Supplemental material for "A total quasi-steady-state formulation of substrate uptake kinetics in complex networks and an example application to microbial litter decomposition"

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S1. Derivation Eq. (A6-b)

Substituting Eq. (A4) into Eq. (12) and taking the zero order approximation $E_{k,0} = E_{k,T}$, yields

$$E_{k,1} + \sum_{l=1}^{l=I} C_{lk,1} = 0 \quad \text{(S1-1)}$$

Dividing Eq. (S1-1) by $K_{S,ik}$ and taking the summation for $k = 1,\cdots,J$, we obtain:

$$\sum_{k=1}^{k=J} \frac{E_{k,1}}{K_{S,ik}} = -\sum_{k=1,l=1}^{k=J,l=I} \frac{C_{lk,1}}{K_{S,ik}} \quad \text{(S1-2)}$$

Similarly, from Eqs. (A4) and (10), one has

$$\sum_{k=1}^{k=I} \frac{S_{k,1}}{K_{S,kj}} = -\sum_{k=1,l=1}^{k=I,l=J} \frac{C_{kl,1}}{K_{S,kj}} \quad \text{(S1-3)}$$

Substitution of Eq. (S1-2) and (S1-3) into Eq. (A5-b) leads to

$$C_{ij,2}\left(1 + \sum_{k=1}^{k=J} \frac{E_{k,0}}{K_{S,ik}} + \sum_{k=1}^{k=I} \frac{S_{k,0}}{K_{S,kj}}\right) = C_{ij,1}\left(\sum_{l=1,n=1}^{n=I,l=J} \frac{C_{nl,1}}{K_{S,il}} + \sum_{k=1,l=1}^{n=I,l=J} \frac{C_{nl,1}}{K_{S,nj}} - \sum_{n=1,l=1}^{n=I,l=J} \frac{K_{S,nl}C_{nl,1}}{K_{S,il}K_{S,nj}}\right) \quad \text{(S1-4)}$$

from which Eq. (A6-b) can be derived.

S2. A synthetic isotope experiment with model S3B1

We applied model S3B1 with the parameter values in Table S1 for a synthetic isotope simulation. From the initial condition, we define the reference isotopic mass fractions for substrate $S_i, i = 2,3$ as

$$R_{S_i,0} = \frac{S_i}{\sum_{k=1}^{k=3} S_k} \quad \text{(S2-1)}$$

At any point in time, the isotope ratio of substrate $S_i, i = 2,3$ is calculated as

$$\delta S_i\left(\text{per mil}\right) = \left(\frac{R_{S_i}}{R_{S_i,0}} - 1\right) \times 1000 \quad \text{(S2-2)}$$

References

Aber, J. D., McClaugherty, C. A. and Melillo, J. M.: Litter decomposition in Wisconsin forests: mass loss, organic-chemical constituents and nitrogen. Report #R3284, School of Natural Resources, University of Wisconsin, Madison, Wisconsin, USA, 1984

Magill, A. H., and Aber, J. D.: Long-term effects of experimental nitrogen additions on foliar litter decay and humus formation in forest ecosystems, Plant Soil, 203, 301-311, doi: 10.1023/A:1004367000041, 1998.

List of Tables

Table S1. Parameter values for the synthetic-isotope experiment with model S3B1. The parameter vectors are presented in the form $\left(K_{S,ij}, k_{ij,2}^{+}, \mu_{ij}\right)$, whose units are, respectively, mg C dm^{-3}, d^{-1}, and none. The numbers in parentheses following the state variables are their initial values, whose units are mg C dm^{-3}. The respiration rate γ_1 is set to 0.03 d^{-1}. The parameters for the substrate kinetics were randomly chosen as in the main text.

