Appendix

Emergent properties of organic matter decomposition by soil enzymes

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Table A1 Model parameter values.

Parameter	Value	Unit	Note
end_time	300		number of iterations
x	100		Grid length
y	100		Grid width
taxa_per_box	0.01		Initial probability of each bacterial taxon occupying a box
n_taxa	1		number of taxa
fb	0		Initial fraction of fungi biomass
n_enzymes	30		Number of enzymes in community
n_uptake	14		Number of uptake transporters
LCI_slope	-0.8		Fractional change in cellulose decay per unit lignocellulose index
n_substrates	12		Number of substrates
Cfrac_b	0.825	mg mg-1	Bacterial C fraction
Nfrac_b	0.16	mg mg-1	Bacterial N fraction
Pfrac_b	0.015	mg mg-1	Bacterial P fraction
Cfrac_f	0.9	mg mg-1	Fungal C fraction
Nfrac_f	0.09	mg mg-1	Fungal N fraction
Pfrac_f	0.01	mg mg-1	Fungal P fraction
Crange	0.09	mg mg-1	Tolerance on C fraction
Nrange	0.04	mg mg-1	Tolerance on N fraction
Prange	0.005	mg mg-1	Tolerance on P fraction
CUE_ref	0.5	mg mg-1	Carbon use efficiency at the reference temperature
CUE_enz	0	mg mg-1	CUE change with enzyme investment
CUE_uptake	0	mg mg-1	CUE change with uptate investment
CUE_temp	-0.016	mg mg-1 ℃-1	CUE temperature sensitivity
Specif_factor	1		Efficiency-specificity
Vmax_Km	1	mg enzyme day cm-3	Slope for Km-Vmax relationship
Vmax_Km_int	0	mg cm-3	Intercept for Km-Vmax relationship
Uptake_Vmax_Km	0.2	mg biomass day cm-3	Slope for uptake Km-Vmax relationship
Uptake_Vmax_Km_int	0	mg cm-3	Intercept for uptake Km-Vmax relationship
dist	1	lattice point	Maximum dispersal distance
direct	0.95		Dispersal direction
max_size_b	2	mg cm-3	C quota threshold for bacterial cell division
max_size_f	50	mg cm-3	C quota threshold for fungal cell division
C_min	0.086	mg cm-3	threshold C concentration for cell death
N_min	0.012	mg cm-3	threshold P concentration for cell death
P_min	0.002	mg cm-3	threshold C concentration for cell death
Death_Rate	0.001		Bacterial death rate
Death_Ratio	0.2		Fungal death ratio
Enz_min	0	mg C cm-3	Initial enzyme present in terms of carbon
Enz_max	0	mg C cm-3	Initial enzyme present in terms of carbon
Enz_per_taxon_min	0		Minimum number of enzymes a taxon can produce
Enz_per_taxon_max	40		Maximum number of enzymes a taxon can produce
Enz_Prod_min	0.00001	mg C mg-1 day-1	Minimum per enzyme production cost as a fraction of C uptake rate
Enz_Prod_max	0.0001	mg C mg-1 day-1	Maximum per enzyme producton cost as a fraction of C uptakte rate
Constit_Prod_min	0.00001	mg C mg-1 day-1	Minimum per enzyme production cost as a fraction of biomass C
Constit_Prod_max	0.0001	mg C mg-1 day-1	Maximum per enzyme production cost as a fraction of biomass C
NormalizeProd	0		Normalize enzyme production for the number of enzyme genes
Enz_C_cost	1	mg mg-1	Per enzyme C cost as a fraction of uptake
Enz_N_cost	0.3	mg mg-1	Per enzyme N cost as a fraction of C cost
Enz_P_cost	0	mg mg-1	Per enzyme P cost as a fraction of C cost
Enz_Maint_cost	5	mg C mg-1 enzyme C	Maintinence cost of enzyme production
Enzyme_Loss_Rate	0.04	day-1	Enzyme turnover rate (Allison 2006)
Enzymes_per_sub	1		Minimum number of enzymes capable of degrading each substrate
Vmax0_min	5	mg substrate mg-1 enzyme day-1	Minimum Vmax for enzyme
Vmax0_max	50	mg substrate mg-1 enzyme day-1	Maximum Vmax for enzyme
Km_min	0.01	mg cm-3	Minimum Km
Km_Ea	20	kj mol-1	Activation energy for Km
NormalizeUptake	0		Normalize uptake investment for the number of uptake genes
Uptake_per_monomer	1		number of transporters per monomer
Uptake_C_cost_min	0.01	transporter mg-1 biomass C	Minimun per enzyme C cost as a fraction of uptake
Uptake_C_cost_max	0.1	transporter mg-1 biomass C	Maximum per enzyme C cost as a fraction of uptake
Uptake_Maint_cost	0.01	mg C transporter-1 day-1	Respiration cost of uptake transporters
Uptake_Vmax0_min	1	mg substrate mg-1 substrate day-1	Minimum uptake Vmax
Uptake_Vmax0_max	10	mg substrate mg-1 substrate day-1	Maximum uptake Vmax
Uptake_Ea_min	35	kj mol-1	Minimum activation energy for uptake
Uptake_Ea_max	35	kj mol-1	Maximum activation energy for uptake
Uptake_Km_min	0.001	mg cm-3	Minimum uptake Km

