Progress Toward a Mechanistic Belowground N Cycle in CLM

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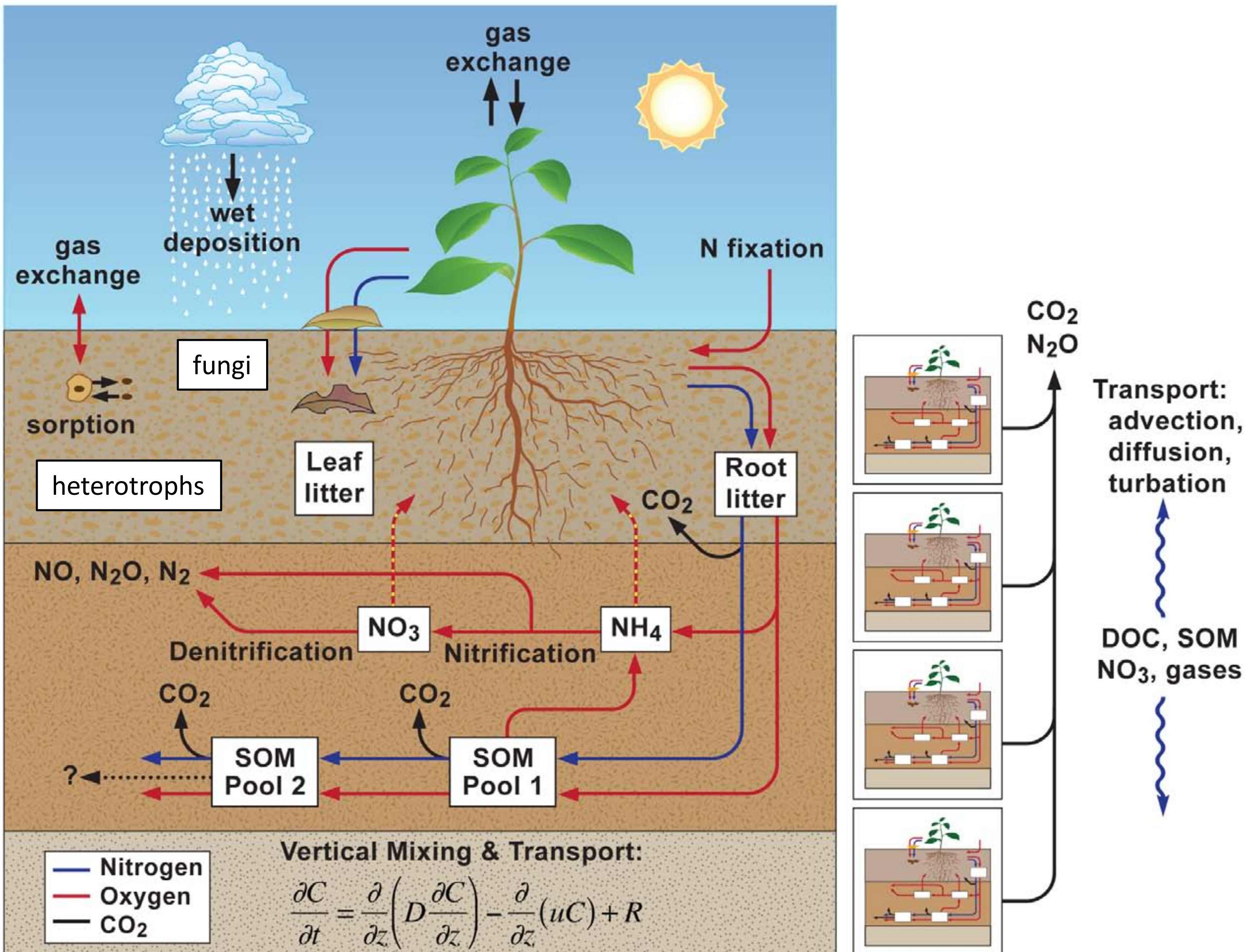
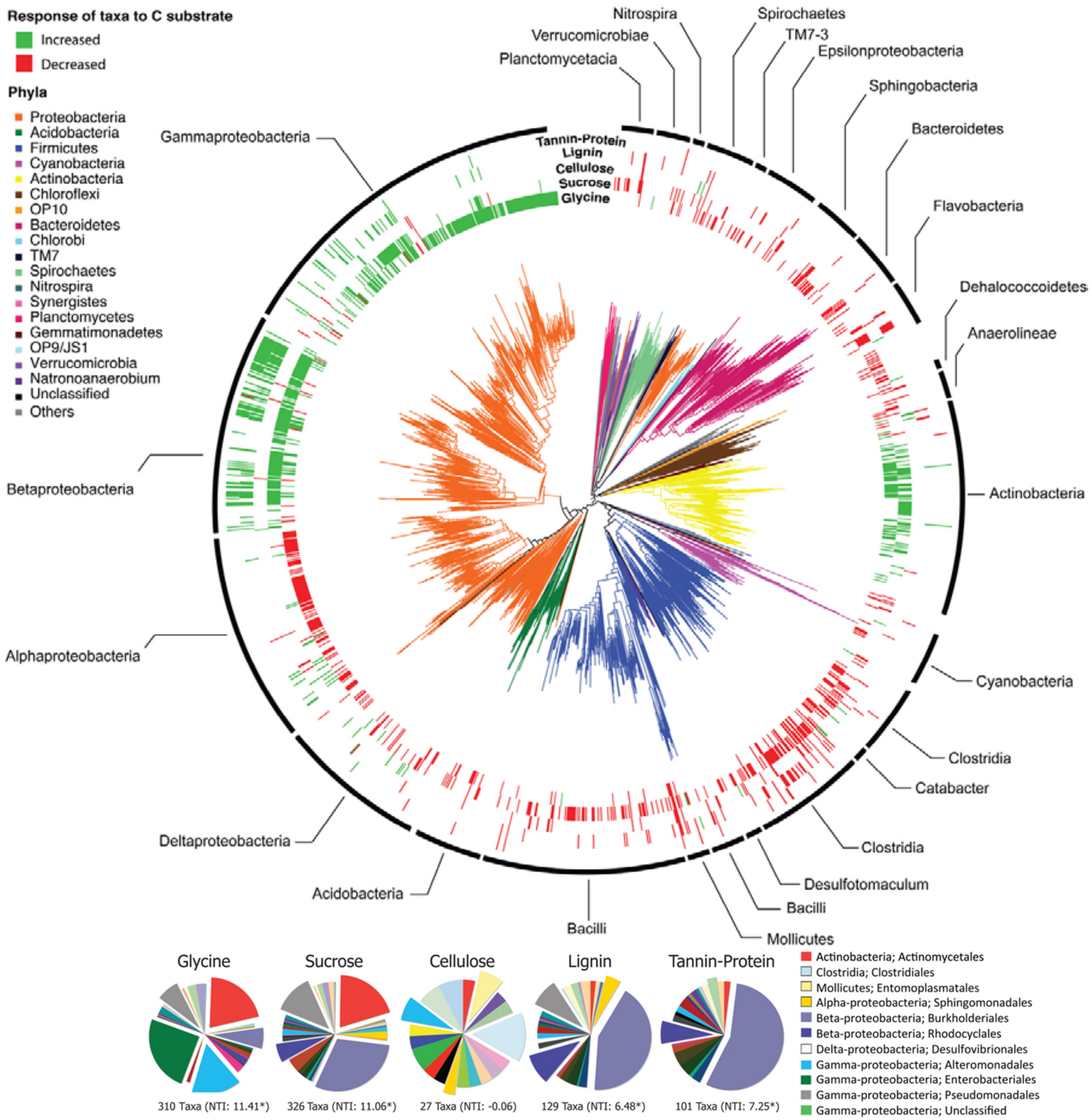


