Microbial physiology is an important control on soil respiration

Including microbial physiology response to temperature and substrate diffusion improves model predictions of soil respiration

Modeling soil respiration using models of varying complexity

Empirical and process-based models of soil respiration

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Key points

* Empirical functions of temperature and soil moisture alone cannot predict rapid changes in soil respiration
* Model predictions of soil respiration are more realistic when including a microbial biomass pool
* The model developed here is a general and parsimonious representation of C and N cycling in soil

# Abstract

Microbial populations are important agents of C and N mineralization in the soil. Soil organic matter can be broken down into monomers by extracellular enzymes and taken up into microbial biomass, where a portion of that matter is eventually mineralized as carbon dioxide or inorganic nitrogen. Most soil decomposition models, including those in earth system models, predict mineralization rates using empirical relationships with soil temperature and moisture, omitting microbes entirely. Though soil temperature and moisture explain a majority of the variation in C efflux measurements, linear combinations of temperature and moisture cannot predict rapid changes in soil C efflux, especially following wet-up events.

After wet-up events, drought-depleted microbial populations grow quickly, creating a positive feedback between increased substrate availability and microbial activity. We found that including a time-dependent microbial biomass pool produced more realistic predictions of soil respiration in a mid-latitude forest. The model developed here incorporates Arrhenius and either Michaelis-Menten kinetics or Equilibrium Approximation Kinetics to determine the effects of temperature and substrate availability on uptake and depolymerization rates, respectively. Microbes allocate substrate to enzyme production and biomass growth depending on the stoichiometry of the monomers that are taken up. Carbon and nitrogen cycling are explicitly tracked, and may be used to predict both C and N pools and fluxes.

Keywords: soil, modeling, decomposition, respiration, microbes

microbial physiology, C cycling, N cycling, diffusion

# Introduction

Soil microorganisms cycle C and N through the biosphere (Schlesinger, 2005), incorporating these elements into cellular materials that are eventually mineralized into carbon dioxide (CO2) and inorganic nitrogen (N). Soil is the largest terrestrial carbon (C) pool, and the flux of CO2 from the soil to the atmosphere is dominated by microbial decomposition ([Schlesinger & Bernhardt, 2013](#_ENREF_29)). Hence, the rate of C mineralized by soil micro-organisms affects the global C cycle.

The rate of C and N mineralization is often correlated with changes in temperature and precipitation, and from this relationship one can construct an empirical relationship between soil temperature, moisture, and mineralization rates (Rodrigo et al., 1997). Empirical soil temperature and moisture functions are used in earth system models for the purpose of predicting future mineralization rates under global change scenarios (Parton et al., 1987). The temperature sensitivity of SOM depoymerization is commonly thought to conform to Arrhenius kinetics ([Lloyd & Taylor, 1994](#_ENREF_23)). However, soil temperature is only the dominant driver of microbial activity when substrate supply is not limiting. When substrate supply is limited by diffusion or oxygen (O2) limitation, then alternative kinetics of substrate and/or enzyme concentration may better constrain mineralization rates (e.g., Michaelis-Menten, Reverse Michaelis-Menten, Equilibrium Chemistry Approximation; Tang et al., 2015).

Despite well-known effects of temperature and substrate supply on the activity of soil microbes, microbial processes have not been modeled explicitly in terrestrial biosphere models. In these models, decomposition rate is determined using a linear rate constant that may vary as a function of temperature or soil moisture ([Bolker *et al.*, 1998](#_ENREF_5), [Jenkinson *et al.*, 1990](#_ENREF_21)). Indeed, none of the models in the Fifth Coupled Model Intercomparison Project (CMIP5), have process-level representation of microbial physiology ([Todd-Brown *et al.*, 2013](#_ENREF_36)). Where they have been included, the models suggest that process-level representation of microbial physiology influences soil C storage at the global scale ([Hararuk *et al.*, 2014](#_ENREF_19), [Tang & Riley, 2015](#_ENREF_35), [Wieder *et al.*, 2013](#_ENREF_39)).