Table A2 Substrate concentrations initialized in DEMENT simulations (mg cm^{-3}).

Substrate	C	N	P
DeadMic	0	0	0
DeadEnz	0	0	0
Cellulose	146.89	0	0
Hemicellulose	85.855	0	0
Starch	12.21	0	0
Chitin	4.9952	0.83254	0
Lignin	48.51	0.40425	0
Protein1	10.6	2.09704	0
Protein2	10.6	2.09704	0
Protein3	10.6	2.09704	0
OrgP1	12.48	0	0.478469
OrgP2	1.8182	0.79745	0.478469

Table A3 Manipulated enzyme production rate scenarios and ECA parameter values. Bold values indicate simulations used in further analyses.

Run	EnzProdConstit	EnzProdInduce	k_2	k_m
1	2	2	17.830	28.603
2	3	3	22.353	73.208
3	4	4	21.473	65.600
4	**5**	**5**	**22.506**	**75.040**
5	6	6	22.929	80.467
6	7	7	24.091	90.833
7	8	8	22.766	81.393
8	9	9	23.244	86.231
9	**10**	**10**	**24.976**	**102.192**
10	11	11	26.746	119.165
11	12	12	26.132	114.029
12	**15**	**15**	**30.561**	**158.196**
13	17	17	32.961	180.897
14	18	18	32.575	177.935
15	**20**	**20**	**33.243**	**189.403**
16	22	22	37.327	227.398
17	25	25	41.945	273.338
18	**30**	**30**	**51.635**	**379.492**

EnzProdConstit, EnzProdInduce: 10^{-5} mg C mg^{-1} day $^{-1}$

k_2: mg substrate mg^{-1} enzyme d^{-1}

k_m: mg cm^{-3}

Table A4 Cellulose enzyme kinetic parameter values for the Michaelis-Menten equation.

Enzyme	**Vmax(mg substrate mg^{-1} enzyme day^{-1})**	**Km (mg cm^{-3})**
1	11.68	13.09
2	19.13	21.44
3	36.72	41.16

Table A5 ECA parameter values of different substrates based on the simulation with enzyme production rates of 15.0×10^{-5} mg C mg^{-1} day^{-1} (both constitutive and inducible).