	S_1 (30)	S_2 (0. 6)	S_3 (0.4)
B_1 (1)	$(20,48,0.5)$	$(19.6,47.84,0.3)$	$(18.8,47.72,0.1)$

Table S2. Best-fit parameters for model S3B3-MM (S3B3 model implemented with M kinetics) by optimizing the simulation outputs to the 77-month red pine litter decomposition experiment data in Melillo et al. (1989). The parameter vectors are presented in the form $\left(K_{S,ij}, k_{ij,2}^{+}, \mu_{ij}\right)$, whose units are, respectively, g C, d^{-1}, and none. The respiratory coefficients (i.e., $\gamma_j, j=1,2,3$ as defined in Eq. (30)) of the three microbes are, respectively, 0.01, 005, and 0.001 d^{-1}. Numbers in the parentheses following the state variables are their initial values, whose units are g C. In doing the calibration, we assumed (i) $K_{S,1j}, j=1,2,3$ are the same for all three microbes; (ii) $K_{S,22}=K_{S,23}$; and (iii) for microbe B_j, $k_{ij,2}^{+}, i=1,2,3$ are the same for all three substrates. By further fixing μ_{ij} to the values in the parentheses, we effectively had 9 total parameters in the calibration.

	S_1 (359)	S_2 (386)	S_3 (255)
B_1	$(48.12,0.5886,0.5)$	$(94.39,0.5886,0.3)$	$(1964.5,0.5886,0.1)$
B_2	$(48.12,0.3995,0.5)$	$(182.26,0.3995,0.3)$	$(1946.2,0.3995,0.1)$
B_3	$(48.12,0.3913,0.5)$	$(182.26,0.3913,0.3)$	$(180.2,0.3913,0.1)$

