PNNL-38840

Leveraging High-resolution Molecular Composition of Soil Organic Matter to Enhance Carbon Cycling Modeling

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Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Abstract

Soils store more carbon than the atmosphere and vegetation combined, yet Earth system models still struggle to predict how this vast reservoir will respond to environmental change. A central limitation is that most soil biogeochemical models represent organic matter using bulk conceptual pools or chemically homogeneous fractions, preventing direct use of rapidly expanding molecular-scale datasets. Here we develop and test a new soil decomposition framework that explicitly integrates high-resolution information on organic matter composition. First, we construct a molecularly informed litter decomposition module in which plant inputs are partitioned into five functional compound classes—carbohydrates, proteins, lignin-like aromatics, lipids, and carbonyls—using a molecular mixing model calibrated to solid-state ^{13}C Nuclear Magnetic Resonance (NMR) spectra. Class-specific kinetics, lignin-dependent physical protection, and substrate-driven microbial carbon use efficiency allow the module to capture metabolic tradeoffs associated with enzyme production and nutrient limitation. We then embed this litter module within a microbially explicit whole-soil model that tracks the transformation of these compound classes through particulate organic matter, dissolved organic matter, mineral-associated organic matter, and microbial biomass. High-resolution Fourier Transform Ion Cyclotron Resonance mass spectrometry (FTICR-MS) data are used to link internal pools to measurable soil organic matter fractions and to constrain key process parameters. Applications at soil-core and ecosystem scales demonstrate that the new model reproduces observed soil respiration dynamics while providing mechanistic attribution of CO_2 fluxes to specific chemical classes and pools. Compared to existing frameworks such as the Community Land Model soil biogeochemistry module and the Millennial model, our approach maintains competitive predictive skill while substantially improving interpretability and opportunities for data–model integration. This work illustrates a viable pathway for leveraging molecular-scale observations to reduce structural uncertainty in soil carbon–climate feedback projections.

Acknowledgments

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Contents

1.0 Introduction

Soils constitute the largest terrestrial reservoir of organic carbon, and the persistence of this pool is a critical regulator of atmospheric CO_2 concentrations and climate. A substantial fraction of long-lived soil organic matter (SOM) exists as mineral-associated organic matter (MAOM), yet the mechanisms governing its formation and, crucially, its vulnerability to destabilization remain a major source of uncertainty in ecosystem and Earth system models. Long-term soil carbon storage is not an intrinsic property of specific molecules, but an emergent outcome of interactions among the chemical diversity of organic inputs, microbial metabolic processing, and physicochemical protection on mineral surfaces. Accurately projecting soil carbon–climate feedbacks therefore requires process-based models that can mechanistically resolve how SOM chemodiversity interacts with microbial communities and minerals.

Over the past decades, soil carbon models have evolved from simple first-order decay formulations with bulk conceptual pools to microbially explicit frameworks that represent biomass dynamics, enzyme-mediated decomposition, and non-linear kinetics. These advances correctly position microbes as the primary agents of carbon transformation and have motivated a shift toward models organized around empirically measurable soil fractions such as particulate organic matter (POM) and MAOM. Despite this progress, most models (Parton et al. 1987; Abramoff et al. 2018; 2022) still treat these fractions as chemically homogeneous reservoirs with fixed decomposition parameters. As a result, they cannot exploit the rapidly growing body of molecular-scale observations that characterize SOM chemodiversity across litter, POM, dissolved organic matter (DOM), MAOM, and microbial biomass (Lehmann and Kleber 2015).

Advanced analytical techniques such as solid-state ^{13}C nuclear magnetic resonance (NMR) spectroscopy and high-resolution Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) now provide detailed information on the molecular makeup of organic matter in plant litter and soil fractions. However, few models directly incorporate these data into their structure or parameterization. Most frameworks represent plant inputs and internal SOM pools using broad chemical groupings or bulk indices, limiting their ability to connect observed changes in molecular signatures to process-level hypotheses, such as shifts in microbial enzyme allocation, resource-use strategies under nutrient limitation, or changes in sorption affinity and desorption rates on mineral surfaces. Likewise, they struggle to explain why chemically similar inputs can follow divergent pathways into respiration versus long-term stabilization, or how environmental change alters the molecular routes by which carbon becomes vulnerable or protected. Integrating molecular data into model structure and parameterization offers a pathway to bridge this divide (Bonanomi et al. 2013), enabling models that are constrained by and comparable to observable chemical metrics.

