Observational benchmarks inform representation of soil organic carbon dynamics in land surface models

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Abstract

Representing soil organic carbon (SOC) dynamics in Earth system models (ESMs) is a key source of uncertainty in predicting carbon climate feedbacks. Machine learning models can help identify dominant environmental controllers and their functional relationships with SOC stocks. The resulting knowledge can be implemented in ESMs to reduce uncertainty and better predict SOC dynamics over space and time. In this study, we used a large number of SOC field observations (n = 54,000), geospatial datasets of environmental factors (n = 46), and two machine learning approaches (Random Forest (RF) and Generalized Additive Modeling (GAM)) to: (1) identify dominant environmental controllers of global and biome-specific SOC stocks, (2) derive functional relationships between environmental controllers and SOC stocks, and (3) compare the identified environmental controllers and predictive relationships with those in Coupled Model Intercomparison Project phase six (CMIP6) models. Our results showed that diurnal temperature, drought index, cation exchange capacity, and precipitation were important observed environmental controllers of SOC stocks. RF model predictions of global-scale SOC stocks were relatively accurate ($R^2 = 0.61$, RMSE = 0.46 kg m$^{-2}$). In contrast, precipitation, temperature, and net primary productivity explained >96% of ESM-modeled SOC stock variability. We also found very different functional relationships between environmental factors and SOC stocks in observations and ESMs. SOC predictions in ESMs may be improved significantly by including additional environmental controls (e.g., cation exchange capacity) and representing the functional relationships of environmental controllers consistent with observations.
Keywords: Environmental controllers, Earth system models, soil organic carbon, net primary productivity, machine learning, model benchmarking

1. Introduction

Soil is the largest actively cycling carbon pool in terrestrial ecosystems and stores almost twice the amount of carbon as in the current atmosphere (Lal, 2016). A small change in soil carbon stocks can lead to large changes in the atmospheric CO$_2$ concentration and future climate change trajectories. Soils also play a crucial role in sequestering atmospheric CO$_2$ as soil organic carbon (SOC) (Hinge et al., 2018). Thus, sequestration, protection, and sustainable management of SOC stocks can be a promising climate mitigation strategy (Lal, 2020). Accurate representation of global SOC storage and its environmental controllers are essential for predicting realistic changes of SOC under different land use and climate change scenarios. Yet, no consensus exists among current Earth system models (ESMs) in representing the spatial distributions of global SOC storage and its fate under future climate change scenarios (Friedlingstein et al., 2014; Arora et al., 2020).

Multiple environmental variables, including climatic and topographic factors, land use history, and edaphic properties, have been identified as possible controllers of SOC storage (Georgiou et al., 2021; Mishra et al., 2022). Current ESMs, however, use the effects of only a limited number of environmental factors in representing SOC storage and dynamics. A recent study that compared SOC stocks from multiple ESMs against observations indicated a large knowledge gap in both ESMs and observations (Georgiou et al., 2021). Therefore, it is important to compare ESM simulations against global SOC observational datasets to evaluate model performance and identify key environmental controllers of global SOC storage.
Benchmarking ESM simulations with observed data is a common approach for model evaluation (Luo et al., 2012; Todd-Brown et al., 2013; Collier et al., 2018). Through comparing model simulations with observations, model strengths, deficiencies, and needed improvements can be identified. The resulting understanding from SOC benchmarking could lead to new ESM land model structures (by identifying key processes) and new parameterizations (by quantifying key relationships between SOC and environmental variables). Thus, benchmarking analysis of ESMs is an effective tool to reduce uncertainties in predicting SOC dynamics and can provide more realistic information for managing SOC under changing climate conditions (Lauer et al., 2017).