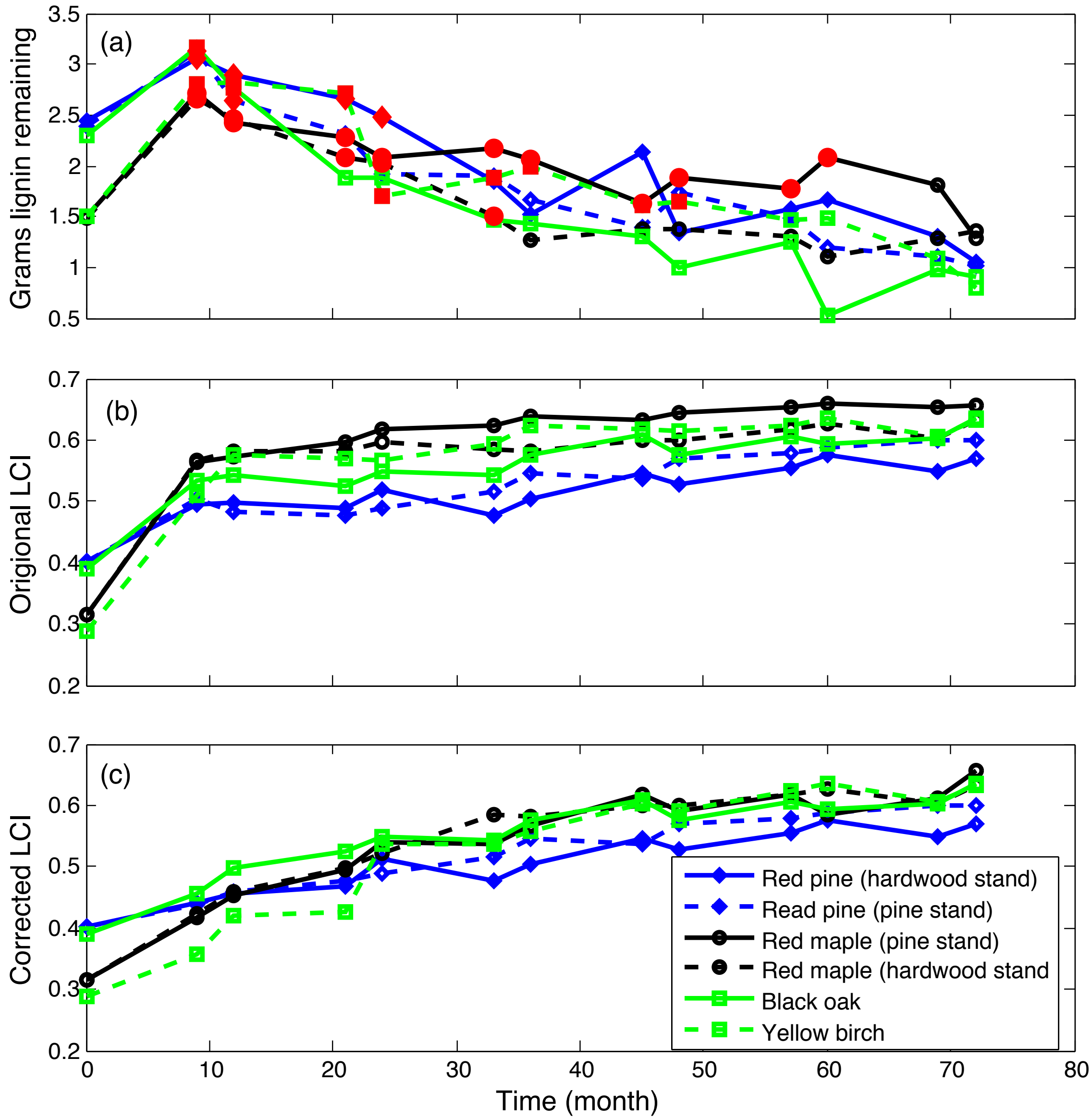

Figure S1. Evolution of lignin in the decomposition experiments documented in Magill et al. (1998). The corrected LCI in panel (c) is derived by replacing the unreasonable lignin data (marked in red) reported in Magill et al. (1998) (that are higher than the initial lignin mass) with the initial lignin mass. We corrected 32 out of 78 (about 40%) data points.

