Supplementary material of Towards resolving poor performance of mechanistic soil organic carbon models

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Soil moisture scalar

We introduce a soil moisture scalar $K(\theta,\psi)$ to MIMICS,

$$K(\theta,\psi) = e^{\lambda\psi} \times \left(k_{a.min} + (1 - k_{a.min}) \times \left(\frac{\phi-\theta}{\phi}\right)^{0.5}\right) \times \left(\frac{\theta}{\phi}\right)^{0.5} \tag{E1}$$

where $e^{\lambda\psi}$ describes the dependence of soil microbial activities on water potential, and λ (kPa^{-1}) is the dependence of biological activity on soil matric potential ψ (kPa). $\left(k_{a.min} + (1 - k_{a.min}) \times \left(\frac{\phi-\theta}{\phi}\right)^{0.5}\right)$ represents the effect of oxygen limitation on microbial activities, and the parameter $k_{a.min}$ is the minimum relative SOC decomposition rate when the soil is fully saturated, and the oxygen supply rate is at its lowest. $\left(\frac{\theta}{\phi}\right)^{0.5}$ represents the effect of diffusion limitation of substrates on SOC decomposition, and θ is soil moisture content (mm mm^{-3}) and ϕ is soil porosity (mm mm^{-3}). More details can be found at (Ghezzehei et al., 2019). We multiplied both V_{max} and microbial turnover rate (τ) by $K(\theta,\psi)$ to represent the effects of soil moisture on microbial growth rates, which include both uptake and turnover (Wieder et al., 2019).

Structure and equations of MES-C

MES-C has two litter pools, metabolic litter (LIT_m) and structural litter (LIT_s), and the decomposition of litter and SOC are governed by two functional types of microbes including *r*-selected (MIC_r) and *K*-selected (MIC_k) microbes. SOC is divided into three parts: light molecule weight carbon (LMWC), mineral associated organic carbon (MAOC) and aggregated organic carbon, where aggregated carbon includes three fractions: aggregated metabolic carbon (AGG_m), aggregated structural carbon (AGG_s) and aggregated mineral associated carbon

(AGG$_{maoc}$). More description and assumptions can be found at Wieder et al., 2015 and Abramoff et al., 2022.

Decomposition of litter follows forward Michaelis-Menten kinetics, and microbial uptake of LMWC follows reversed Michaelis-Menten kinetics. Both kinetics are dependent on temperature sensitive maximum reaction velocities and half saturation constants calculated as,

$$V_{max} = e^{(V_{slope} \times T + V_{int})} \times a_v \times V_{mod} \tag{E2}$$

$$K_m = e^{(K_{slope} \times T + K_{int})} \times a_k \times K_{mod} \tag{E3}$$

The fluxes from donor to receiver pools are calculated as,

$$LIT_m - MIC_r = LIT_m \times V_{max[r1]} \times K(\theta, \psi) \times MIC_r / (K_{m[r1]} + MIC_r) \tag{E4}$$

$$LIT_s - MIC_r = LIT_s \times V_{max[r2]} \times K(\theta, \psi) \times MIC_r / (K_{m[r2]} + MIC_r) \tag{E5}$$

$$LMWC - MIC_r = MIC_r \times V_{max[r3]} \times K(\theta, \psi) \times LMWC / (K_{m[r3]} + LMWC) \tag{E6}$$

$$MIC_r - SOC = MIC_r \times {\tau_r}^2 \tag{E7}$$

$$LIT_m - MIC_k = LIT_m \times V_{max[k1]} \times K(\theta, \psi) \times MIC_k / (K_{m[k1]} + MIC_k) \tag{E8}$$

$$LIT_s - MIC_k = LIT_s \times V_{max[k2]} \times K(\theta, \psi) \times MIC_k / (K_{m[k2]} + MIC_k) \tag{E9}$$

$$LMWC - MIC_k = MIC_k \times V_{max[k3]} \times K(\theta, \psi) \times LMWC / (K_{m[k3]} + LMWC) \tag{E10}$$

$$MIC_k - SOC = MIC_k \times {\tau_k}^2 \tag{E11}$$

$$LMWC - MAOC = K(\theta, \phi) \times k_{adsorp} \times LMWC \times (1 - MAOC / Q_{max}) \tag{E12}$$

$$MAOC - LMWC = k_{desorp} \times MAOC / Q_{max} \tag{E13}$$

$$AGG_m - LIT_m = k_{ab} \times K(\theta, \phi) \times AGG_m \tag{E14}$$

$$AGG_s - LIT_s = k_{ab} \times K(\theta, \phi) \times AGG_s \tag{E15}$$

$$AGG_{maoc} - MAOC = k_{ab} \times K(\theta, \phi) \times AGG_{maoc} \tag{E16}$$