gas exchange
wet deposition
gas exchange
N fixation
fungi
sorption
heterotrophs
Leaf litter
Root litter
CO_2
NO, N_2O, N_2
NO_3
NH_4
Denitrification
Nitrification
CO_2
CO_2
SOM Pool 2
SOM Pool 1
?
Nitrogen
Oxygen
CO_2
Vertical Mixing & Transport:
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial z}(uC) + R$$
CO_2
N_2O
Transport:
advection,
diffusion,
turbation
DOC, SOM
NO_3, gases

Soil bacteria exhibit differential growth responses to carbon substrates of varying chemical recalcitrance



- Only growing bacteria were targeted (BrdU captured DNA) analyzed by PhyloChip microarrays
- Growth response of ~2,200 bacterial taxa compared following addition of C substrates of varying chemical recalcitrance.
- Organisms responding to 'labile' C were phylogenetically clustered
- Organisms responding to 'recalcitrant' C were phylogenetically dispersed.

Goldfarb et al (2011). Frontiers in Terrestrial Microbiology, 2:94.

Atmosphere

Lamarque et al., 2011

Table 4. Continued.

MACR + O3 → .8*CH3(
+ .215*OH
MACRO2 + NO → NO2
+ .25*CH3COCHO + .5(
MACRO2 + NO → 0.8*(

Table 4. Continued.

NO2 + HO2 + M → HO2NO2 + M

HO2NO2 + OH → H2O + NO2 + O2
HO2NO2 + M → HO2 + NO2 + M

C-1 Degradation (Methane, CO, CH2O and

CH4 + OH → CH3O2 + H2O
CH3O2 + NO → CH2O + NO2 + HO2
CH3O2 + HO2 → CH3OOH + O2
CH3OOH + OH → CH3O2 + H2O

Odd hydrogen reactions

H + O2 + M → HO2 + M

H + O3 → OH + O2
H + HO2 → 2*OH
H + HO2 → H2 + O2
H + HO2 → H2O + O
OH + O → H + O2
OH + O3 → HO2 + O2
OH + HO2 → H2O + O2
OH + OH → H2O + O
OH + OH + M → H2O2 + M

Table 4. Continued.

Heterogeneous reaction
N2O5 → 2*HNO3
NO3 → HNO3
NO2 → 0.5*OH + 0.5*N
HO2 → 0.5*H2O2

O1D reactions with halog

O1D + CFC11 → 3*CL
O1D + CFC12 → 2*CL
O1D + CFC113 → 3*CL
O1D + HCFC22 → CL
O1D + CCL4 → 4*CL
O1D + CH3BR → BR
O1D + CF2CLBR → BR
O1D + CF3BR → BR

Table 4. Continued.

Continued.

Stratospheric only photolysis

CH4 + hv → H + CH3O2
CH4 + hv → 1.44*H2 + .18*CH2O + .18*O + .(
+ .05*H2O
H2O + hv → OH + H
H2O + hv → H2 + O1D
H2O + hv → 2*H + O
CL2 + hv → 2*CL
OCLO + hv → O + CLO
CL2O2 + hv → 2*CL
HOCL + hv → OH + CL
HCL + hv → H + CL
CLONO2 + hv → CL + NO3
CLONO2 + hv → CLO + NO2
BRCL + hv → BR + CL
BRO + hv → BR + O
HOBR + hv → BR + OH
BRONO2 + hv → BR + NO3
BRONO2 + hv → BRO + NO2
CH3CL + hv → CL + CH3O2
CCL4 + hv → 4*CL
CH3CCL3 + hv → 3*CL
CFC11 + hv → 3*CL
CFC12 + hv → 2*CL
CFC113 + hv → 3*CL
HCFC22 + hv → CL
CH3BR + hv → BR + CH3O2
CF3BR + hv → BR
CF2CLBR + hv → BR + CL
CO2 + hv → CO + O

Odd-Oxygen Reactions

O + O2 + M → O3 + M
O + O3 → 2*O2
O + O + M → O2 + M
O1D + N2 → O + N2
O1D + O2 → O + O2
O1D + H2O → 2*OH
O1D + H2 → HO2 + OH
O1D + N2O → N2 + O2
O1D + N2O → 2*NO
O1D + CH4 → CH3O2 + OH
O1D + CH4 → CH2O + H + HC

Table 4. Continued.

