research Journals Number: 1 Primary_atype: Research Publisher: Na-
842   ture Publishing Group Subject_term: Carbon cycle Subject_term_id: carbon-
843   cycle) doi: 10.1038/s41467-018-04971-6

844   Young, I. M., Blanchart, E., Chenu, C., Dangerfield, M., Fragoso, C., Grimaldi,
845   M., . . . Monrozier, L. J. (1998). The interaction of soil biota and
846   soil structure under global change. *Global Change Biology*, *4*(7), 703–
847   712. Retrieved 2022-06-10, from https://onlinelibrary.wiley
848   .com/doi/abs/10.1046/j.1365-2486.1998.00194.x (_eprint:
849   https://onlinelibrary.wiley.com/doi/pdf/10.1046/j.1365-2486.1998.00194.x)
850   doi: 10.1046/j.1365-2486.1998.00194.x

851   Zurmühl, T., & Durner, W. (1996). Modeling Transient Water

852   and Solute Transport in a Biporous Soil. *Water Resources Re-*

853   *search*, *32*(4), 819–829. Retrieved 2021-09-13, from `https://`

854   `onlinelibrary.wiley.com/doi/abs/10.1029/95WR01678` (_eprint:

855   https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/95WR01678) doi:

856   10.1029/95WR01678

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

Supplementary Information

Table 1: Parameters used in the modeling framework.

Symbols	Description	Values	Units	Sources
U_{max}	Maximum microbial uptake rate (Figure 3)	1	(d^{-1})	(Moyano et al., 2013)
U_{max}	Maximum microbial uptake rate (Figure 4)	0.38	(d^{-1})	This study
p	SOC-microorganism collocation factor	0.794	(-)	(Yan et al., 2018)
m_s	Cementation exponent for DOC diffusion	1.5	(-)	(Yan et al., 2018)
n_s	Saturation exponent for DOC diffusion	2	(-)	(Yan et al., 2018)
m_g	Cementation exponent for O_2 diffusion	1.5	(-)	(Yan et al., 2018)
n_g	Saturation exponent for O_2 diffusion	2	(-)	(Yan et al., 2018)
DOC_b	Bulk concentration of DOC (Figure 3)	1	$(g\ C\ m^{-3})$	(Moyano et al., 2013)
O_b	Bulk concentration of O_2 (Figure 3)	1	$(g\ m^{-3})$	(Moyano et al., 2013)
K_{DOC}	Half saturation constant of DOC	0.05	$(g\ C\ m^{-3})$	(Moyano et al., 2013)
K_{O_2}	Half saturation constant of O_2	0.005	$(g\ m^{-3})$	(Moyano et al., 2013)
a_{tex}	Shape parameter of textural porosity	0.286	(-)	(Smettem & Kirkby, 1990)
a_{str}	Shape parameter of structural porosity	1.5	(-)	(Smettem & Kirkby, 1990)
θ_r	Residual water content	0.01	(-)	(Smettem & Kirkby, 1990)
θ_m	Water content between micro- and macropororsity	0.33	(-)	(Smettem & Kirkby, 1990)
θ_s	Water content at saturation	0.65	(-)	(Smettem & Kirkby, 1990)
α	Shape parameter	580	(-)	This study
β	Shape parameter	6	(-)	This study
$K_{s,tex}$	Saturated hydraulic conductivity for textural component	0.1	$(m\ d^{-1})$	This study
$K_{s,tot}$	Total saturated hydraulic conductivity	1	$(m\ d^{-1})$	This study
ϕ_{tex}	Textural porosity	0.5	(-)	This study

Symbols	Description	Values	Units	Sources
ϕ_{tot}	Total porosity	0.6	(-)	This study
p_i	Proportion of C input to POM	0.66	(-)	(Abramoff et al., 2022)

References

Abramoff, R. Z., Guenet, B., Zhang, H., Georgiou, K., Xu, X., Viscarra Rossel, R. A., ... Ciais, P. (2022, January). Improved global-scale predictions of soil carbon stocks with Millennial Version 2. *Soil Biology and Biochemistry*, *164*, 108466. Retrieved 2022-02-02, from https://www.sciencedirect.com/science/article/pii/S0038071721003400 doi: 10.1016/j.soilbio2021.108466

Moyano, F. E., Manzoni, S., & Chenu, C. (2013, April). Responses of soil heterotrophic respiration to moisture availability: An exploration of processes and models. *Soil Biology and Biochemistry*, *59*, 72–85. Retrieved 2021-08-25, from https://www.sciencedirect.com/science/article/pii/S0038071713000138 doi: 10.1016/j.soilbio.2013.01.002

Smettem, K. R. J., & Kirkby, C. (1990, September). Measuring the hydraulic properties of a stable aggregated soil. *Journal of Hydrology*, *117*(1), 1–13. Retrieved 2021-10-17, from https://www.sciencedirect.com/science/article/pii/002216949090084B doi: 10.1016/0022-1694(90)90084-B

Yan, Z., Bond-Lamberty, B., Todd-Brown, K. E., Bailey, V. L., Li, S., Liu, C., & Liu, C. (2018, July). A moisture function of soil heterotrophic respiration that incorporates microscale processes. *Nature Communications*, *9*(1), 2562. Retrieved 2021-08-25, from https://www.nature.com/articles/s41467-018-04971-6 (Bandiera_abtest: a Cc_license_type: cc_by Cg_type: Nature Research Journals Number: 1 Primary_atype: Research Publisher: Nature Publishing Group Subject_term: Carbon cycle Subject_term_id: carboncycle) doi: 10.1038/s41467-018-04971-6