## *Model Description*

### ReSOM

#### Table 1. Equations governing the change in each carbon pool over time in the ReSOM model. All pools are in units of carbon mass per soil volume (g C m-3). Additional pool, flux, and parameter values are defined in Table S1. For full equations, additional parameters, and model development see Tang and Riley [2015].

|  |
| --- |
| **Pool Description Differential equation** |
| *S* polymeric organic carbon (1)  *D* monomeric organic carbon (2)  *D*ads adsorbed monomeric organic carbon (3)  *X* reserve microbial biomass (4)  *B* structural microbial biomass (5)  *E* extracellular enzymes (6)  *E*ads adsorbed extracellular enzymes (7)  where:  *I*S polymeric input flux (g C m-3 d-1)  *I*D monomeric input flux (g C m-3 d-1)  *F*S polymeric depolymerization flux (g C m-3 d-1)  *F*D monomeric uptake flux (g C m-3 d-1)  *F*Dads adsorption flux of monomers (g C m-2 d-1)  *F*Eads adsorption flux of enzymes (g C m-2 d-1)  *Y*X yield coefficient for reserve biomass (unitless)  *f*E fraction of decayed extracellular enzymes contributing to the polymer pool (unitless)  B1 microbial mortality rate (d-1)  E enzyme turnover rate (d-1)  Dads turnover rate of adsorbed monomers (d-1)  Eads turnover rate of adsorbed enzymes (d-1)  ** metabolic turnover rate (d-1)  *g* growth rate (d-1)  *p*E enzyme production rate (d-1) |

The ReSOM model computes depolymerization of polymers, sorption of monomers and enzymes, and uptake of monomers (i.e., microbial assimilation) using Equilibrium Chemistry Approximation (ECA) kinetics, a generalization of Michaelis-Menten (MM) kinetics [*Tang and Riley*, 2013]. ECA is more accurate than MM kinetics in approximating the law of mass action kinetics, which underlies both approaches [*Michaelis and Menten*, 1913; *Tang and Riley*, 2013; *Tang*, 2015]. ECA kinetics represents decomposition and substrate uptake as a competition between minerals and SOC for enzymes, and minerals and microbes for low molecular weight C, respectively. Two advantages of the ECA approach are the ability to (i) include distinct temperature-dependent effects on mineral sorption and microbial processes (i.e., decomposition, uptake, and maintenance) based on well-established kinetic theory and (ii) represent the multi-consumer, multi-substrate competitive environment in a computationally efficient manner. Thus, depolymerization (*F*S) and uptake (*F*C) are defined as

(8)

(9)

where *E* is the extracellular enzyme pool, *S* is the polymeric organic carbon pool, *B* is the structural microbial biomass pool, *D* is the monomeric organic carbon pool, and *M* is the mineral sorption capacity (i.e., Qmax), *V*max is the maximum rate of each process, *z* is a scaling parameter for transporter density, and *k* is the affinity parameter for decomposition (*k*ES), uptake (*k*BD), sorption to enzymes (*k*ME), and sorption to monomers (*k*MD).

Plant inputs estimated from site-level NPP are partitioned based on [*Tang and Riley*, 2015] into polymer and monomer pools, respectively, where the polymer pool represents polymeric compounds in litter (e.g., cellulose, hemicellulose, lignin) and the monomer pool represents intracellular material, easily-leached monomeric compounds in litter, and root exudates.

Adsorption (*F*Dads, *F*Eads) and desorption (*F*Ddes, *F*Edes) rates of monomers (10, 12) and enzymes (11, 13) depend on mineral surfaces and competing processes:

(10)

(11)

(12)

(13)

where Dads and Eads are defined in Table 1.

The temperature-dependent processes are grouped into three categories: (i) equilibrium reactions, (ii) non-equilibrium reactions, and (iii) enzyme-mediated reactions. Some processes such as depolymerization and uptake may have equilibrium, non-equilibrium, and enzyme-mediated components affecting different parameters (e.g., binding affinity, maximum rate, and fraction of active enzymes, respectively). Equilibrium reactions include reversible binding (enzyme-polymer, microbe-monomer, enzyme-mineral, monomer-mineral) and microbial maintenance.