Here we develop a process-based modeling framework, CRUMB (Chemically Resolved Unified Microbial Biogeochemistry), that explicitly integrates molecular-scale information on organic matter composition into both litter and whole-soil models. First, we construct a litter decomposition module in which plant inputs are partitioned into five functional compound classes—carbohydrates, proteins, lignin-like aromatics, lipids, and carbonyls—informed by the NMR data. We then embed this module within a microbially explicit soil model that tracks the transformation of these compound classes through POM, DOM, MAOM, and microbial biomass, and that can be constrained with high-resolution FTICR-MS measurements. Applications at soil-core and ecosystem scales, including comparison with existing frameworks such as the CLM soil biogeochemistry module (Lawrence et al. 2019) and the Millennial model (Abramoff et al. 2018; 2022), demonstrate how molecularly explicit structure improves both predictive performance and interpretability.

2.0 Model Development

2.1 Conceptual Framework

Our overarching goal is to represent how the chemical diversity of plant inputs and SOM shapes decomposition, microbial activity, and carbon storage in a way that can be directly constrained by molecular-scale measurements. The framework couples three core elements: (1) chemically resolved plant litter inputs, (2) microbially mediated transformations among SOM pools, and (3) interactions between organic matter and mineral surfaces that give rise to MAOM.

At the ecosystem level, plant inputs enter the soil as above- and belowground litter and root exudates. These inputs differ in their molecular composition, ranging from labile carbohydrates and proteins to more slowly decomposing lignin-rich and lipid compounds. Microbial communities process this chemically diverse input, investing carbon and nutrients into extracellular enzymes that depolymerize complex substrates, assimilating a fraction of the released DOM into biomass while respiring the remainder as CO_2. Microbial necromass, together with residual plant-derived fragments, contributes to POM and can further associate with mineral surfaces to form MAOM. Environmental conditions such as temperature and moisture modulate the rates of these processes.

The conceptual framework treats SOM persistence as an emergent property of these coupled biological and physicochemical processes rather than as an intrinsic feature of particular molecules. Chemical diversity enters the model explicitly through the representation of distinct organic compound classes, while microbial physiology is represented through carbon use efficiency, enzyme allocation, and nutrient constraints. Organo-mineral interactions are represented through sorption, desorption, and exchange processes that transfer organic matter between POM, DOM, and MAOM. High-resolution molecular data, including solid-state ^{13}C NMR for plant litter and FTICR-MS for soil fractions, provide the empirical basis for defining the relevant compound classes and for constraining the distribution and turnover of these classes across pools.

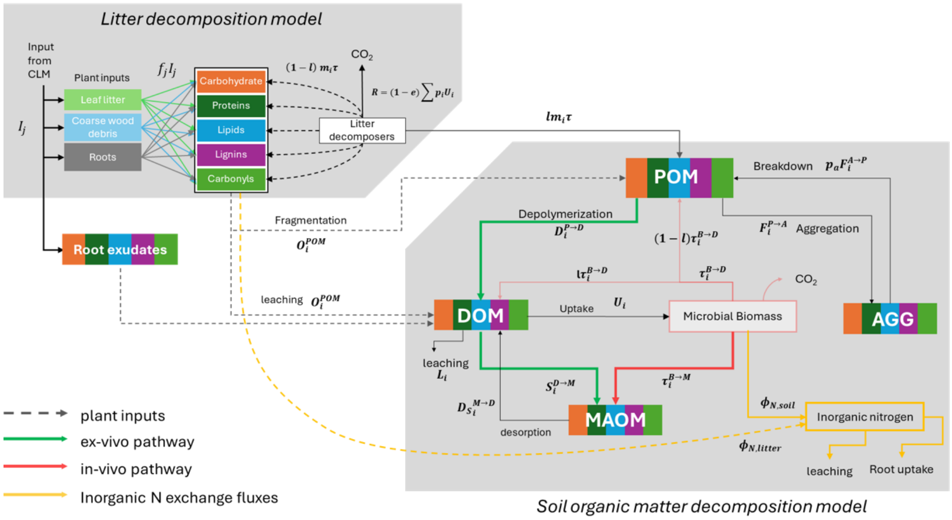

Figure 1. Conceptual structure of the CRUMB model. Plant inputs from CLM are partitioned into five functional chemical classes (carbohydrates, proteins, lipids, lignins, carbonyls) using the litter decomposition module, which simulates microbially mediated decay

and CO_2 release. Chemically resolved litter and root exudates feed into soil organic matter pools—particulate organic matter (POM), dissolved organic matter (DOM), aggregate-associated organic matter (AGG), and mineral-associated organic matter (MAOM)—each represented as the same five compound classes. Inorganic nitrogen dynamics (mineralization, leaching, and root uptake) are coupled to carbon flows, allowing CRUMB to link molecular composition, microbial activity, and mineral interactions to emergent soil C and N cycling.

