EcoENzYme (EEZY) model diagrams and code

TITLE:

*A theoretical model of C- and N-acquiring exoenzyme activities, which balances microbial demands during decomposition*

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**Sector 01 Main C fluxes**



Biom\_C(t) = Biom\_C(t - dt) + (GrowC - Hc) \* dt

INIT Biom\_C = 1 { microbial biomass mg C }

INFLOWS:

GrowC = GrwC { C input for microbial growth }

OUTFLOWS:

Hc = Kt\*Biom\_C { Microbial death/turnover; fixed proportion/d }

C1(t) = C1(t - dt) + (in\_C1 - Dc1) \* dt

INIT C1 = 500 { mg soil organic carbon pool 1; this substrate has N }

INFLOWS:

in\_C1 = Dc1 { at steady state, inputs equal outputs }

OUTFLOWS:

Dc1 = dC1dt

C2(t) = C2(t - dt) + (in\_C2 - Dc2) \* dt

INIT C2 = 1000-C1 { mg soil organic carbon pool 2; this substrate has no N }

INFLOWS:

in\_C2 = Dc2 { at steady state, inputs equal outputs}

OUTFLOWS:

Dc2 = dC2dt

DOC(t) = DOC(t - dt) + (Dc1 + Dc2 - GrowC - EPc1 - EPc2 - Respiration - Overflow) \* dt

INIT DOC = 0 { solubilized-dissolved organic carbon }

INFLOWS:

Dc1 = dC1dt

Dc2 = dC2dt

OUTFLOWS:

GrowC = GrwC { C input for microbial growth }

EPc1 = Ep1 { amount of C used in enzyme 1 production }

EPc2 = Ep2 { amount of C used in enzyme 2 production }

Respiration = Rg+ReT+Rm { C flux for growth respiration and overflow metabolism }

Overflow = Ro

Enz\_C1(t) = Enz\_C1(t - dt) + (EPc1 - ELc1) \* dt

INIT Enz\_C1 = { Initial enzyme 1 pool } 0.02\*Biom\_C

INFLOWS:

EPc1 = Ep1 { amount of C used in enzyme 1 production }

OUTFLOWS:

ELc1 = K\*Enz\_C1 {{ enzyme 2 turnover; fixed proportion/d }

Enz\_C2(t) = Enz\_C2(t - dt) + (EPc2 - ELc2) \* dt

INIT Enz\_C2 = 0.02\*Biom\_C { Exoenzyme C2 pool }

INFLOWS:

EPc2 = Ep2 { amount of C used in enzyme 2 production }

OUTFLOWS:

ELc2 = K\*Enz\_C2 { enzyme 2 turnover; fixed proportion/d }

C\_in = Dc1+Dc2

K = 0.05 { enzyme turnover coefficient/d }

Km = 0.01 { microbial maintenance respiration coefficient/d }

Kt = 0.012 { microbial biomass turnover coefficient/d }

Rm = Km\*Biom\_C { maintenance respiration }

**Sector 02 Enzyme allocation**



alpha = alpha\_1

alpha\_1 = max(0,min(1, 1/2\*(CN1\*Vmax1\*CUE1\*K2+Et\*CN1\*Vmax1\*CUE1+Et\*CN1\*Vmax2\*CUE2-CN1\*Vmax2\*CUE2\*K1-CNm\*K2\*Vmax1-CNm\*Vmax1\*Et+(-2\*CNm\*Vmax1\*Et\*CN1\*Vmax2\*CUE2\*K1+2\*Et\*CN1^2\*Vmax1\*CUE1\*Vmax2\*CUE2\*K1+2\*CNm\*K2\*Vmax1\*CN1\*Vmax2\*CUE2\*K1-2\*CNm\*K2\*Vmax1\*Et\*CN1\*Vmax2\*CUE2-2\*CN1^2\*Vmax1\*CUE1\*K2\*Vmax2\*CUE2\*K1+2\*CN1^2\*Vmax1\*CUE1\*K2\*Et\*Vmax2\*CUE2-4\*CNm\*Vmax1^2\*Et\*CN1\*CUE1\*K2-2\*CNm\*Vmax1\*Et^2\*CN1\*Vmax2\*CUE2+2\*Et^2\*CN1^2\*Vmax1\*CUE1\*Vmax2\*CUE2+CNm^2\*Vmax1^2\*Et^2+CNm^2\*K2^2\*Vmax1^2+2\*Et\*CN1^2\*Vmax1^2\*CUE1^2\*K2-2\*CNm\*K2^2\*Vmax1^2\*CN1\*CUE1+2\*CN1^2\*Vmax2^2\*CUE2^2\*K1\*Et-2\*CNm\*Vmax1^2\*Et^2\*CN1\*CUE1+2\*CNm^2\*Vmax1^2\*Et\*K2+Et^2\*CN1^2\*Vmax1^2\*CUE1^2+CN1^2\*Vmax1^2\*CUE1^2\*K2^2+CN1^2\*Vmax2^2\*CUE2^2\*K1^2+Et^2\*CN1^2\*Vmax2^2\*CUE2^2)^(1/2))/Et/(CN1\*Vmax1\*CUE1+CN1\*Vmax2\*CUE2-CNm\*Vmax1) ))