$$MAOC - AGG_{maoc} = k_{ma} \times K(\theta, \phi) \times MAOC \tag{E17}$$

$$LMWC - F_l = k_l \times K(\theta, \phi) \times LWMC \tag{E18}$$

Thus, changes in C pools can be described using the following equations,

$$\frac{dLIT_m}{dt} = I_m \times (1 - f_m) - E4 - E8 + E14 \tag{E19}$$

$$\frac{dLIT_s}{dt} = I_s \times (1 - f_s) - E5 - E9 + E15 \tag{E20}$$

$$\frac{dMIC_r}{dt} = (MGE[1] \times E4) + (MGE[2] \times E5) + (MGE[1] \times E6) - E7 \tag{E21}$$

$$\frac{dMIC_k}{dt} = (MGE[3] \times E8) + (MGE[4] \times E9) + (MGE[3] \times E10) - E11 \tag{E22}$$

$$\frac{dLMWC}{dt} = f_a[r] \times E7 + f_a[k] \times E11 + E13 - E6 - E10 - E12 - E18 \tag{E23}$$

$$\frac{dMAOC}{dt} = f_c[r] \times E7 + f_c[k] \times E11 + E16 + E12 - E13 - E17 \quad \text{(E24)}$$

$$\frac{dAGG_m}{dt} = I_m \times f_m - E14 \quad \text{(E25)}$$

$$\frac{dAGG_s}{dt} = I_s \times f_s - E15 \quad \text{(E26)}$$

$$\frac{dAGG_{maoc}}{dt} = E17 - E16 \quad \text{(E27)}$$

Table S1 MES-C parameters, values and units used in this study

Parameter	Description	Value	Units	Reference
V_{slope}	Regression coefficient (E2)	0.063	ln(mg C_s (mg MIC)$^{-1}$ h^{-1}) °C^{-1}	(Wieder et al., 2015)
V_{int}	Regression intercept (E2)	5.47	ln(mg C_s (mg MIC)$^{-1}$ h^{-1})	Same as above
a_V	Tuning coefficient (E2)	8×10^{-6}		Same as above
$V_{mod\text{-}r}$	Modifies V_{max} for fluxes into MIC_r (E2)	10,2,10[a]		Same as above
$V_{mod\text{-}K}$	Modifies V_{max} for fluxes into MIC_K (E2)	3,3,2[b]		Same as above
K_{slope}	Regression coefficient (E3)	0.017, 0.027, 0.017 [a,b]		Same as above
K_{int}	Regression intercept (E3)	3.19		Same as above
a_k	Tuning coefficient (E3)	10		Same as above
$K_{mod\text{-}r}$	Modifies Km for fluxes into MIC_r (E3)	0.125,0.5,0.25×P_{scalar} [a]		Same as above
$K_{mod\text{-}K}$	Modifies Km for fluxes into MIC_K (E3)	0.5,0.25,0.167×P_{scalar} [b]		Same as above
P_{scalar}	Physical protection scalar used in K_{mod}	$(2.0 \times e^{-2\sqrt{f_{clay}}})^{-1}$		Same as above
τ_r	r-selected microbial biomass turnover rate (E7)	$5.2 \times 10^{-4} \times e^{0.3(f_{met})} \times \tau_{mod}$	h^{-1}	Same as above
τ_k	K-selected microbial biomass turnover rate (E11)	$2.4 \times 10^{-4} \times e^{0.1(f_{met})} \times \tau_{mod}$		Same as above
τ_{mod}	Modifies microbial turnover rate	$0.6 < \sqrt{NPP/100} < 1.3$		This study
f_{met}	Partitioning of litter inputs to LIT_m	0.85-0.013 (lignin/N)		(Wieder et al., 2015)
k_{adsorp}	Binding affinity of LMWC (E12)	1/24.0 × f_{pH}	h^{-1}	(Abramoff et al., 2022)
f_{pH}	pH regulation on binding affinity	$e^{-0.186\times pH-0.216}$		Same as above
Q_{max}	Maximum sorption capacity (E12)	$0.6 \times \%claysilt$ [c]	mg C (g soil)$^{-1}$	(Georgiou et al., 2022)
$K(\theta,\phi)$ [d]	Moisture scalar (E12)	$(\theta/\phi)^{0.5}$		(Ghezzehei et al., 2019)
k_{desorp}	Desorption rate (E13)	1/6.0/24.0	h^{-1}	(Wang et al., 2013)