Figure 1 illustrates the main components and fluxes in this framework. Plant inputs, characterized by their molecular composition, enter the soil and are partitioned into chemically defined litter pools. Microbial activity transforms these pools into POM, DOM, and MAOM while generating CO_2. DOM serves as the immediate substrate for microbial uptake and as the exchange medium between particulate and mineral-associated pools. MAOM is formed by sorption and association of organic molecules with mineral surfaces and can be destabilized through desorption and displacement processes, returning carbon to more reactive pools. This conceptual structure underlies the more detailed, chemically resolved decomposition framework described in the next section.

2.2 Chemically Resolved Decomposition Framework

The chemically resolved decomposition framework implements the conceptual model above using explicit state variables for organic matter pools, microbial biomass, and inorganic nitrogen, together with class-specific kinetics and regulatory functions.

The model tracks carbon in five compound classes—carbohydrates, proteins, lignin-like aromatics, lipids, and carbonyl-rich compounds—that are present in plant litter and are propagated, in transformed form, through soil pools. Plant litter inputs are partitioned into these classes using a molecular mixing approach informed by solid-state ^{13}C NMR spectra of leaves, roots, and woody debris. For each litter type, the mixing model provides the initial mass of each compound class, ensuring that the model's representation of input chemistry is quantitatively linked to measurable NMR features.

Within the soil column, organic carbon is stored in three primary SOM pools (POM, DOM, and MAOM), along with a microbial biomass pool and an inorganic nitrogen pool. POM contains relatively large organic particles derived from partially decomposed plant residues and microbial necromass; MAOM represents organic molecules associated with mineral surfaces; and DOM consists of soluble compounds that mediate exchanges among POM, MAOM, and microbes. Each SOM pool carries information on the relative abundance of the five compound classes, allowing the model to represent class-specific decomposition and transfer rates.

Decomposition is modeled as enzyme-mediated transformation of organic matter into DOM and CO_2. For litter and POM, class-specific depolymerization rates are parameterized using first-order kinetics, modified by protection and accessibility functions (Figure 2A). Lignin-rich material provides physical and chemical shielding to embedded carbohydrates and proteins; this effect is represented using a sigmoidal protection function that decreases the effective decay rate of these labile classes as the lignin fraction increases (Chakrawal et al. 2024). DOM compounds are subject to sorption and desorption between solution and mineral surfaces, controlling their residence time in MAOM and their availability for microbial uptake.

Microbial physiology is represented through carbon use efficiency (CUE), enzyme allocation, and nutrient constraints (Chakrawal et al. 2022). Microbes take up DOM and allocate it to growth, maintenance, and enzyme production. Maximum CUE depends on the average oxidation state of carbon in the available substrates and can be reduced by the energetic cost of producing oxidative enzymes required to degrade more recalcitrant compounds. Nitrogen availability further modifies CUE through overflow respiration and altered enzyme allocation when microbes experience N limitation or excess. These regulatory mechanisms allow the model to capture tradeoffs between rapid exploitation of labile substrates and investment in accessing more protected carbon.