Models that represent microbial physiology vary in complexity. Some conflate soil organic matter (SOM) decomposition with microbial uptake and mineralization, or make the simplifying assumption that these rates are identical (MIMICS, CORPSE).

Many soil decomposition models ignore the role of N in regulating C mineralization and vice-versa (REFS). Some use soil N concentration to empirically modify mineralization rates (REFS), while others do not consider N (Allison et al., 2010; Sulman et al., 2014; Wang et al., 2013). Microbes utilize C and N in plant litter and root exudates, as well as free monomers that have been cleaved from polymeric soil organic matter by extracellular enzymes ([Brzostek & Finzi, 2011](#_ENREF_6), [Frey *et al.*, 2013](#_ENREF_18)). Plant input and soil organic matter C-to-N ratios (C:N) range from # to #, and are significantly higher than that of microbial biomass (8-15) and extracellular enzymes (~3; REFS). As a result, microbial populations are often N-limited. This may explain why an increase in C-rich plant inputs can induce microbial population growth and nutrient limitation, which results in the production of extracellular enzymes that decompose SOM (i.e., priming; Brzostek et al. 2013, Kuzyakov, 2010).

Our objective was to develop a coupled C-and-N model that is general, parsimonious, and robust when challenged with rapid changes in temperature and substrate supply. We did this by building in complexity from empirical and semi-mechanistic models to a mechanistic microbial physiology model that integrates temperature, soil moisture, and substrate stoichiometry over time. We tested different model structures against a common dataset of heterotrophic soil respiration measurements in a mid-latitude forest located in central Massachusetts, USA. We discuss the parametric sensitivity of the final model and the affect of different kinetics assumptions. Lastly, we performed a theoretical nutrient addition experiment, to demonstrate the potential priming affects due to changes in substrate stoichiometry.

# Methods

## 2.1 Model descriptions

### 2.1.1 Empirical regression

We fit a multivariate linear regression to soil temperature and moisture to predict the C efflux, FC,

FC = a\*T + b\*θ + c [1]

where T is soil temperature at 10 cm depth, θ is volumetric soil moisture at 2 – 8cm depth, and a-c are fit coefficients. This model makes no assumption that the coefficient or model form relates to decomposition processes, so parameters cannot be estimated independently. As a result, the parameters in this model (a-c) will be determined by fitting to the validation dataset.

### 2.1.2 Dual Arrhenius and Michaelis-Menten Model

The Dual Arrhenius and Michaelis-Menten Model (DAMM) simulates the effects of soil temperature, soil moisture and substrate supply on soil organic matter (SOM) depolymerization. Depolymerization is affected by soil temperature according to Arrhenius kinetics. Soil water content modifies the supply of two substrates, oxygen and a generalized C-containing substrate, both of which affect depolymerization using a Michaelis-Menten (i.e., dual Monod) kinetic approximation,

Depolymerization rate = [3]

where VmaxS is the maximum reaction rate, [S] is the C-substrate concentration, kMS is the half-saturation constant for the C-substrate, [O2] is the oxygen concentration, and kMO2 is the half-saturation constant for oxygen. Oxygen concentration limits the depolymerization rate when soil water content is high, and C-substrate supply limits depolymerization when soil water content is low because the substrate cannot diffuse to the reaction site. A complete description of the model equations and default parameters are available in Davidson et al. (2012).

### 2.1.3 DAMM and the Microbial Carbon and Nitrogen Physiology Model

The DAMM model was combined with a microbial-explicit C and N cycling model, appropriately named the Microbial Carbon and Nitrogen Physiology Model (MCNiP), described in Finzi et al. (2015). The combined model tracks seven pools, soil organic C (SOC) and N (SON), dissolved organic C (DOC) and N (DON), microbial biomass C (BiomassC) and N (BiomassN), and extracellular enzymes (Enz; Figure 1).