The temperature dependence of these reactions is based on Eyring’s transition state theory [*Eyring*, 1935; *Tang and Riley*, 2013],

(14)

where *T*0 is the reference temperature, set to the mean annual temperature, *K(T*0*)* is the reference affinity, Δ*G*EQ is the Gibbs free energy change of the equilibrium reaction, *R* is the gas constant, and *T* is the current temperature. Maximum reaction rates for depolymerization and monomer uptake are classified as non-equilibrium or forward reactions. The temperature dependence of the forward reaction is

(15)

where *V(T*0*)* is the reference maximum rate for the forward reaction and Δ*G*NEQ is the Gibbs free energy change of the non-equilibrium reaction.Enzyme-mediated processes considered in this model include depolymerization of polymers by extracellular enzymes and uptake of monomers by transporter proteins. Enzyme-mediated processes are governed by a temperature-dependent optimum, which affects the fraction of enzymes that are active (i.e., conformationally able to bind to substrates), defined by

(16)

(17)

(18)

where *f*act is the fraction of enzymes that are active at a given temperature and varies between 0 and 1 (Figure S2), Δ*G*E is the Gibbs free energy change of the enzyme reaction, Δ*H\** is the enthalpy change at the convergence temperature for enthalpy (*T\**H), Δ*S\** is the entropy change at the convergence temperature for entropy (*T\**S), Δ*C*P is the change in heat capacity, *n* is the average number of amino acid residues in an enzyme, and *N*CH is the average number of non-polar hydrogen atoms per amino acid residue. From [*Murphy et al.*, 1990; *Ratkowsky et al.*, 2005; *Schipper et al.*, 2014], we defined parameters for amino acid traits (*n, N*CH*,* Δ*H\**) that result in a thermal optimum at 290 K.

Water control on decomposition due to diffusion limitation on substrate access is imposed by modifying the decomposition rate directly. Litter, woody debris, and polymeric carbon decomposition as well as microbial and enzyme turnover are limited depending on the soil water potential following [*Wilson and Griffin*, 1975]

(19)

If the soil water potential is lower than the minimum soil water potential for the given soil, decomposition does not occur. A Michaelis-Menten relationship estimates the oxygen limitation on decomposition based on its bulk concentration

(20)

where is set to 0.22 mol m-3 following [*Arah and Kirk*, 2000]. Water limitation due to transport emerges via interactive effects between dissolved organic carbon in the aqueous phase and microbial biomass. The BeTR reactive transport module determines the availability of aqueous phase C in any given depth layer due to diffusive and advective transport.

### ELMv1 and BeTR

### Model Integration

The 0-D microsite version of the ReSOM model was first translated from Matlab into Fortran 90. The model predictions are computed by solving a series of ordinary differential equations. At the microsite level where computational efficiency is not a concern, each flux was stored as a new variable, and the change in each C pool (dC/dt) was computed by adding and subtracting component fluxes from each pool. In the integrated ELM-BeTR-ReSOM model, component fluxes are stored as values in a matrix rather than as standalone variables, as in the cascade matrix of ELM- and CLM-Century, and the general matrix representation of soil models [*Sierra, Carlos; Muller*, 2014]. As shown in [*Sierra, Carlos; Muller*, 2014], linear and nonlinear models can be represented with general matrix representation. For each C pool, there is a corresponding nitrogen (N) and phosphorus (P) pool. Transfers between pools are controlled by C dynamics as defined below, and N and P are transferred according to their stoichiometry as follows.

Microbial uptake is controlled by soil temperature, diffusion, and concentration of C monomers in the aqueous phase. Microbes take up monomer N and P in the same stoichiometric ratio as they occur in the aqueous phase. Monomers are then transferred to the microbial reserve pool that is used to construct microbial biomass and enzymes. Microbial biomass and enzyme stoichiometry is maintained; therefore, if there is insufficient N or P to construct microbial biomass and enzymes, N and P can be immobilized from the NH4 and soluble P pools, respectively. Currently, microbes are given priority over plants for these nutrients, but in the future they will compete for nutrients using the ECA framework currently used for nitrification, denitrification, and P cycling [*Zhu et al.*, 2016, 2017]. If there is insufficient N or P in the aqueous soil pools, then growth is limited. If there is excess C, N or P, these elements can be mineralized as CO2, NH4 and soluble P, respectively.

We converted ReSOM from the representation shown in Table 1 (i.e., a mass balance of individual fluxes) to a general matrix representation using the the form:

where dC/dt is the change in a vector of C pools, I is the input matrix, T is the transfer matrix representing all flows of C between pools, and O is the output matrix.

If we let ,

The O matrix can be further decomposed into N(C) and C, a matrix of decay rates and a vector of the C pools.

let

let

In order to verify this matrix representation is identical to the representation from Table 1, we can set the dCO2/dt composed of individual fluxes,

equal to the dCO2/dt derived from the general matrix representation,

=

and check that the expressions are equal to each other:

1. =
2. =
3. =
4. =
5. =
6. =
7. =
8. =
9. =
10. =

The ELMv1-BetR-ReSOM model development branch can be found in the repository: https://github.com/rabramoff/sbetr/tree/rzacplsbetr.