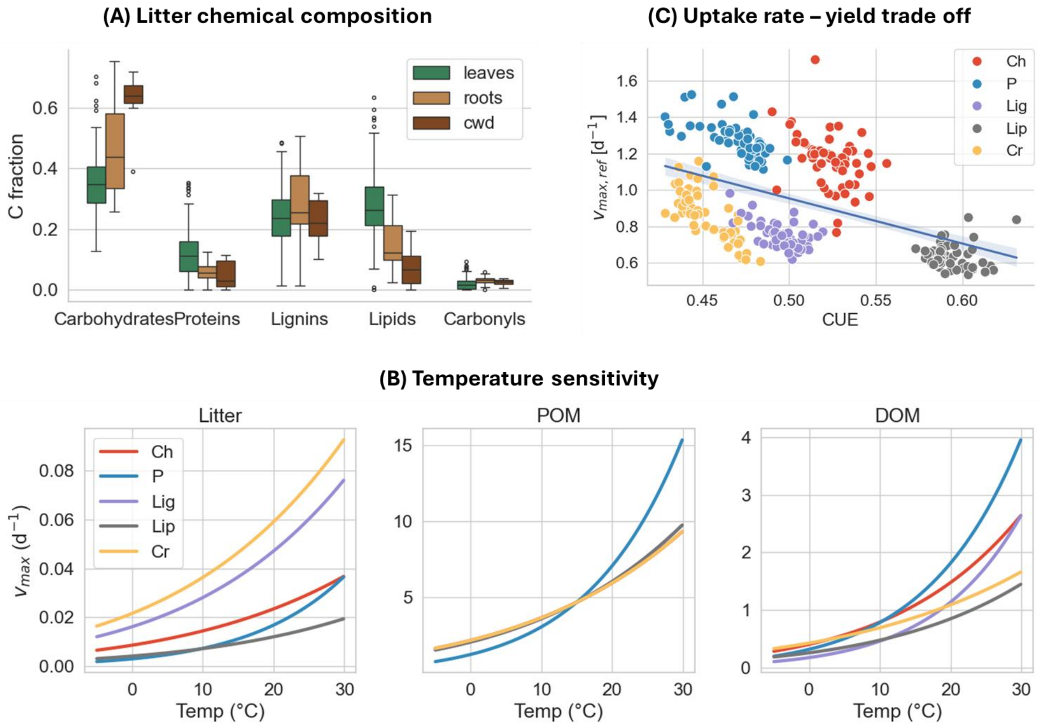

Figure 2. Parameterization of chemically specific processes in CRUMB. Legend in panel B and C are Ch: carbohydrates, P:proteins, Lig: lignin-like aromatics, Lip: lipids, and Cr: carbonyl-rich compounds.

High-resolution FTICR-MS measurements of soil fractions inform the distribution of compound classes within POM, DOM, and MAOM and are used to constrain key parameters controlling sorption, desorption, and class-specific turnover (Figure 2). This linkage enables direct comparison between modeled pool composition and observed molecular signatures and supports calibration against both fluxes and composition.

Together, the chemically resolved pool structure, class-specific kinetics, and microbial regulation schemes provide a mechanistic basis for simulating how molecular composition shapes decomposition dynamics and carbon persistence. The following sections apply this framework to litter- and soil-core-scale experiments and to an ecosystem-scale application at the KONZ NEON site.

2.3 Numerical Implementation and Parameterization

CRUMB is implemented as a system of ordinary differential equations that track the mass of carbon in each pool and molecular class over time. The model is designed to be modular, with separate but coupled components for litter inputs, microbial biomass dynamics, POM and DOM transformation, and MAOM formation and loss. Simulations are typically run at time steps appropriate to the application: sub-daily to daily time steps for capturing microbial dynamics and sorption–desorption processes, aggregated to monthly or annual outputs for comparison with many observational datasets.

The numerical solution employs standard ODE solvers with adaptive time-stepping to ensure stability and efficiency, particularly when coupling relatively fast microbial and sorption processes with slower changes in bulk soil carbon stocks. Environmental drivers such as temperature and moisture can be incorporated as modifiers of rate constants, depending on data availability and application scale. Boundary conditions include prescribed litter and root inputs, and, when run at ecosystem scale, inputs from the Community Land Model (Lawrence et al. 2019; Lombardozzi et al. 2023).

Parameterization draws on multiple data sources. For the litter module, we use ^{13}C NMR datasets that provide functional group distributions for a wide range of litter types and decomposition stages, combined with litter mass loss and CO_2 flux measurements. These datasets are used to estimate class-specific decomposition rate constants, lignin shielding parameters, and relationships between CUE and substrate oxidation state. For soil pools, NMR measurements of POM and MAOM fractions inform initial compositions and constraints on class transitions, while FTICR-MS data on DOM and bulk SOM inform relative reactivity and sorption behavior of different compound classes.

Overall, the numerical implementation and parameterization strategy are designed to balance model complexity with observational constraints, ensuring that the added molecular detail in CRUMB is both scientifically meaningful and empirically grounded.

3.0 Soil-Core Scale Application

3.1 Root-Exudate Experiment and Model Setup

To illustrate how CRUMB can be used to test hypotheses about chemical controls on soil organic carbon (SOC) dynamics at the soil-core scale, we conducted a numerical experiment focused on root exudates. The experiment represents a single vertically uniform soil layer (i.e., a one-dimensional soil core without explicit depth structure) in which total soil C stocks and MAOM are tracked over time. All environmental drivers (temperature, moisture), soil physical properties, and model parameters were held constant across simulations; only the molecular composition of root exudates was varied.