Soil temperature and moisture inputs constrain the rate of unprotected SOM depolymerization and uptake of dissolved organic matter (DOM) to the microbial biomass pool. Arrhenius kinetics controls the rate of SOM depolymerization to DOM, and the supply of SOM and enzymes also affects the rate via Equilibrium Approximation kinetics, a generalization of Michaelis-Menten kinetics,

Depolymerization rate = [4]

where VmaxS is the maximum reaction rate, [SOM] is the concentration of SOM, [Enz] is the concentration of extracellular enzyme at the reaction site, and kMdep is the half-saturation constant for SOM. Microbial uptake of DOM is limited by both DOM concentration and oxygen concentration,

Uptake rate = [5]

where VmaxD is the maximum reaction rate, [DOM] is the concentration of DOM, kMupt is the half-saturation constant for SOM. C or N uptake is partitioned in the microbial pool to maintenance, growth, and enzyme production. Enzyme production can be limited either C or N according to Liebig’s law of the minimum (sensu Schimel and Weintraub 2003).

Enzyme production = *q* \* UPTN [N-limited] [14]

Enzyme production = *p* \* (CUE\*UPTC) / CNe [C-limited] [15]

Where *q* and *p* are partitioning coefficients, UPTC and UPTN are the C and N taken up in the current time step, CUE is carbon use efficiency, and CNe is the C:N of enzymes. Inputs to the model include litter and root exudate C and N, temperature and soil moisture. Outputs used in this study are rates of C mineralization (i.e. C efflux) and N mineralization. Litter is partitioned to SOM and DOM pools at each timestep (h-1). Root exudates enter the DOM pool only.

Model parameters were identical to original DAMM and MCNiP parameters, excepting the following: AuptC\_N, EauptC\_N, AC\_N, EaC\_N, KmC\_N. In DAMM, these parameters were fit to the validation dataset, so in order to make a more independent assessment of DAMM-MCNiP’s capability we estimated AuptC\_N, EauptC\_N, AC\_N, and EaC\_N from independent measurements of β-glucosidase activity from organic and mineral soil ([Davidson *et al.*, 2012](#_ENREF_12), [Finzi *et al.*, 2015](#_ENREF_15)). Because we cannot experimentally distinguish between depolymerization kinetics and uptake kinetics, each pair of A and Ea values are identical. KmC\_N was estimated such that at standard temperature, 293 K (20ºC), and the mean soil moisture value for this site, 0.229 cm3 H2O cm-3 soil, KmC\_N was equal to the initial available substrate SOM concentration (sensu Davidson *et al.* 2012). In contrast to Allison *et al.* (2010) and MCNiP, we did not choose a Km larger than the available SOM pool. Microbes in MCNiP have access to the entire SOM pool, so without a Km value that is high relative to the SOM pool size, substrate will always be saturating. Our parameterization allows for substrate to saturate a reaction site, for example, if substrate is temporarily mobilized during a wet-up event ([Birch, 1958](#_ENREF_4), [Davidson *et al.*, 2014](#_ENREF_13)). Additional comments on parameter value sources and complete equations for DAMM-MCNiP can be found in Appendices A1 and A2, respectively.

We spun up the model for 1000 years. DAMM-MCNiP pools update over time, so it was important that we simulate a full year of soil temperature and moisture data during spin-up. We reconstructed a full year of soil temperature measurements from growing season data using a linear fit to nearby Fisher Meterological Station measurements of soil temperature collected at 15-minute intervals (REF hf001-10). We fit hourly averaged soil temperature at 10cm depth to our measurements (R2 = 0.86, P < 0.001). We used this fit to estimate soil temperature at 10 cm at our site for the remainder of the year (Figure A1). The fit of measured soil moisture to precipitation did not explain much variation (R2 = 0.02, P < 0.001), so we instead fit soil moisture to gage height (i.e., water surface height above a specified altitude) measurements at Black Gum Swamp, which drains an area adjacent to our site (REF hf070-04). The Black Gum Swamp gage had the best fit to data out of the gages on the Prospect Hill Tract of Harvard Forest (R2 = 0.14, P < 0.001). Water stage changes as a result of drainage from soil, and though it does not explain much variation in soil moisture data, we believe it provides a reasonable estimate of soil moisture values for the purpose of model spin-up (Figure A2).