Substrate	**k_2**	**k_m**	**RMSE**
Cellulose	30.561	158.196	0.029
Chitin	31.578	51.798	0.002
DeadEnz	10.027	7.717	0.004
Hemicellulose	48.030	90.618	0.019
Lignin	14.826	27.247	0.009
OrgP1	43.331	100.000	0.012
OrgP2	73.453	100.000	0.003
Protein1	35.204	100.000	0.021
Protein2	26.128	100.000	0.029
Protein3	48.722	100.000	0.011
Starch	34.229	100.000	0.016
Total	17.806	1177.599	0.178

Note: parameter values of substrates from OrgP1 through Starch are derived from fits with an upper bound of 100.0 for each parameter to avoid overfitting and should be interpreted with caution.

k_2: mg substrate mg^{-1} enzyme d^{-1}

k_m: mg cm^{-3}

RMSE: mg cm^{-3} d^{-1}

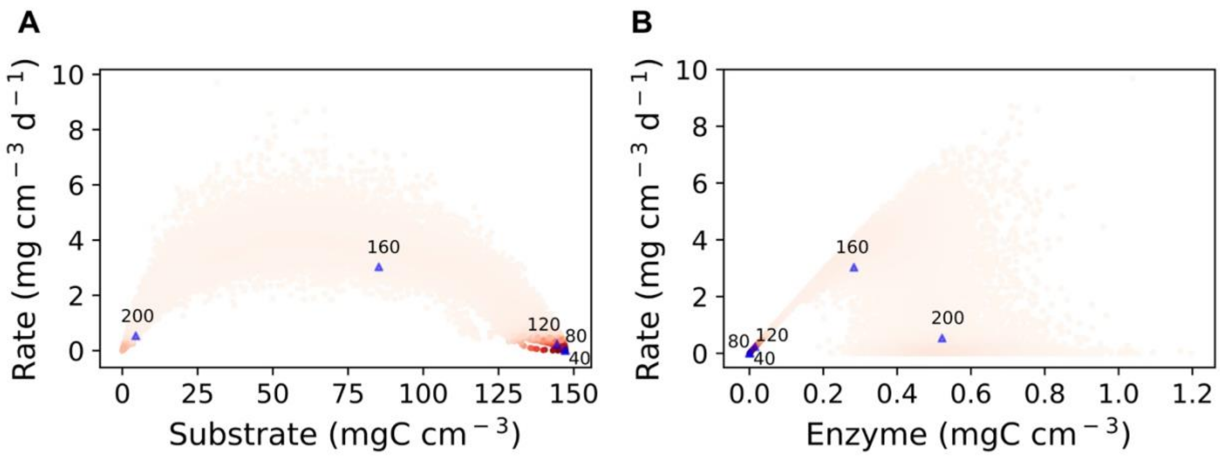

Fig.A1 Degradation rate versus substrate and enzyme concentration over the 100×100 spatial grid with data from specific dates plotted together. Points represent grid box data on days 40, 80, 120, 160, and 200 from the simulation with enzyme production rates of 15.0×10^{-5} mg C mg^{-1} day^{-1} (both constitutive and inducible). High intensity of red denotes high density of points based on kernel density distribution. Blue points denote the means for each day.