Exudates were prescribed as a constant fraction of daily GPP simulated by CLM directly to the DOM pool, with identical total C input among scenarios. We compared three exudate chemistries: (1) carbohydrate-rich exudates, (2) “mixed” exudates with class proportions similar to typical plant root exudate mixtures, and (3) carbonyl-rich exudates representing organic-acid–dominated inputs. In a second set of simulations, we altered only the sorption–desorption parameters for carbonyl compounds to represent “fast ligand displacement,” in which organic acids more efficiently displace pre-existing MAOM from mineral surfaces. This design isolates the effect of exudate chemistry and its interaction with mineral desorption rates on MAOM and total SOC stocks.

3.2 Results and Discussion

CRUMB predicts that the chemical composition of root exudates strongly influences both MAOM formation and net SOC balance, even when the total quantity of exudate C is held constant (Figure 3). When exudates are dominated by carbohydrates, MAOM stocks increase most rapidly, and total SOC shows the largest net gain over the 20-year simulation. Mixed exudates also lead to a net increase in MAOM and SOC, but at a lower rate. In contrast, carbonyl-rich exudates (representing organic acids) produce markedly smaller gains in MAOM under the default, slower desorption scenario and, when desorption is accelerated, can even lead to net MAOM losses.

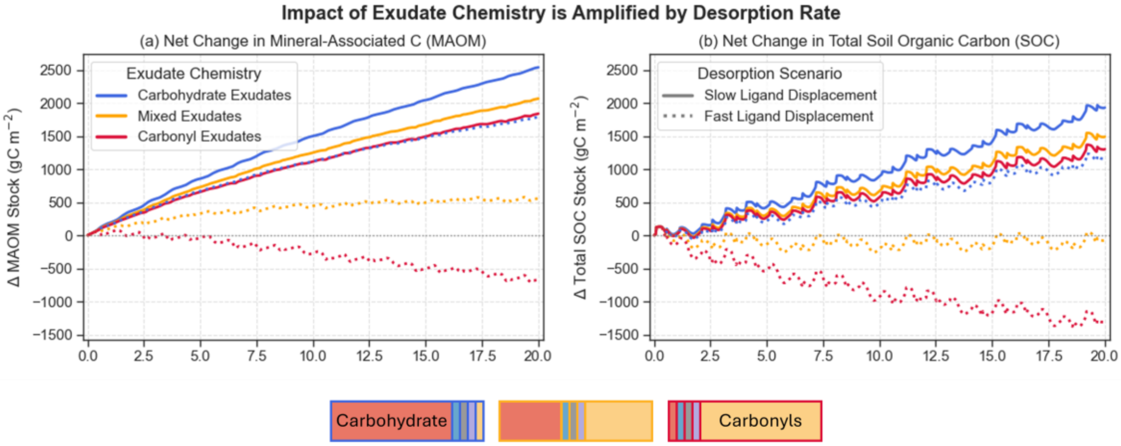

Figure 3. Effect of root exudate chemistry and desorption rate on soil carbon. Simulated changes in (a) mineral-associated organic matter (MAOM) and (b) total soil organic

carbon (SOC) over time for carbohydrate-, mixed-, and carbonyl-rich exudates under slow (solid lines) and fast (dotted lines) ligand–driven desorption.

The right panel of Figure 3 shows that the consequences of exudate chemistry are amplified when carbonyl-rich exudates are allowed to more effectively displace existing MAOM from mineral surfaces. Under this “fast ligand displacement” scenario, simulations with carbonyl-dominated exudates exhibit substantial net losses of total SOC relative to their initial state, whereas carbohydrate-dominated exudates still result in net SOC gains. Mixed exudates occupy an intermediate position, with SOC changes near zero or slightly negative under fast desorption. These patterns arise because carbonyl-rich exudates both (i) provide less efficient substrate for microbial growth (lower C use efficiency) and (ii) preferentially promote desorption and mineral dissolution, liberating previously stabilized MAOM carbon that is then respired.

Taken together, the soil-core exudate experiment demonstrates how CRUMB’s chemically resolved structure can be used to explore mechanistic hypotheses that connect molecular-scale traits of exudates to emergent soil C outcomes. The simulations support the hypothesis that organic-acid–rich exudation in N-limited soils can drive net SOC loss despite continued C inputs, whereas carbohydrate-rich exudation favors MAOM accumulation and SOC gain (Bölscher et al. 2025). More broadly, these results highlight that the sign and magnitude of root exudate effects on SOC depend not only on exudate quantity but also on their molecular composition and on the kinetics of ligand-promoted desorption from mineral surfaces—processes that are explicitly represented in CRUMB but are absent or highly simplified in conventional soil carbon models.