ALKOOH + OH → ALKO2
XO2 + NO → NO2 + HO2 + .5*CO + .25*GLYOXAL + .25*HY(
+ .25*CH3COCHO + .25*GLYALD
XO2 + NO3 → NO2 + HO2 + 0.5*CO + .25*HYAC + 0.25*GLY
+ .25*CH3COCHO + .25*GLYALD
XO2 + HO2 → XOOH
XO2 + CH3O2 → .3*CH3OH + 0.8*HO2 + .7*CH(
+ .1*GLYOXAL + .1*CH3COCHO + .1*GLYALD
XO2 + CH3CO3 → 0.5*CO + CH3O2 + HO2 + C
+ .25*HYAC + .25*CH3COCHO + .25*GLYALD
XOOH + OH → H2O + XO2
XOOH + OH → H2O + OH

C-7 Degradation

TOLUENE + OH → .25*CRESOL + .25*HO2 + .7
TOLO2 + NO → .45*GLYOXAL + .45*CH3COCH(
+ .9*HO2
TOLO2 + HO2 → TOLOOH
TOLOOH + OH → TOLO2
CRESOL + OH → XOH
XOH + NO2 → .7*NO2 + .7*BIGALD + .7*HO2

C-10 Degradation

C10H16 + OH → TERPO2
C10H16 + O3 → .7*OH + MVK + MACR + HO2
C10H16 + NO3 → TERPO2 + NO2
TERPO2 + NO → .1*CH3COCH3 + HO2 + MVK + MACR + N
TERPO2 + HO2 → TERPOOH
TERPOOH + OH → TERPO2

Radon/Lead

Odd Bromine Reactions

BR + O3 → BRO + O2
BR + HO2 → HBR + O2
BR + CH2O → HBR + HO2 + CO
BRO + O → BR + O2
BRO + OH → BR + HO2
BRO + HO2 → HOBR + O2
BRO + NO → BR + NO2
BRO + NO2 + M → BRONO2 + M

BRO + CLO → BR + OCLO
BRO + CLO → BR + CL + O2
BRO + CLO → BRCL + O2
BRO + BRO → 2*BR + O2
HBR + OH → BR + H2O
HBR + O → BR + OH
HOBR + O → BRO + OH
RO + NO3

Table 4. Continued.

Ice aerosol reactions

N2O5 → 2*HNO3
CLONO2 → HOCL + HNO3
BRONO2 → HOBR + HNO3
CLONO2 + HCL → CL2 + HNO3
HOCL + HCL → CL2 + H2O
HOBR + HCL → BRCL + H2O

eactions with Cl, OH
2 + CO + 2*HCL
. + H2O + HO2
H2O + 3*CL
L + H2O + CF2O
l + H2O + HO2

tions

+ HNO3
+ HNO3
CLONO2 + HCL → CL2 + HNO3
HOCL + HCL → CL2 + H2O
HOBR + HCL → BRCL + H2O

Nitric acid di-hydrate reactions

N2O5 → 2*HNO3
CLONO2 → HOCL + HNO3
CLONO2 + HCL → CL2 + HNO3
HOCL + HCL → CL2 + H2O
BRONO2 → HOBR + HNO3

e Reactions
CLO + O2
HCL + H
→ HCL + H
+ HCL + O2
+ OH + CLO
→ HCL + H
+ CH3O2 +
CL + O2
→ CL + HO2
→ HCL + O2
→ O2 + HO
→ NO2 + CL
+ M → CLO