## 2.2 Sensitivity analysis

We conducted a global variance-based sensitivity analysis in order to calculate the sensitivity of C efflux to 18 of the parameter values listed in Table 1. We used the SOBOL sampling method to calculate a first-order sensitivity index,

[3]

where pi is the *i*th parameter, p~i are all parameters that are not the *i*th parameter, VAR is the variance, and E is the expectation (Saltelli et al., 2010). For each parameter, we sampled across a range of the parameter’s default value +/– 10% with 60,000 model evaluations. We also computed the Root Mean Squared Error (RMSE) for each model evaluation compared against C efflux data from Harvard Forest. We performed this analysis in Matlab 2015b, using the toolbox SAFE R1.1 (Pianosi et al., 2015).

## 2.3 Model performance

To test model performance, we used measurements of soil temperature, moisture, and C efflux from a trenching experiment at Harvard Forest, MA. A 5 x 5 m trench was dug to 1 m depth in November 2008 in a mixed hardwood stand on the Prospect Hill tract of Harvard Forest. Automated measurements of C efflux were collected from April through October 2009. We used C efflux from trenched plots as an estimate of heterotrophic respiration. This dataset is described in greater detail in Davidson *et al.* (2012).

Linear regression was used to fit the output predicted by each model with C efflux measurements from trenching and to estimate the RMSE of the model fit. We computed the correlation coefficient (Pearson’s ρ) between model-predicted C efflux and temperature or soil moisture. All analyses were conducted in R Statistical Software (R Development Core Team, 2013).

## 2.4 DAMM-MCNiP priming test

# 3. Results

## 3.1 Sensitivity analysis

Of the parameters included in the sensitivity analysis, activation energy of depolymerization (eaDep) was by far the most sensitive parameter (Figure 2a), followed by eaUpt when eaDep is excluded from the analysis (Figure 2b). The RMSE for each model evaluation plotted against eaDep show that the RMSE sharply increases at values below 61 kJ mol-1, and slowly increases at values above 63 kJ mol-1 (Figure 2c).

## 3.2 Model performance

From a visual inspection of the model output, all three models capture the seasonality of C efflux well, except for the fall season where DAMM-MCNiP over-predicts C efflux rates (Figure 3a, gray shading). DAMM-MCNiP otherwise appears to capture short time-scale variability of measured C efflux well, especially large wet-up events.

The empirical regression model of C efflux explained 56% of the variation in the data (P < 0.001, R2adj = 0.56, RMSE = 0.19), but systematically underestimates the C efflux with a slope (β) of the relationship between predicted and measured efflux < 1 (β = 0.55, Figure 3b). DAMM explains slightly less variation in the dataset (P < 0.001, R2adj = 0.52, RMSE = 0.31), but is also less biased (β = 0.85). DAMM-MCNiP explains 19% of the variation in the dataset (P < 0.001, R2adj = 0.19, RMSE = 0.36) and underestimates the C efflux (β = 0.45). Both the variance explained (P < 0.001, R2adj = 0.38, RMSE = 0.32) and the bias (β = 0.64) change significantly when the fall is excluded from the dataset (Figure 3c).

## 3.3 DAMM-MCNiP priming test

# 4. Discussion

Sensitivity analyses showed a minimum in model RMSE for eaDep ranges between 61 – 63 kJ mol-1, suggesting that the true range of activation energies in the soil are similar to those estimated by Davidson et al. (2012) using beta-glucosidase assays (eaDep ≈ 59 – 64 kJ mol-1). It also suggests that beta-glucosidase is more abundant and/or active in these soils than phenol oxidase, which in the same study was estimated to have an activation energy of ~32 kJ mol-1. It would be more accurate to assay the full suite of enzymes at work in the soil, but given the limitations of laboratory incubations, these analyses indicate that a beta-glucosidase assay may be sufficient to estimate the activation energy of heterotrophic decomposition.