4.0 Ecosystem-Scale Application

4.1 Model Setup at the KONZ NEON site

We applied the new soil decomposition model at the ecosystem scale using one of the NEON sites, Konza Prairie Biological Station (KONZ), as a testbed. KONZ is a mesic grassland characterized by strong seasonality in temperature and moisture, with pronounced growing-season pulses in soil CO_2 efflux. This site provides continuous eddy-covariance and chamber-based measurements of soil respiration that we used for model evaluation.

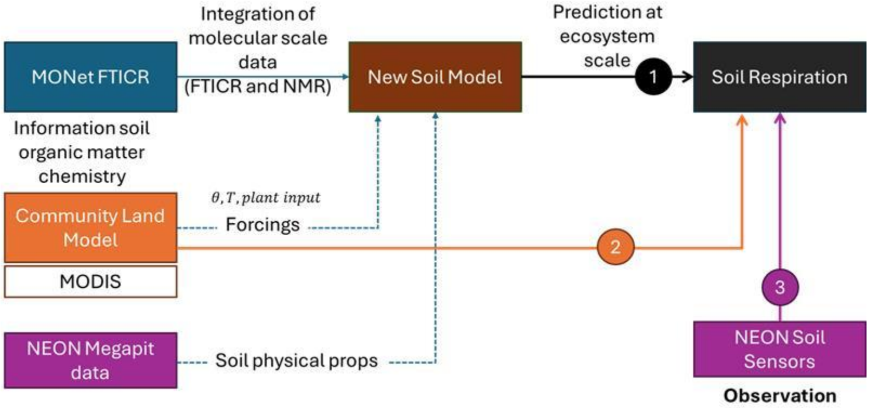

Figure 4. Simulation comparison between 1) the new CRUMB model; 2) the Community Land Model; 3) the measurement from NEON flux towers.

The new model was configured as a single soil layer representing the active rooting zone. Meteorological and plant productivity forcings were derived from a site-specific configuration of the Community Land Model (CLM), which provided time series of soil temperature, soil moisture, and plant litter inputs. Aboveground litter, belowground litter, and root exudates were partitioned into the five model compound classes including carbohydrates, proteins, lignin-like aromatics, lipids, and carbonyl-rich compounds. Root exudates were represented as a chemically labile mixture dominated by carbohydrate and carbonyl compounds, consistent with their composition as sugars and low-molecular-weight organic acids.

Within the soil, the model tracked carbon in the three SOM pools (POM, DOM, MAOM) and microbial biomass, each carrying information on compound-class composition. Decomposition and transfer fluxes among pools were governed by class-specific kinetics, lignin-dependent protection, microbial carbon use efficiency (CUE) linked to substrate chemistry and enzyme costs, and nitrogen constraints. Environmental scalars derived from CLM soil temperature and moisture modified decomposition and sorption/desorption rates.

For comparison, we also ran both the native CLM soil model and the Millennial model version 2 (Figure 4). All models were spun up under repeating climate and input conditions until soil C and N pools reached quasi-steady state. The evaluation period covered 2018–2021, during which modeled daily soil respiration was compared with NEON soil CO_2 efflux measurements. In addition to total respiration, the new model produced diagnostically useful outputs by attributing CO_2 production to the five compound classes.

4.2 Results and Discussion

Figure 5 summarizes the KONZ ecosystem-scale results. Panel A compares daily soil respiration from the three models with NEON measurements. All models reproduce the broad seasonal pattern of soil CO_2 efflux: low winter fluxes, rising rates in spring as soils warm and wet, and pronounced growing-season peaks. However, their dynamics differ in magnitude and temporal structure.