Currently ESMs predict SOC stocks primarily with model representations that depend on soil temperature, moisture, and belowground net primary production (Todd-Brown et al., 2013). ESMs capture the positive correlation between NPP and precipitation, resulting in high SOC stocks for areas with high NPP in moist regions (Sun et al., 2016). Higher temperature increases soil respiration, which, in the short-term, reduces SOC storage. In the longer-term, increased soil respiration can release nutrients, leading to increased plant growth, belowground carbon inputs, and thereby SOC stocks; the balance of these factors can take centuries to manifest (Mekonnen et al., 2022). Soil respiration temperature sensitivity is often defined based on $Q_{10}$ or Arrhenius equations in ESMs (Wynn et al., 2006), although low- and high-temperature modifications to these relationships are likely needed (Jiang et al., 2013; Azizi-Rad et al., 2022).

In a previous U.S. continental-scale study, we derived empirical non-linear relationships between SOC and environmental factors that produced comparable prediction accuracy to a random forest (RF) machine learning approach (Mishra et al., 2022). We apply a similar approach in this study in both global field observations and ESMs to (1) identify key observed environmental controllers of, and functional relationships with, global SOC stocks and (2) evaluate ESMs with these...
observational benchmarks. Simulated SOC stocks from three CMIP6 ESMs (i.e., Community Earth System Model (CESM, Hurrell et al., 2013); U.K. Earth System Model (UKESM, Sellar et al., 2019); Beijing Climate Center model (BCC, Xiao-Ge et al., 2019) were benchmarked with 50,000 SOC profile observations across the globe. We used a machine learning (i.e., random forest) approach with 46 environmental factors to identify the key environmental controllers of SOC stocks at the global scale. We then applied a generalized additive model (GAM) to derive the predictive relationships between these key environmental factors and SOC stocks in observations and ESM simulations. Specific objectives of this study were to: (1) identify dominant environmental controllers of SOC stocks in field observations and CMIP6 ESMs, (2) derive observed and ESM-modeled functional relationships between environmental factors and SOC stocks, and (3) analyze these functional relationships to inform needed improvements in ESM representations of SOC dynamics.

2. Materials and Methods

2.1 Soil organic carbon stock observations

We used two datasets of SOC stocks for the topsoil layer (i.e., 0 – 30 cm) and the whole soil profile (i.e., 0 – 100 cm). The World Soil Information Service (WoSIS) compiled SOC profiles across the globe after quality assessment. The 2019 snapshot of the WoSIS dataset contained 111,380 soil profiles with SOC content information (unit: g C g-soil^{-1}) at different soil depths (Batjes et al., 2020). We estimated the SOC stock (g C m^{-2}) at different soil layers using:

\[ \text{SOC Stock} = \text{SOC Content} \times \left(1 - \frac{G}{100}\right) \times BD \times D \]  

(1)

where G is the coarse fragment fraction (%); BD is the bulk density of soil (g m^{-3}); and D is the soil layer depth (m).
When the measured bulk density value was absent from the dataset, we used a pedo-transfer function (Yigini et al., 2018) to estimate the soil bulk density:

\[ BD = \alpha + \beta \times \exp(-\gamma \times OM) \]  

(2)

Where OM is organic matter, equivalent to SOC×1.724, with SOC content in percent (%); \( \alpha, \beta, \) and \( \gamma \) are fitting parameters. We found \( \alpha = 0.32, \beta = 1.30, \) and \( \gamma = 0.0089 \) after fitting WoSIS data to this equation.

Another dataset we used in this study was compiled from Mishra et al. (2021). This dataset contained 2,546 soil profiles with SOC stock (g C m\(^{-3}\)) information from permafrost regions in North America, northern Eurasia, and the Qinghai-Tibet Plateau. In total, we used 113,926 soil profile observations from these two data sources. SOC stocks of different soil layers were then summed to SOC stocks in 0 – 30 cm and 0 – 100 cm depth intervals. Because not all these soil profiles covered the whole 0 – 30 cm or 0 – 100 cm intervals, we used a total of 54,000 soil profiles that included SOC stock information for both depth intervals. The geographical distributions of soil profiles used in this study are shown in Figure 1. Because SOC stock values across the globe were highly skewed, we used a natural logarithm transformation in this study.