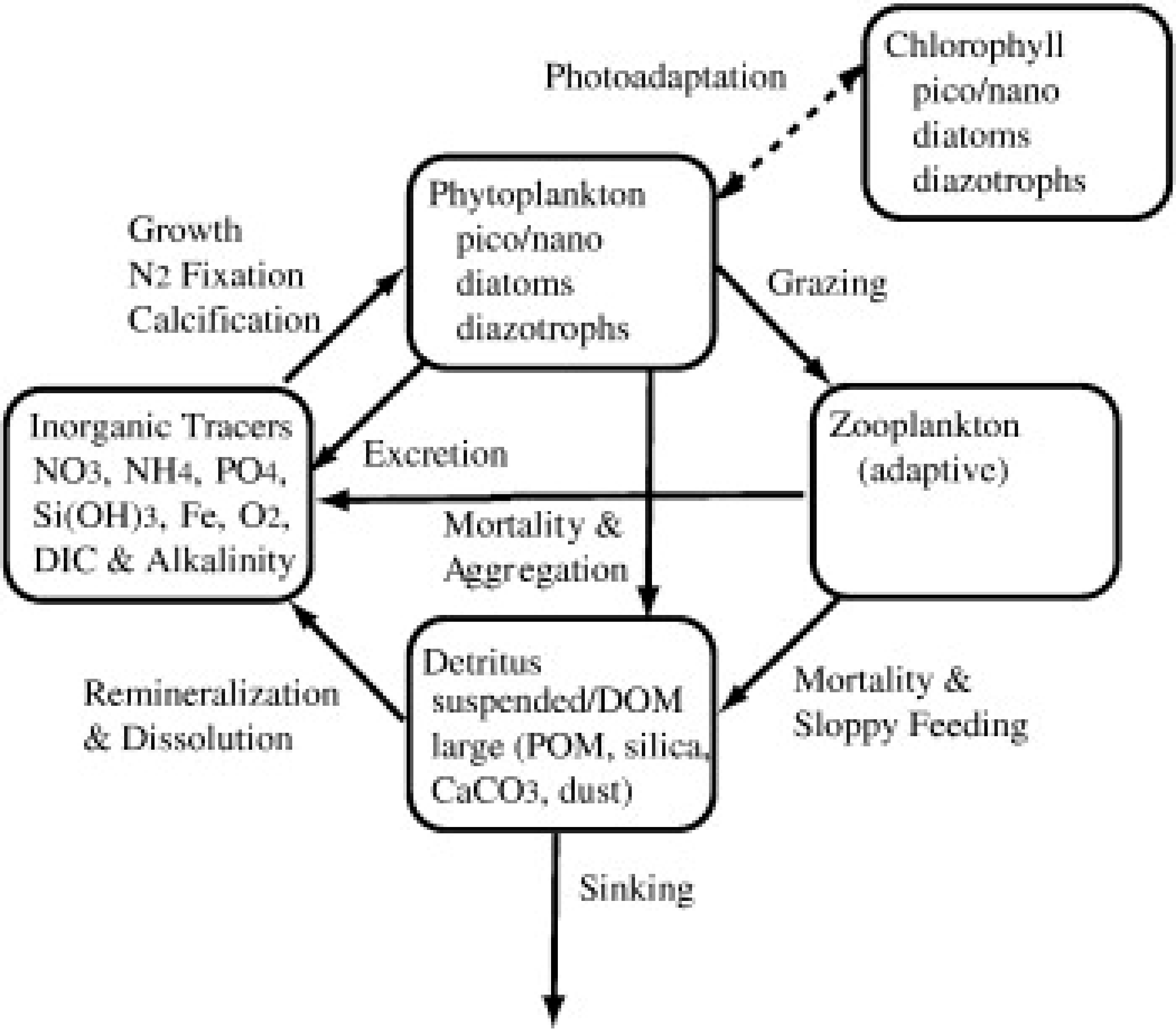
→ 2*CL + O
→ CL2 + O
→ CL + OC
+ M → CL2