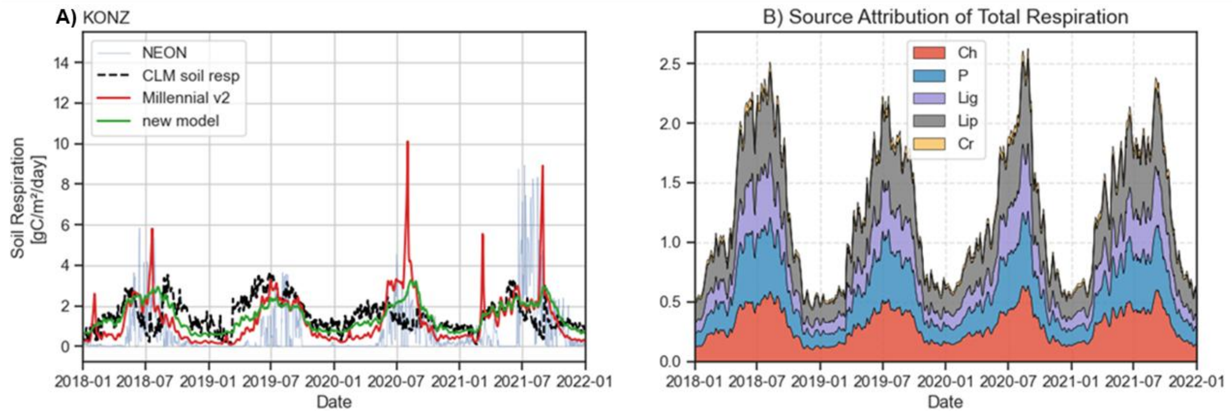

Figure 5. Comparison of modeled and observed soil respiration at the KONZ NEON site (A) and source attribution of total respiration by chemical class in the new model (B). Legend in panel B are Ch: carbohydrates, P:proteins, Lig: lignin-like aromatics, Lip: lipids, and Cr: carbonyl-rich compounds.

The CLM soil model tracks the seasonal envelope of respiration but tends to underestimate peak growing-season fluxes during some periods of high microbial activity. Millennial v2 captures certain pulse events but exhibits sharp, high-magnitude spikes in respiration following wetting events that are not supported by the smoother NEON observations. These spikes reflect the strong priming-like responses produced by its representation of substrate pulses and microbial dynamics. In contrast, the new model reproduces both the magnitude and timing of seasonal respiration more faithfully. It captures the onset and decline of growing-season fluxes, avoids the extreme transient peaks seen in Millennial v2, and produces a closer alignment with NEON measurements over multiple years.

Some of the remaining differences among the model trajectories can be attributed to their representation of soil vertical structures. Because the new model aggregates the soil column into a single layer, it implicitly averages strong vertical gradients in temperature, moisture, and substrate availability that are resolved explicitly in CLM.

Figure 5B demonstrates a key advantage of the molecularly explicit framework: the ability to attribute total soil respiration to specific compound classes. At KONZ, carbohydrates and proteins dominate CO_2 production during the early growing season, reflecting rapid microbial utilization of labile litter and root-derived inputs when conditions are favorable. As the season progresses, a growing share of respiration arises from the slow turnover of lignin-rich and lipid-associated material stored in POM and MAOM. Carbonyl-rich compounds contribute a smaller but persistent fraction of total respiration, consistent with their role as both labile substrates and agents of desorption from mineral surfaces. This decomposition of the bulk flux into chemically distinct sources is an emergent property of the class-specific kinetics and microbial regulation encoded in the model.

The KONZ application illustrates several broader implications of incorporating molecular composition into ecosystem-scale soil models. First, the new framework maintains predictive skill comparable to, and in some cases better than, existing soil biogeochemistry schemes while providing richer mechanistic diagnostics. Instead of treating soil respiration as a single aggregate signal, the model links temporal patterns in CO_2 efflux to the consumption of specific compound classes across litter, POM, DOM, and MAOM pools. Second, because internal state variables and fluxes are defined in terms of the same compound classes measured by NMR and FTICR-MS, the model provides a direct pathway for integrating site-specific molecular data into initialization, calibration, and evaluation. Finally, the KONZ results highlight the need to consider vertical structure jointly with process representation: extending the chemically resolved framework to a multi-layer soil column will be essential for fully leveraging its capabilities within land surface and Earth system models.

5.0 Conclusion and Future Work

The work described here demonstrates a viable approach for integrating molecular-scale information on organic matter composition into process-based models of litter and soil carbon dynamics. By combining a ^{13}C NMR–informed litter decomposition module with a microbially explicit whole-soil framework that can be constrained with FTICR-MS measurements, we link plant input chemistry to the formation, transformation, and loss of carbon in particulate, dissolved, and mineral-associated pools. This structure allows the model to represent key microbial tradeoffs associated with enzyme production and nutrient limitation, and to associate decomposition kinetics with measurable compound classes rather than bulk, chemically homogeneous pools.

Applications at soil-core and ecosystem scales show that the molecularly explicit model can reproduce observed respiration dynamics while providing additional diagnostic power. At the KONZ NEON site, for example, the new framework performs comparably to or better than existing soil biogeochemistry schemes such as the CLM soil model and Millennial v2, and uniquely attributes total soil CO_2 efflux to specific chemical classes. This capability strengthens the connection between modeled state variables and modern analytical datasets, enabling more direct testing of hypotheses about substrate use, mineral–organic interactions, and the conditions under which carbon becomes stabilized or destabilized.