*Empirical, semi-empirical, and mechanistic models*

The regression model is an empirical fit, and it is therefore likely that the coefficients will not apply to different biomes, ecosystems, plant types, and management strategies. DAMM is semi-empirical and performs well. However, with no parameter fitting, the process-based model DAMM-MCNiP performs reasonably well at this site, which is impressive. Empirical fits contain little predictive information, but process-based models are theoretically more powerful for two reasons. First, they can predict responses to nonlinear (e.g., chemical, biological, and geophysical) processes. Second, process-based models can provide information on multiple pools and fluxes. The empirical regression provides no information on C and N pools, while the process-based model generates testable hypotheses for DOC concentrations, enzyme activities, N mineralization rates, and other pools and fluxes.

# 5. Acknowledgements

# 6. Figures

# 7. Tables

**Table 1.** Model parameter abbreviations, units, and default values. Parameter values included in the sensitivity analysis are marked with an asterisk (\*).

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | Units | Default Value | Description |
| rootDOC | mg cm-3 | input | Root exudates |
| T | K | input | temperature in Kelvin |
| θ | cm3 H2O cm-3 soil | input | volumetric water content |
| BD | g cm-3 | 0.8 | bulk density |
| PD | g cm-3 | 2.52 | particle density |
| O2frac\* | L O2/ L air | 0.209 | volume fraction of O2 air |
| Cfrac\* | g C cm-3/ g C cm-3 | 0.000414 | fraction of unprotected SOM, using soluble substrate estimated from Magill et al., 2000 |
| dLiq\* | - | 3.17 | diffusion coefficient for unprotected SOM and DOM in liquid |
| dGas\* | - | 1.67 | diffusion coefficient for O2 in air |
| kmO2\* | cm3 O2 cm-3 air | 0.121 | Michaelis constant for O2 |
| R | kJ K-1 mol-1 | 0.0083145 | universal gas constant |
| p\* | - | 0.5 | proportion of assimilated C allocated to enzyme production |
| q\* | - | 0.5 | proportion of assimilated N allocated to enzyme production |
| a\* | - | 0.5 | proportion of enzyme pool acting on SOC pool (1-a = proportion acting on SON pool) |
| initSOC | mg cm-3 | 53.8846 | initial SOC pool |
| initSON | mg cm-3 | 1.7936 | initial SON pool |
| initDOC | mg cm-3 | 0.0021 | initial DOC pool |
| initDON | mg cm-3 | 0.0011 | initial DON pool |
| initBiomassC | mg cm-3 | 1.8699 | initial microbial biomass C |
| initBiomassN | mg cm-3 | 0.1870 | initial microbial biomass N |
| litterC | mg cm-3 hr-1 | 0.0005 | litter input to SOC pool |
| initEnz | mg cm-3 | 0.0341 | initial enzyme pool |
| inputDOC | mg cm-3 hr-1 | 0.0005 | litter input to DOC pool |
| death\* | hr-1 | 0.00015 | microbial turnover rate |
| enzLoss\* | hr-1 | 0.001 | enzyme turnover rate |
| micToSom\* | mg mg-1 | 0.5 | fraction of dead microbial biomass |
| aDep\* | mg SOM cm-3 (mg Enz cm-3)-1 h-1 | 1.0815\*1011 | Vmax intercept for SOM depolymerization |
| aUpt\* | mg DOC cm-3 (mg biomass cm-3)-1 h-1 | 1.0815\*1011 | Vmax intercept for DOC uptake |
| kmDep\* | mg cm-3 | 0.0025 | Km for SOM depolymerization |
| kmUpt\* | mg cm-3 | 0.3 | Km for DOC uptake |
| CUE\* | mg mg-1 | 0.31 | Carbon use efficiency |
| eaDep\* | kJ mol-1 | 61.77 | Ea for SOM depolymerization |
| eaUpt\* | kJ mol-1 | 61.77 | Ea for DOC uptake |
| cns | - | 27.6 | C:N of soil |
| cnl | - | 50 | C:N of litter |
| cnm | - | 10 | C:N of microbial biomass |
| cne | - | 3 | C:N of enzymes |
| cnex | - | 27.6 | C:N of root inputs |