→ CLO + O
→ H2O + CL
CL + OH
→ CLO + OH
→ HCL + C
→ H2O + C
O → CLO +
OH → HOC
CL → CL2 +

+ .5*CH3CO
NO2
+ HO2
2
2 + 2*GLYO
O2 + CO +
O2 + CH3CH
3 + NO2 + M
+ NO3

O2 + M

Ocean BGC



Doney et al., 2009

Belowground N Cycle Goals in CLM

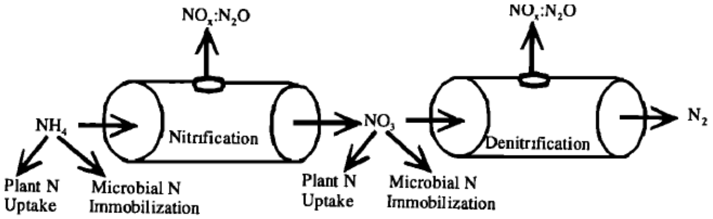
- Represent belowground N dynamics in a mechanistic way
- Biological processes
  - Nitrification
  - Denitrification
  - Mineralization, interaction with C dynamics
  - Fixation
  - Biological populations
- Physical and chemical processes
  - Advection (vertical, horizontal)
  - Gas production (CO_2, N_2O, CH_4, NO)
  - Stabilization (aggregation, mineral interactions, etc.)
  - Multi-phase (aqueous, gaseous, sorbed)
  - pH, redox, oxygen
- Current version of CLM4 contains little mechanistic representation of these processes

Two Parallel Paths for Improving CLM's Belowground N Cycle Representation

- CLM4.5
- CLM4-BeTR

CLM4.5

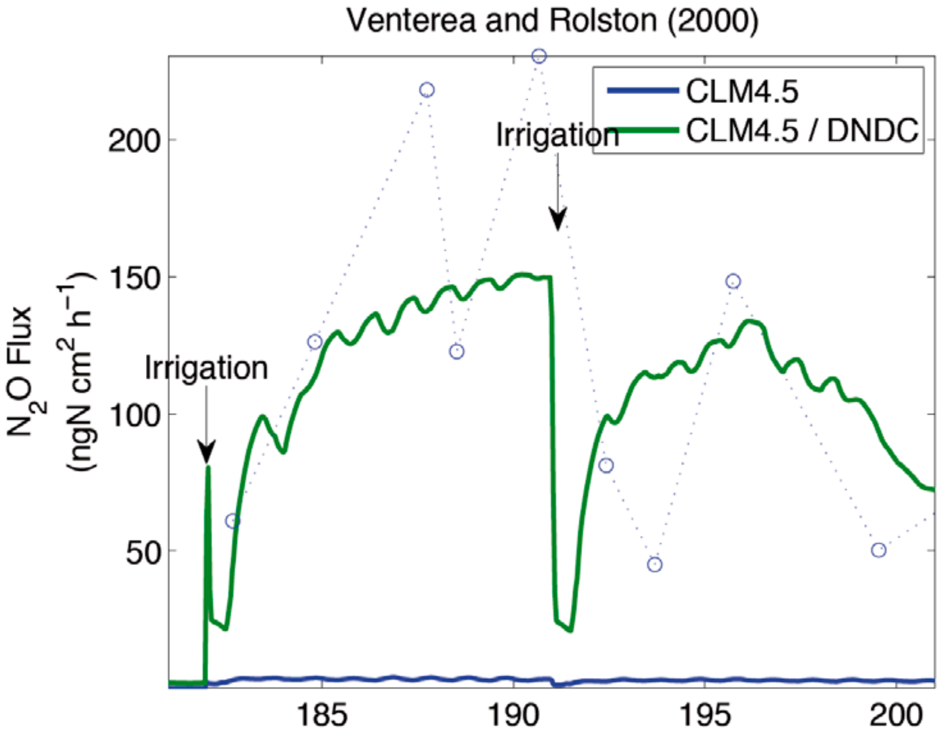
- C cascade
  - Century structure currently included
  - Easily modified structure and parameters
- Vertical discretization
  - Each layer has the complete C & N cascade
  - Surface and root litter
  - Radiocarbon, ^{13}C
  - Mixing, cryoturbation



- Century nitrification (Parton et al., 2001), denitrification (DelGrosso et al., 2000), N_2O emissions
  - Nitrification rate: $FNO_3 = Net_{min} * K_1 + K_{max} * NH_4 * F(t) * F(WFPS) * F(pH)$
  - N_2O production: $FN_2O = K_2 * FNO_3$
  - Denitrification rate: $D_t = \min[F_d(NO_3), F_d(CO_2)] F_d(WFPS).$
  - N_2O production: $R_{N2/N2O} = F_r(NO_3/CO_2) F_r(WFPS).$