Several challenges remain before such molecularly informed models can be applied routinely at regional and global scales. Molecular composition data from NMR and FTICR-MS are still limited in spatial and temporal coverage, requiring assumptions or statistical representations of chemotypes where direct measurements are unavailable. The coupling of multi-element stoichiometry, microbial traits, and multiple chemical classes also raises questions of parameter identifiability, especially when confronted with sparse observational constraints. Finally, the computational complexity of fully resolving chemical classes and microbial regulation may be prohibitive for long integrations in Earth system models without further model reduction.

Future work will focus on expanding and simplifying this framework in parallel. On the one hand, applying the model across diverse sites and soil types—particularly where depth-resolved molecular data are available—will help evaluate the generality of its parameterizations and reveal where chemical detail most improves predictive skill. On the other hand, we aim to extend the current single-layer formulation to a vertically resolved, multi-layer soil column so that depth gradients in temperature, moisture, and substrate availability can be represented consistently with land surface models such as CLM. This will allow a more direct, like-for-like comparison of process representations and help isolate the effects of molecularly explicit decomposition from those of vertical discretization. In parallel, we will develop reduced-complexity representations or emulators that preserve the essential controls of SOM chemodiversity and microbial physiology while being tractable for use in land and Earth system models. Together, these efforts will move toward soil carbon models that are simultaneously mechanistic, data-constrained, and scalable, thereby reducing uncertainty in projections of soil carbon–climate feedbacks.

6.0 References

Abramoff, Rose, Xiaofeng Xu, Melannie Hartman, et al. 2018. “The Millennial Model: In Search of Measurable Pools and Transformations for Modeling Soil Carbon in the New Century.” *Biogeochemistry* 137 (1): 51–71. https://doi.org/10.1007/s10533-017-0409-7.

Abramoff, Rose Z., Bertrand Guenet, Haicheng Zhang, et al. 2022. “Improved Global-Scale Predictions of Soil Carbon Stocks with Millennial Version 2.” *Soil Biology and Biochemistry* 164 (January): 108466. https://doi.org/10.1016/j.soilbio.2021.108466.

Bölscher, Tobias, Zoe G. Cardon, Mariela Garcia Arredondo, et al. 2025. “Vulnerability of Mineral-Organic Associations in the Rhizosphere.” *Nature Communications* 16 (1): 5527. https://doi.org/10.1038/s41467-025-61273-4.

Bonanomi, Giuliano, Guido Incerti, Francesco Giannino, Antonio Mingo, Virginia Lanzotti, and Stefano Mazzoleni. 2013. “Litter Quality Assessed by Solid State 13C NMR Spectroscopy Predicts Decay Rate Better than C/N and Lignin/N Ratios.” *Soil Biology and Biochemistry*, Special Issue: Interactions of Soil Minerals with Organic Components and Microorganisms VII and Enzymes in the Environment IV, vol. 56 (January): 40–48. https://doi.org/10.1016/j.soilbio.2012.03.003.

Chakrawal, Arjun, Salvatore Calabrese, Anke M. Herrmann, and Stefano Manzoni. 2022. “Interacting Bioenergetic and Stoichiometric Controls on Microbial Growth.” *Frontiers in Microbiology* 13 (May). https://doi.org/10.3389/fmicb.2022.859063.

Chakrawal, Arjun, Björn D. Lindahl, and Stefano Manzoni. 2024. “Modelling Optimal Ligninolytic Activity during Plant Litter Decomposition.” *New Phytologist* 243 (3): 866–80. https://doi.org/10.1111/nph.19572.

Lawrence, David M, Rosie A Fisher, Charles D Koven, et al. 2019. “The Community Land Model Version 5: Description of New Features, Benchmarking, and Impact of Forcing Uncertainty.” *Journal of Advances in Modeling Earth Systems* 11 (12): 4245–87. https://doi.org/10.1029/2018MS001583.

Lehmann, Johannes, and Markus Kleber. 2015. “The Contentious Nature of Soil Organic Matter.” *Nature* 528 (7580): 60–68. https://doi.org/10.1038/nature16069.

Lombardozzi, Danica L., William R. Wieder, Negin Sobhani, et al. 2023. “Overcoming Barriers to Enable Convergence Research by Integrating Ecological and Climate Sciences: The NCAR–NEON System Version 1.” *Geoscientific Model Development* 16 (20): 5979–6000. https://doi.org/10.5194/gmd-16-5979-2023.

Parton, W. J., D. S. Schimel, C. V. Cole, and D. S. Ojima. 1987. “Analysis of Factors Controlling Soil Organic Matter Levels in Great Plains Grasslands.” *Soil Science Society of America Journal* 51 (5): 1173–79. https://doi.org/10.2136/sssaj1987.03615995005100050015x.

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