2.2 Environmental predictors of SOC stocks

The storage and cycling of SOC are controlled by multiple environmental factors. In this study, we used observations of 46 environmental variables, which represented major soil forming factors (McBratney et al., 2003.). Twenty-one of the 46 environmental variables were climatic variables, including annual average temperature, precipitation, evapotranspiration, drought severity index, and statistics for different temporal scales (e.g., during the wettest and driest quarter in a year). Thirteen of the 46 variables described soil properties (e.g., clay content, sand content, silt content, soil texture, pH, and cation exchange capacity). Six variables represented topographic factors (e.g.,
Six variables represented land use and land cover types. All the categorical variables were converted to integer variables and the environmental variables were resampled to a common 1 km resolution. The environmental factors, their original spatial resolution, and data sources are provided in the supporting information (Table S1).

2.3 Selection of dominant environmental controllers of SOC stocks

We used RF to select dominant environmental predictors of SOC stocks within biomes and at global scale in both observations and ESMs. RF is an ensemble learning method, which is an extension of the classical Classification and Regression Trees (CART). Building a collection of uncorrelated CARTs through bootstrapping the samples and applying the random subspace method at each branch of the trees, RF improves the prediction performance (Breiman, 2001; Wiesmeier et al., 2011; Mishra et al., 2020). RF is well known for its strength in modeling highly nonlinear relationships between the predictors and is robust to overfitting (Chagas et al., 2016). Moreover, RF is not very sensitive to the choice of the hyperparameters, which makes RF one of the most popular off-the-shelf model for many classification and regression problems.

In this study, we trained the RF model using SOC content as a response variable and environmental factors as predictors. The model performance was evaluated using the coefficient of determination ($R^2$) and root mean square error (RMSE). A 10-fold cross-validation was used to compute $R^2$ and RMSE. Biome-specific analyses were conducted on a subset of the global dataset. For biome classification, we used the IGBP land classes (Loveland and Belward, 1997). The “Random-Forest” package in R was used to train a RF model using all the observed environmental factors in the dataset and to identify dominant environmental controllers of SOC stocks. Prior to fitting into the final model, we performed a potential collinearity test among the environmental variables by
calculating pairwise correlations and variance influence factors. Predictors showing a variance influence factor (VIF) value greater than 10 were omitted, leaving 14 uncorrelated environmental predictors of SOC stocks in the observations.

2.4 Generalized additive model

Generalized additive model (GAM) is an extension of generalized linear models, which employs spline functions to model nonlinear relationships between predictor and response variables (Arnold et al., 2013). In GAM, the relationship between predictor and response variable can be modeled as (Hastie and Tibshirani, 1987):

\[
Y = C + \sum_{i=1}^{p} f_i(X_i)
\]  

(3)

Here, Y is the response variable (SOC), C is a constant, X_i are the environmental controller variables, f_i is a spline function for X_i, and p is the total number of environmental controllers. We used the “mgcv” package in R to build GAMs for the observations as well as CMIP6 ESMs (Arnold et al., 2013). The performance of GAMs was evaluated by using R^2 and RMSE.

2.5 Earth system model outputs

We downloaded and aggregated the SOC and environmental controller data from three ESMs that participated in CMIP6: Community Earth System Model (Hurrell et al., 2013.), U.K. Earth System Model (Sellar et al., 2019), and Beijing Climate Center model (Xiao-Ge et al., 2019). These ESMs included most of the environmental factors used by CMIP6 ESMs. ESMs did not report depth-dependent soil carbon projections, making direct comparison with depth-dependent SOC observations difficult. The majority of land models used in ESMs were designed to simulate topsoil
carbon for topsoil depth; thus, we assumed that the simulated soil carbon is contained within 1 m of soil profile to simplify comparison with observations.