# 6. References

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# 7. Supplement

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Type** | **Symbol** | **Units** | **Definition** | **Default Value** |
| **Pool** | S | g C m-3 | Polymeric organic carbon | - |
|  | D | g C m-3 | Monomeric organic C | - |
|  | Dads | g C m-3 | Adsorbed monomeric organic C | - |
|  | B | g C m-3 | Microbial structural biomass | - |
|  | X | g C m-3 | Microbial reserve biomass | - |
|  | E | g C m-3 | Extracellular enzymes | - |
|  | Eads | g C m-3 | Adsorbed extracellular enzymes | - |
|  | M | g C eqv m-3 | Mineral surfaces | - |
| **Flux** | IS | g C m-3 d-1 | Polymeric input | - |
|  | ID | g C m-3 d-1 | Monomeric input | - |
|  | FS | g C m-3 d-1 | Depolymerization | - |
|  | FD | g C m-3 d-1 | Uptake | - |
|  | FDads | g C m-3 d-1 | Monomer adsorption | - |
|  | FEads | g C m-3 d-1 | Enzyme adsorption | - |
|  | RCO2 | g C m-3 d-1 | Respiration | - |
|  | Fr | g C m-3 d-1 | C overflow | - |
| **Parameter** | B1 | d-1 | Mortality rate | - |
|  | Dads | d-1 | Turnover of adsorbed monomers | 0.006 |
|  | Eads | d-1 | Turnover of adsorbed enzymes | 0.006 |
|  | fE | - | Fraction of decayed extracellular enzyme contributing to polymer pool | 0.2 |
|  | E | d-1 | Enzyme turnover rate | 0.0061 |
|  | YX | - | Yield rate of enzyme from reserve metabolites | 0.8 |
|  | κ | d-1 | Metabolic turnover rate | 0.0537 |
|  | g | d-1 | Growth rate | - |
|  | pE | d-1 | Enzyme production rate | - |
|  | m | d-1 | Maintenance rate | - |
|  | KEQ (T) | g C | Affinity parameter at dynamic equilibrium | - |
|  | K(T0) | g C | Affinity parameter at reference temperature | - |
|  | GEQ | kJ mol-1 | Gibbs energy change at equilibrium | - |
|  |  |  | for the enzyme-mineral adsorption affinity parameter | 20 |
|  |  |  | for the monomer-mineral adsorption affinity parameter | 20 |
|  |  |  | for reserve export | 0 |
|  | VNEQ (T) | d-1 | Maximum non-equilibrium rate parameter | - |
|  |  | d-1 | for monomer adsorption | 0.01 |
|  |  | d-1 | for enzyme adsorption | 0.001 |
|  | V(T0) | d-1 | Maximum rate parameter at reference temperature | - |
|  | GNEQ | kJ mol-1 | Gibbs energy change at non-equilibrium | - |
|  | GE | kJ mol-1 | Gibbs energy change of enzyme reaction | - |
|  | R | J K-1 mol-1 | Gas constant | 8.314 |
|  | T | K | Temperature | - |
|  | T0 | K | Reference temperature | - |
|  | fact | - | Fraction enzymes active at temperature T | - |
|  | H\* | J mol-1 | Enthalpy change at T\*H | 5312.072 |
|  | S\* | J K-1 mol-1 | Entropy change at T\*S | 18.1 |
|  | T\*H | K | Convergence temperature for enthalpy | 373.6 |
|  | T\*S | K | Convergence temperature for entropy | 385.2 |
|  | CP | J mol-1 | Heat capacity change | - |
|  | n | - | Number of amino acid residues for an enzyme | 183 |
|  | NCH | - | Average number of non-polar hydrogen atoms per amino acid residue | 5.524 |
|  | VE,max | d-1 | Maximum rate of polymer degradation | 2.4133 |
|  | kES | g C | Affinity parameter for enzymatic polymer degradation | 200 |
|  | kME | g C | Affinity parameter for surface adsorption of enzymes | 50 |
|  | z | - | Scaling parameter for transporter density | 0.05 |
|  | VB,max | d-1 | Maximum rate of monomer assimilation | 10.9343 |
|  | kBD | g C | Affinity parameter for microbial monomer uptake | 1 |
|  | kMD | g C | Affinity parameter for mineral surface adsorption of monomers | 25 |

#### Table S1. Parameter and pool values for ReSOM. Default values are taken from [*Tang and Riley*, 2015], with the exception of GEQ for the enzyme- and monomer-mineral adsorption binding affinity parameters, as well as the reserve export affinity parameter which we do not consider temperature sensitive in these model runs. These model versions also include nonequilibrium maximum reaction rates for adsorption, which are not included in the original model.



#### Table S2. Schematic of file structure.