k_{ab}	Breakdown rate of soil aggregate carbon (E14)	1.14×10^{-5}	h^{-1}	Same as above
k_{ma}	Rate of aggregate formation from MAOC (E17)	4.57×10^{-6}	h^{-1}	Same as above
k_l	Leaching rate of LMWC	0.0015/24	h^{-1}	(Abramoff et al., 2022)
f_m	Fraction of metabolic litter inputs transferred to AGG_m (E18)	0.5		This study
f_s	Fraction of structural litter inputs transferred to AGG_s (E19)	0.5		This study
MGE	Microbial growth efficiency (E20)	$0.55, 0.25, 0.75, 0.35\times T_{scalar}$[e]	mg mg^{-1}	(Wieder et al., 2015)
T_{scalar}	Temperature regulation on MGE	$e^{(-0.015\times f_T)}$		
f_a	Fraction of τ partitioned to LWMC (E22)	$1-f_c$		(Wieder et al., 2015)
f_c	Fraction of τ partitioned to MAOC (E23)	$0.1\times e^{-3(f_{met})}, 0.3\times e^{-3(f_{met})}$[f]		Same as above

[a] For LIT_m, LIT_s and LMWC fluxes entering MIC_r, respectively.

[b] For LIT_m, LIT_s and LMWC fluxes entering MIC_K, respectively.

[c] %claysilt represents soil clay and silt content.

[d] θ is soil moisture (mm^3 mm^{-3}) and ϕ is soil porosity (mm^3 mm^{-3}).

[e] The first two values correspond to C fluxes into MIC_r, the second two values correspond to C fluxes into MIC_K.

[f] For MIC_r and MIC_K, respectively.

Table S2 The optimised MIMICS parameters (dimensionless) and their value ranges

Parameter	Definition	Range
xav	A scaling factor for V_{max}	0.1-10.0
xak	A scaling factor for K_m	0.5-20.0
xdesorp	A scaling factor for SOC desorption rate	0.1-2.0
xbeta	An exponent of the biomass-dependent mortality rate of microbes	1.0-2.0
xdiff	A scaling factor for SOC diffusion coefficient in soils	0.1-10.0
xnpp	A scaling factor for litter input represented by NPP	0.5-2.0

Table S3 The optimised MES-C parameters (dimensionless) and their value ranges

Parameter	Definition	Range
xak	A scaling factor for K_m	0.1-10.0
xfm	A scaling factor for metabolic litter inputs entering AGG_m	0.1-5.0
xtvp	A scaling factor for aggregated C breakdown rate	0.1-10.0
xtvc	A scaling factor for aggregation formation rate from MAOC	0.1-10.0
xqmax	A scaling factor for maximum adsorption capacity	0.5-5.0
xnpp	A scaling factor for litter input represented by NPP	0.5-2.0

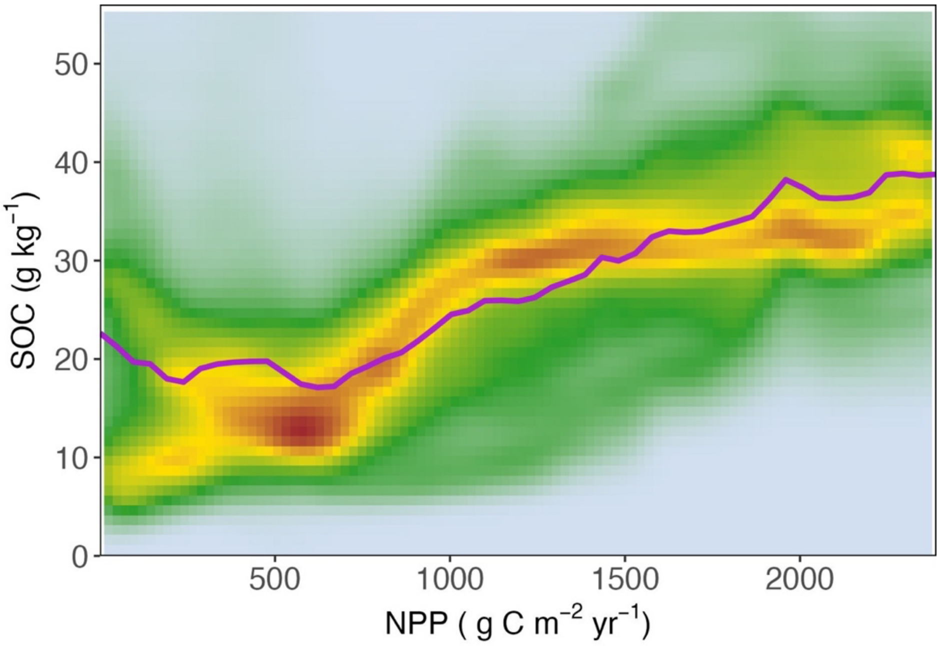

Figure S1. Density representation of ICE with respect to different predictors and observed SOC in natural ecosystems. The purple curves represent the mean partial dependence across all instances. Note that SOC greater than 56 g kg^{-1} (around 1% of data) are not shown here.

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