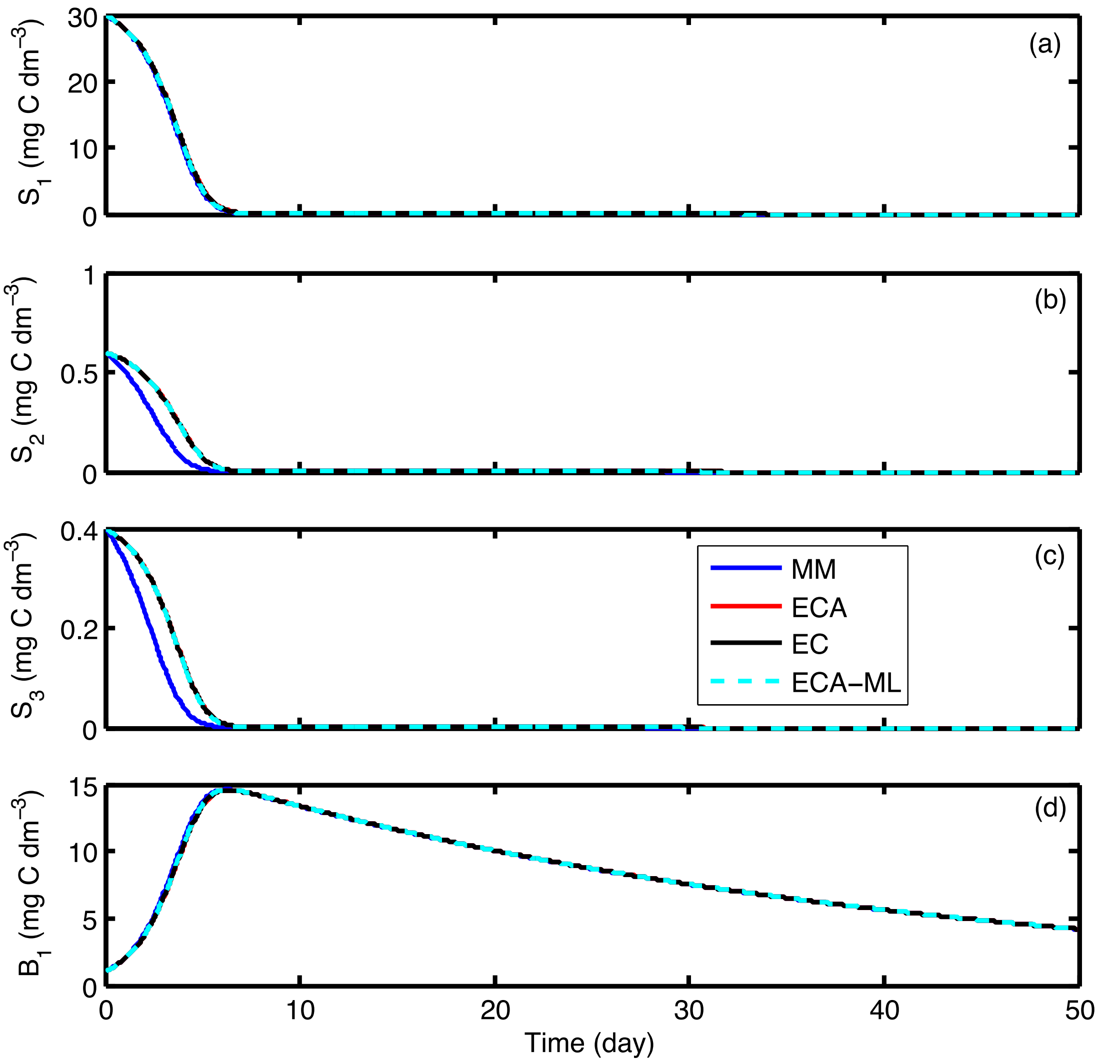

Figure S2. Time series of relevant state variables simulated from the synthetic-isotope simulation experiment by applying the three different substrate uptake functions to microbial model S3B1. Relevant parameters are specified in Table S1.