Et = Enz\_C1+Enz\_C2 { calculate the total enzyme pool size }

gamma\_1 = if DOC>0 then max(0,min(1,(-Enz\_C1 + alpha\*Enz\_C1 + alpha\*Enz\_C2 + alpha\*Ke\*DOC)/(Ke\*DOC))) else 0 { fraction of total enzyme PRODUCTION allocated to Enz\_1 }

ratio\_E2:E1 = Enz\_C2/Enz\_C1

Vmax1 = kd1\*C1 { maximum rate of SOC1 decay }

Vmax2 = kd2\*C2 { maximum rate of SOC2 decay }

**Sector 03 Enzyme C production and respiration**



CNm = 7.16 {Microbial C:N ratio}

CUE1 = 0.5

CUE2 = 0.5 { Place right hand side of equation here... }

Ep1 = min(Ke\*DOC,CNm\*DON)\*gamma\_1 { enzyme 1 production; limited by C and N }

Ep2 = min(Ke\*DOC,CNm\*DON)-Ep1 { enzyme 2 production; limited by C and N }

Epct = Ep1+Ep2 { total amount of C used for enzyme 1+2 production }

Ke = 0.05 { Fraction of C-uptake allocated to exoenzyme production }

Re1 = Ep1\*((1-CUE1)/CUE1\*Dc1/(Dc1+Dc2) + (1-CUE2)/CUE2\*Dc2/(Dc1+Dc2)) { Respiratory cost of enzyme 1 production }

Re2 = Ep2\*((1-CUE1)/CUE1\*Dc1/(Dc1+Dc2) + (1-CUE2)/CUE2\*Dc2/(Dc1+Dc2)) { Respiratory cost of enzyme 2 production }

ReT = Re1+Re2 { total respiration for enzyme production }

**Sector 04 Decay rates**



dC1dt = kd1\*Enz\_C1/(K1 + Enz\_C1) { SOC1 solubilization by enzyme action }

dC2dt = kd2\*Enz\_C2/(K2 + Enz\_C2) { SOC2 solubilization by enzyme action }

dCTdt = dC1dt+dC2dt

K1 = 0.3 { enzyme activity half-saturation constant }

K2 = 0.3 { Place right hand side of equation here... }

kd1 = 1 { Place right hand side of equation here... }

kd2 = 1.0 { Place right hand side of equation here... }

**Sector 05 Nitrogen flow routine**



Biom\_N(t) = Biom\_N(t - dt) + (GrowN - loss) \* dt

INIT Biom\_N = Biom\_C/CNm { microbial N content }

INFLOWS:

GrowN = GrwN { DON uptake into microbial biomass }

OUTFLOWS:

loss = Hc/CNm {Death/turnover N}

DON(t) = DON(t - dt) + (Dn - GrowN - EPn1 - EPn2 - Mnzn) \* dt

INIT DON = 0 { solublized-dissolved organic N }

INFLOWS:

Dn = Dc1/CN1 { SON solubilization }

OUTFLOWS:

GrowN = GrwN { DON uptake into microbial biomass }

EPn1 = En1o { amount of DON used in enzyme 1 production }

EPn2 = En2o { amount of DON used in enzyme 2 production }

Mnzn = DON-GrwN-EpnT

Enz\_N1(t) = Enz\_N1(t - dt) + (EPn1 - ELn1) \* dt

INIT Enz\_N1 = Enz\_C1/CNm { initial N content of enzyme 1 }

INFLOWS:

EPn1 = En1o { amount of DON used in enzyme 1 production }

OUTFLOWS:

ELn1 = ELc1/CNm { Exoenzyme 1 turnover N }

Enz\_N2(t) = Enz\_N2(t - dt) + (EPn2 - ELn2) \* dt

INIT Enz\_N2 = Enz\_C2/CNm { initial N content of enzyme 2 }

INFLOWS:

EPn2 = En2o { amount of DON used in enzyme 2 production }

OUTFLOWS:

ELn2 = ELc2/CNm { Exoenzyme 1 turnover N }

SON1(t) = SON1(t - dt) + (in\_N - Dn) \* dt

INIT SON1 = C1/CN1 { N content of soluble organic carbon pool 1 }

INFLOWS:

in\_N = in\_C1/CN1 { Inputs of organic N }

OUTFLOWS:

Dn = Dc1/CN1 { SON solubilization }

N\_out = EPn1+EPn2+GrowN+Mnzn

**Sector 06 Microbial growth & respiration**



C1\_growth = C\_for\_growth\*CUE1\*Dc1/(Dc1+Dc2) { growth from SOC1-C }

C2\_growth = C\_for\_growth\*CUE2\*Dc2/(Dc1+Dc2) { growth from SOC2-C }

C\_available = C1\_growth+C2\_growth { total C available for growth }

C\_demand\_for\_growth = max(0,(DON-EpnT)\*CNm) { C demand given N availability }

C\_for\_growth = max(0,DOC-Rm-Epct-ReT) { DOC left after enzyme production and maintenance }

GrwC = max(0 , min( C\_available , C\_demand\_for\_growth )) { microbial growth C }

Rg = GrwC\*((1-CUE1)/CUE1\*Dc1/(Dc1+Dc2) + (1-CUE2)/CUE2\*Dc2/(Dc1+Dc2)) { Respiratory cost of microbial growth }

Ro = max(0,DOC-(Epct+GrwC+ReT+Rg+Rm)) { overflow metabolism }

**Sector 07 Enzyme N production and N immobilization**



En1o = Ep1/CNm { DON immobilized in enzyme 1 production }

En2o = Ep2/CNm { DON immobilized in enzyme 2 production }

Epnot = En1o+En2o { total DON immobilized by production of enzymes 1+2 }

EpnT = Epnot { total N immobilization in enzymes production }

GrwN = GrwC/CNm { DON used for biomass production }

**Sector 09 CN ratios; Given and estimated**



CN1 = 5

CNs = 25

CNs\_1 = CN1\*(C2+C1)/C1 { C:N ratio of total litter substrate }