3. Results

3.1 Descriptive statistics of SOC observations

The average global SOC stock in the 0 - 1 m depth interval was 13.5 kg C m$^{-2}$, ranging from 0.14-435.3 kg C m$^{-2}$. Summary statistics of SOC stocks at global scale and within different biomes is presented in Table 1. The standard deviation showed a similar spread in SOC stock values in croplands (n=21820), savannas (n=9807) and grasslands (n=5938). However, in forests (n=12164) and shrublands (n=3769), the standard deviation was higher indicating a large range in SOC stock values. Distributions of total SOC stocks in different biomes are presented in Figure 2. Across different biomes, forests contain the largest organic carbon content globally, with a mean value of 15.9 kg C m$^{-2}$ and standard deviation 20.7 kg C m$^{-2}$.

3.2 Dominant environmental controllers of SOC stocks in observations and ESMs

At the global scale, we found that diurnal temperature, drought severity index, annual temperature, and cation exchange capacity are the dominant environmental controllers of SOC stocks in observations (Figure 3). By including all the environmental controllers, the RF model explained 61% of observed global spatial SOC variation. $R^2$ ranged from 48% in savannas to 65% in croplands (Table 2) and the importance of key environmental controllers varied between biomes (Figure 4). In croplands, precipitation, drought, diurnal temperature, and cation exchange capacity were identified as the dominant controllers of SOC stocks. In grasslands, annual temperature, cation exchange capacity, and sand content were the dominant controllers. In forests, cation exchange capacity, precipitation, and temperature were dominant controllers. In
shrublands, annual temperature, soil pH, and cation exchange capacity were the most important controllers. In savannas, soil related variables, temperature, and precipitation were the most important controllers. Across all land cover types, we found that cation exchange capacity and seasonal climatic variables were the dominant environmental controllers of SOC stocks.

In contrast, the RF model with 8 environmental variable predictors made near-perfect predictions of ESM simulated SOC stocks (average $R^2 = 0.95$, $R^2$ values for UKESM, CESM, and BCC model were 0.99, 0.89, and 0.98, respectively). In contrast to the results obtained from the observed SOC stocks, the dominant controllers of ESM simulated SOC stocks were annual temperature, net primary productivity (NPP), and annual precipitation (Figure 5). In particular, NPP was by far the most dominant predictor of SOC stocks in the UKESM.

3.2 Predictive relationships between environmental factors and SOC stocks

Dominant environmental controllers of observed SOC stocks identified by the RF model were used in GAM to derive predictive relationships. We retrieved explicit analytical expressions by fitting the splines derived from GAM in the observation dataset. Notwithstanding its role as the sole carbon source to soil, our results did not show NPP as a strong controller on observed SOC stocks (Figure 6a). In contrast with field observations, all ESMs showed significant dependence (exponential increase) of SOC stocks on NPP. Our results also showed that observed SOC stocks increased almost linearly with observed annual precipitation (Figure 6b). In contrast, ESMs show different relationships between SOC and precipitation. We found a nonlinearly increasing SOC with precipitation in CESM, an initial sharply increasing and then decreasing relationship in UKESM, and a decreasing relationship in BCC ESM. On the relationship between SOC storage and soil texture and elevation, ESMs do not capture the
observed relationships. Our results indicated that observed SOC stocks decreased with clay
content in the interval between 0 and 20%, and then increased with clay content above 20%
(Figure 6c). Observed SOC stocks increased with silt content up to 55% and then decreased
(Figure 6d).

SOC stock functional relationships differed between the three ESMs and in many cases
differed with the relationships we derived from observations. In terms of the effects of annual
temperature on modeled SOC storage, we found that SOC stocks decreased with annual
temperature and were most sensitive to temperature in the range between 0 and 10°C (Figure 6e).
However, while the three ESMs captured the general negative relationship between SOC storage
and temperature, none of them correctly described the varying sensitivity of SOC in different
temperature ranges (especially in extreme temperature ranges <0°C and >20°C). In representing
the control of elevation on SOC storage, only UKESM showed consistent patterns with
observations, where SOC storage remained stable when the elevation was lower than 2000 m and
decreased when the elevation was higher than 2000 m (Figure 6f).