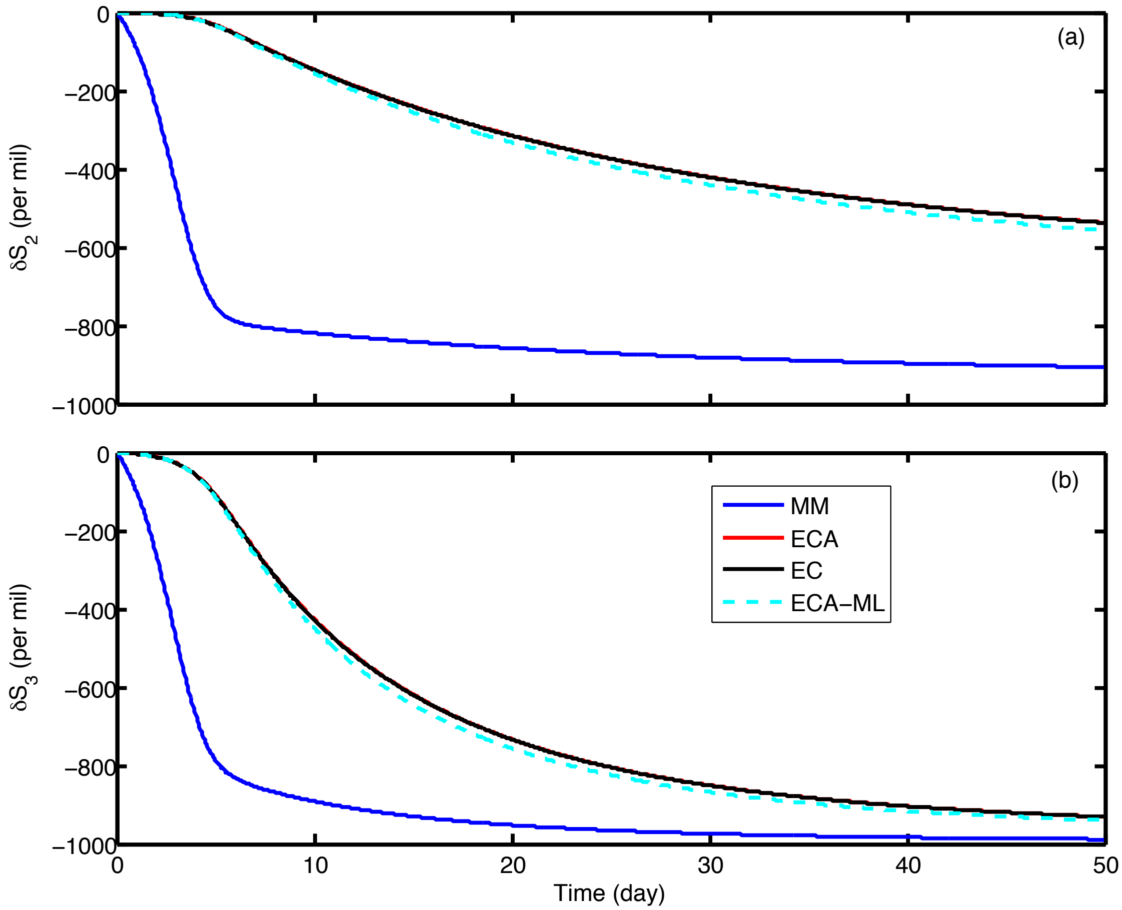

Figure S3. Temporal evolution of the synthetic-isotopic signatures of pool S2 and S3 simulated from model S3B1 using different substrate uptake functions. Relevant parameters are specified in Table S1.

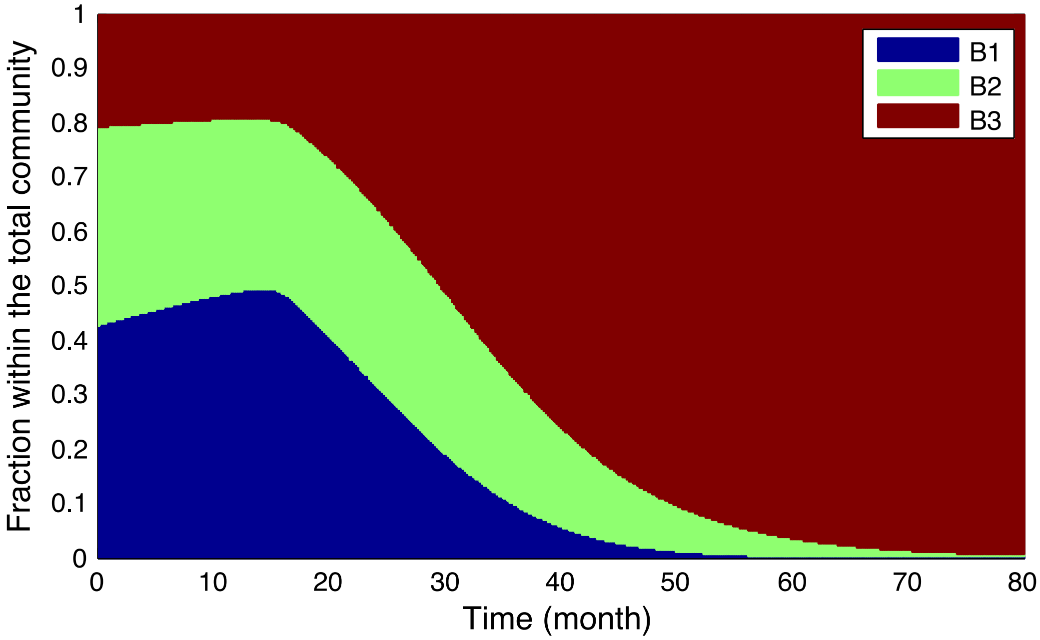

Figure S4. Model (S3B3-ECA) predicted microbial community structure for the 77-month litterbag experiment. Relevant model parameters are in Table 5.