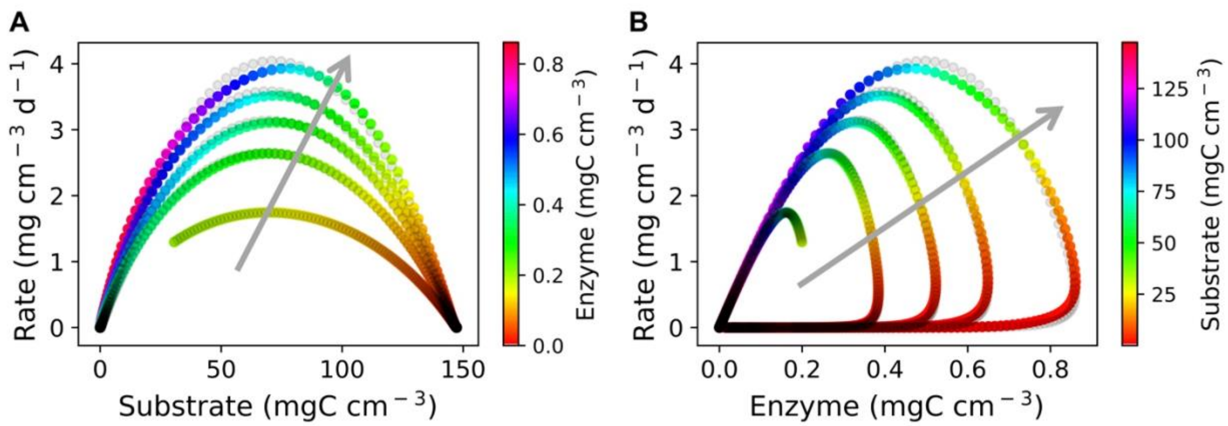

Fig.A2 Cellulose degradation rate as a function of both substrate and enzyme concentration. Similar to **Fig.4**, grey points follow the best fit ECA equation (see **Table A3** for the parameter values). Points in color represent averages over the grid of each day with colors denoting enzyme (**A**) or substrate concentration (**B**). In contrast to **Fig.4,** the ECA equation is fitted with data from five simulations with different enzyme production rates (5×10^{-5}, 10×10^{-5}, 15×10^{-5}, 20×10^{-5}, and 30×10^{-5} mg C mg^{-1} day^{-1}, which are selected from scenarios in **Table A3**). The arrow in grey points toward increasing enzyme production rates across the simulations.

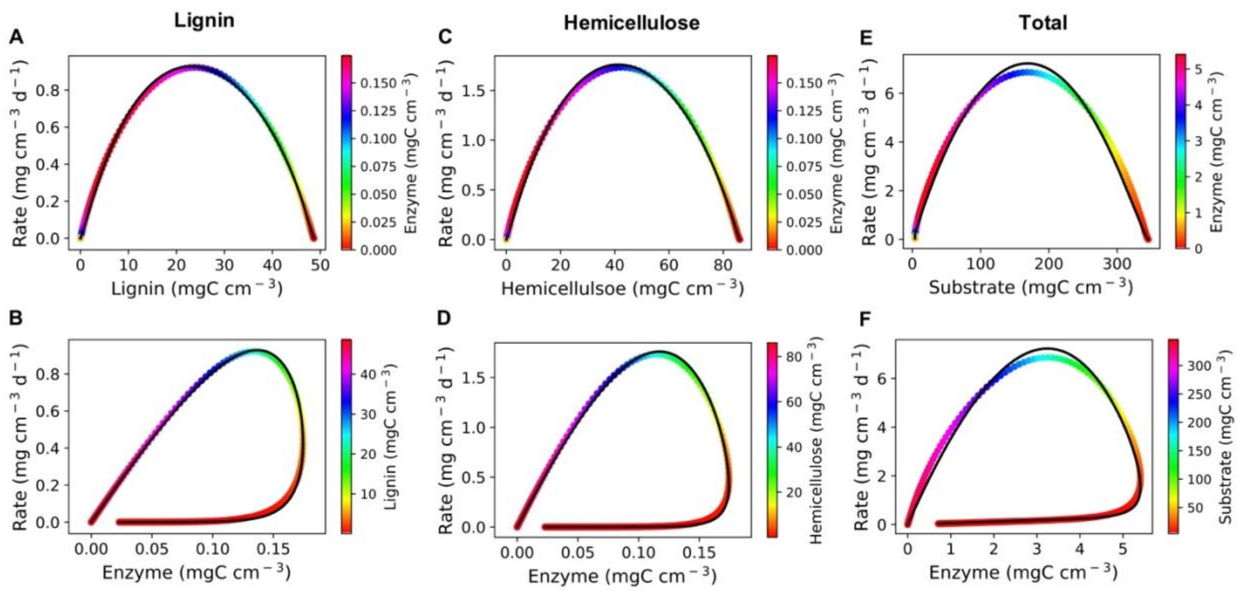

Fig.A3 Same as Fig.4 but for different substrates. A,B) Lignin (RMSE= 0.009 mg cm^{-3} d^{-1}); **C,D)** hemicellulose (RMSE= 0.019 mg cm^{-3} d^{-1}); and **E,F)** all substrates in the system (RMSE= 0.178 mg cm^{-3} d^{-1}). See **Table A5** for ECA parameter values and all other substrates.