Discussion

Previous studies have suggested that the spatial variation of SOC is dependent on multiple
environmental factors such as climatic and edaphic variables, geography, and vegetation. Here,
we found that climatic variables (i.e., temperature and precipitation) are the most important
controllers of global SOC stocks, followed by edaphic variables (i.e., cation exchange capacity),
topography (i.e., elevation), and vegetation (i.e., NPP). Using boosted regression trees, Luo et al.
(2021) studied edaphic and climatic controls on SOC dynamics at different soil depths and found
that soil type and climatic variables are the most important variables in explaining the SOC
stocks (Luo et al., 2021). In this study, we found that seasonal climatic variables such as diurnal temperature range and precipitation seasonality are among the most important environmental controllers in explaining the spatial variation of SOC stocks. This result indicates the critical role of seasonal and interannual climatic variables in understanding SOC dynamics.

The importance of climatic variables on global SOC storage emerges from close links with processes that affect ecosystem productivity and soil microbial processes. Consistent with our findings, Wiesmeier et al. (2014) reported climatic variables (temperature and precipitation) as significant controllers of SOC stocks up to 1 m depth in German soils under oceanic climate (Wiesmeier et al., 2014). Sreenivas et al. (2014) used RF to predict the SOC variability across semi-arid and humid areas of India in the top 30 cm of soil and found that the top three environmental controllers were land cover, mean temperature of hottest months, and mean annual precipitation (Sreenivas et al., 2016). In our analysis, the overall relative importance of climatic variables was significantly higher than other variables at the global and biome scales.

Soil properties were identified as the second most important controllers of global SOC stocks. Soil properties impact various processes that govern soil carbon dynamics. For example, soil properties impact microbial activity, porosity, and oxygen availability in the soil profile, which directly or indirectly control soil water dynamics, plant growth, and SOC stocks.

Consistent with our findings, Luo et al. (2021) reported that sand content, silt content, and soil pH were significant controllers of SOC stocks in all soil depths globally.

The Palmer drought severity index, which indicates low soil moisture availability, was a dominant controller of global SOC stocks. Consistent with our findings, Li et al. (2021) reported that soil particle size and soil water content were the most influential predictors of SOC variation (Li et al., 2021). Soil drought, indicating more negative soil water potential and low soil
hydraulic conductivity, can cause tree mortality (Anderegg et al., 2012). Climate extremes like droughts can impact the structure, composition, and functioning of terrestrial ecosystems and can thereby severely affect the regional carbon cycle (Frank et al., 2015).

Cation exchange capacity is a soil property that indicates the active soil surface to which SOC may be adsorbed, and polyvalent metal cations can play a significant role in SOC stabilization by binding organic compounds to mineral surfaces (O’Brien et al., 2015; Solly et al., 2020). O’Brien et al., (2015) found that exchangeable soil Ca$^{2+}$ is a significant predictor of SOC stocks. This relationship is supported by the mechanism that Ca$^{2+}$ and Mg$^{2+}$ promote clay flocculation and bind organic matter to clay surfaces. Solly et al. (2020) reported that SOC and cation exchange capacity are significantly related in both topsoil and subsoil with strong positive relationship.

After climatic factors and cation exchange capacity, topography and vegetation (NPP) were important controllers of observed global SOC stocks. Effects of NPP on observed SOC stocks was found to be small (~6% in 0-100 cm soil depth). Similar to our findings, Luo et al. (2021) reported NPP explaining about 10% of the variation of SOC stocks. NPP delivers the primary inputs of carbon to soil and NPP generally increases with moisture, temperature, and CO$_2$ up to a certain limit (Todd-Brown et al., 2013). NPP also depends on the availability of soil nutrients. Most ESMs overestimate the increase in SOC pools in response to NPP increases (Todd-Brown et al., 2013). The effects of NPP on SOC also depend on biome type and soil depths (Luo et al., n.d.; Georgiou et al., 2021). The contribution of NPP on SOC stocks mostly depends on how much NPP ends up in the soil and how it is translocated to different soil depths. Georgiou et al. (2021) reported a saturating relationship of SOC stocks with increasing NPP in a
global observational dataset. However, Chen et al., (2018) reported high SOC stocks with increasing productivity and soil water holding capacity (Chen et al., 2018).