1. Abstract
   1. Take home: Need to model substrate supply and microbial pools in order to represent seasonal C fluxes.
      1. Tried with various temperature relationships, empirical temp and moisture relationships, doesn’t work. Need updating pools.
      2. I can see why a function is more attractive, easier to fit etc, but necessary to have updating pools.
      3. MCNiP adds inertia.
2. Intro
   1. C important, substrate supply is important
   2. Birch effect theory – fast pulse after rain
   3. Important to represent diffusion constraints on substrate supply, even in a relatively wet ecosystem such as HF.
3. Methods
   1. Short description of HF data collection (include Kathleen?)
      1. Soil respiration
      2. Litter inputs and C:N (archive)
      3. Root exudates & turnover (me)
   2. Model equations
   3. Model diagnostics
      1. How sensitivity analysis
         1. SOBOL
         2. GLUE
   4. Model run lengths, spin-up, defaults
      1. Fake soil moisture data, timeline of response to pulse
         1. We isolated the first rain event of the year on DATE, and repeated it 1-4 times.
         2. We ran the model under idealized dry conditions (vwc = 0.15) and pulsed the same volume of water into the soil either in one slow pulse, or in 4 fast pulses within a weeklong span to test the affect of rain frequency on DOC accumulation.
            1. with soil moisture reaching a maximum over 2 days and diminishing to a minimum after 6 days. We repeated this pulse 1-4 times.
      2. Damm & damm-mcnip comparison
4. Results
   1. Model diagnostics
      1. **Activation energy is very important (in all models)**
   2. Fake moisture run (run all models, esp. damm and dmc)
      1. Need DAMM to respond to water
      2. Need MCNiP to “remember” growth induced by water
      3. Figure(s)
         1. **Track DOC**
         2. **Mic**
         3. **SOC**
   3. Model comparison with HF data
      1. **Comparison figure**
      2. **Regression/residuals figures?**
   4. Priming demo (will this fit?)
      1. Potential application of model
      2. **Priming figure that is now pulse change in C:N**
5. Discussion
   1. Model diagnostics & fake moisture run
      1. Parsimonious
      2. Activation energy important in all models
      3. Decomposition is major control on downstream processes such as uptake and respiration, implying that the representation of these processes could be simplified.
   2. Model comparison and priming demo
      1. Model sensitivity to soil moisture better in dmc compared to damm
         1. Need to model soil efflux
      2. Including N brings down C efflux due to limitation
      3. Something about N pulse experiment.
   3. Conclusions and Implications
      1. We developed simple model with water, temp, microbes, N
      2. Needs
         1. Recycling N pool
         2. Plant coupling
         3. Minerals
         4. Parameter estimation
      3. Flexible, easy to use, requires only temp, moisture and inputs.
      4. No oscillations?

\*\*\*Try instead of priming figure:

1. Steady state SOC at different temperature values/soil moisture values/C:N
2. CUE?
3. Can make flying carpet if need

\*\*\*After model comparison figures, before priming

1. Model root litter decomposition?
2. Model leaf litter decomposition?
3. Model variation in C efflux due to variation in root exudates measured over the year (is the range in C efflux right?)

\*\*\*Before model comparison figures

1. Compare linear regression based models using temp and moisture scalars (a la other ESMs) to show that they can’t reproduce C efflux measurements.
   1. Find the paper that Bill Riley sent me about this.
      1. Found it, now do some lit search to supplement (find more and more recent equations).
      2. Century (parton et al 1987 sssaj), Roth, Daycent, CLM-cn (Bonan et al 2013 GCB)