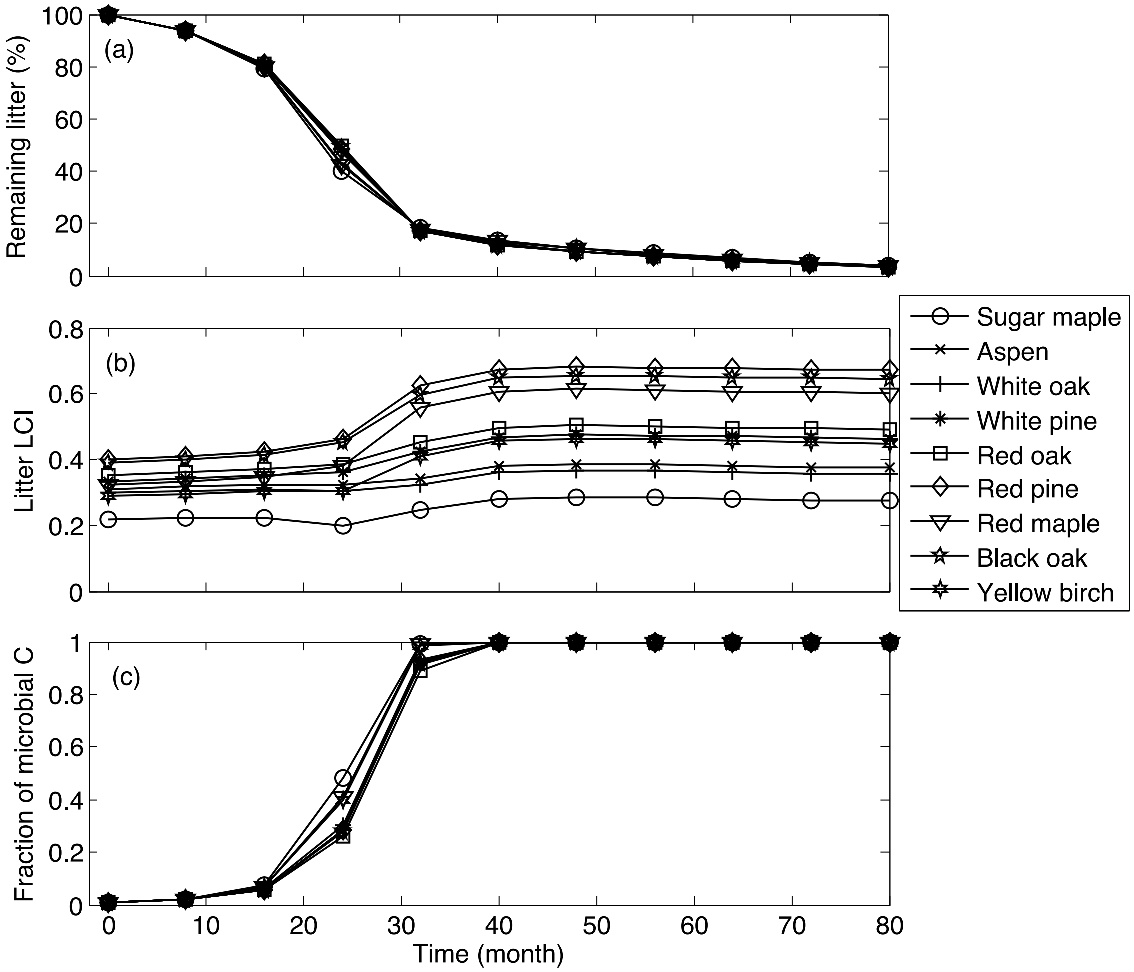

Figure S5. Model (S3B3-MM: models S3B3 implemented with MM kinetics) predicted temporal evolution of litter decomposition dynamics for the 9 different litters in Table 4. Model parameters are in Table S2.