The three CMIP6 ESMs we analyzed predicted SOC stocks mostly as a function of temperature, precipitation, and NPP. These ESMs simulated positive correlations between SOC stocks and NPP (Figure 5a), resulting in high SOC stocks in areas with high NPP in most regions (Shi et al., 2013; Sun et al., 2016). In these ESMs, effects of temperature and precipitation on SOC stocks are driven by soil respiration. Most current ESMs simulate the response of soil respiration to temperature using either a Q_{10} or Arrhenius equation (Wynn et al., 2006), such that a higher temperature causes more soil respiration, and, all else equal, eventually reduces SOC stocks (Figure 5b). Our results showed diverse control of precipitation on SOC stocks in different ESMs. Todd-Brown et al. (2013) showed that ESM soil respiration either increases monotonically with precipitation, or first increases to a plateau under optimal precipitation and then decreases with further increasing precipitation. Consistent with those results, the ESMs we analyzed in this study showed different dependence of SOC storage on annual precipitation.

In this study, we found that, in comparison to the patterns that emerged from observations, ESMs have distinctively different emergent relationships between environmental factors and SOC stocks. These results could either result from unrealistic parameterization or missing critical processes in model representation. Our results show that observed global SOC stocks are controlled not only by temperature, precipitation, and NPP. Effects of other environmental factors, such as drought severity index and cation exchange capacity should also be considered in future representations of SOC dynamics in ESMs. It is also imperative to compare observational data and ESM simulations to improve model structures and parameterization.
5. Conclusion

Our results document disagreement between environmental controllers of SOC stocks in observations and ESM land models. Specifically, NPP, annual temperature, and annual precipitation have dominant control in modeled SOC stocks. In contrast, diurnal temperature, drought index, annual temperature, cation exchange capacity, and other soil related variables are the dominant controllers of observed SOC stocks. Using field observations and data for environmental factors, machine learning techniques predict about 60% of the variability in observed global SOC stocks, while in ESMs, only a few environmental factors predict about 95% of the variability in predicted SOC stocks. Comparisons of derived functional relationships between the environmental factors and SOC stocks in observations and ESM models also show discrepancies. These discrepancies indicate the importance of efforts to benchmark ESM land models and to improve the mechanistic representations that are affected by the observed dominant environmental controllers. Such an effort could decrease disagreements between observed and modeled SOC stocks.

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References


Figures and Tables

Figure 1. Spatial and statistical distributions of 54,000 soil organic carbon profiles used in this study.
Figure 2: Boxplot of soil organic carbon content (logarithmic scale) for each biome or land cover type analyzed in this study. The horizontal line in the middle of the boxes is the median while their lower and upper limits correspond to the first and third quartiles.
Figure 3: Importance of different environmental factors to predict the global soil organic carbon stocks in observations.
Figure 4: Strengths and importance of environmental controllers of observed SOC stocks within different biomes.
Figure 5: Importance of different environmental factors on global soil organic carbon stocks in three CMIP6 earth system models.
Figure 6: Predictive relationships between environmental factors and soil organic carbon stocks in observations (black line) and CMIP6 earth system models (different colors).
Table 1: Descriptive statistics of global soil organic carbon stocks at 0-100 cm depth interval.

<table>
<thead>
<tr>
<th>Location</th>
<th>Depth (cm)</th>
<th>Minimum (kgC m$^{-2}$)</th>
<th>Maximum (kgC m$^{-2}$)</th>
<th>Mean (kgC m$^{-2}$)</th>
<th>Median (kgC m$^{-2}$)</th>
<th>Standard Deviation (kgC m$^{-2}$)</th>
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<td>435.3</td>
<td>13.5</td>
<td>9.5</td>
<td>18.2</td>
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<td>9.5</td>
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Table 2: Prediction accuracies of Random Forest models across biomes and at global scale in predicting SOC stocks.

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<th>Location</th>
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