Evaluating BG N Cycle Predictions

- Plants complicate interpretation of N observations for soil BGC processes
- Use N observations before emergence or in controls
  - Isolates soil BGC
  - Many such studies exist, often with measurements of NO_3, NH_4 concentrations, rates, and gas fluxes



- Baseline model fails to reproduce rates or gas fluxes
- Adding microbial activity and updating parameterizations improved dynamics

Rate Dependence on Θ and T Uncertain

- Multi-model comparison (Rodrigo et al. 1997):

$$h(T,\theta) = f_T g_\theta$$

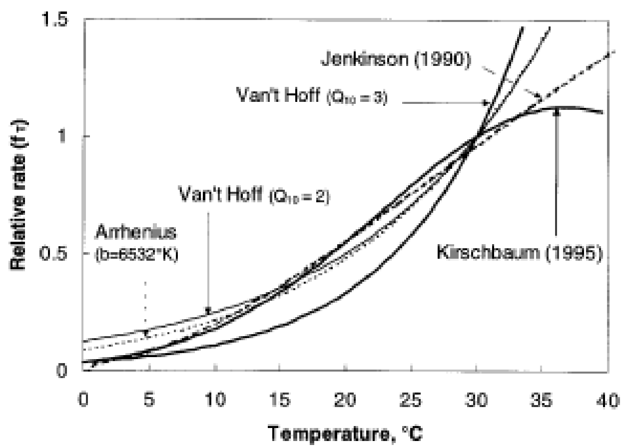
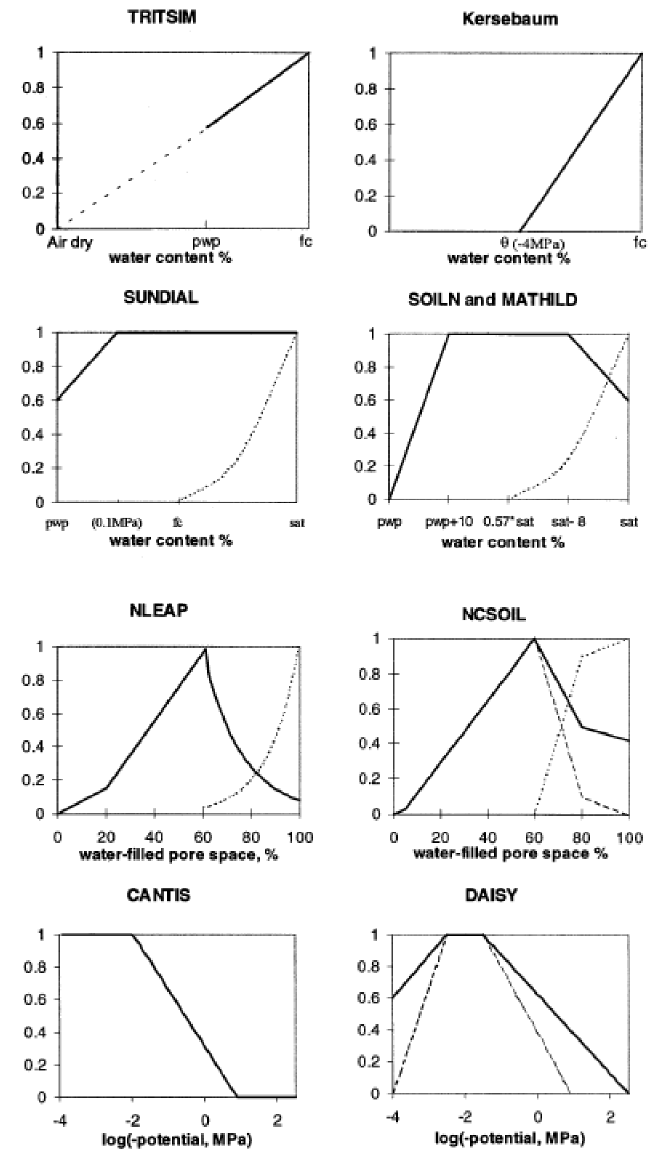
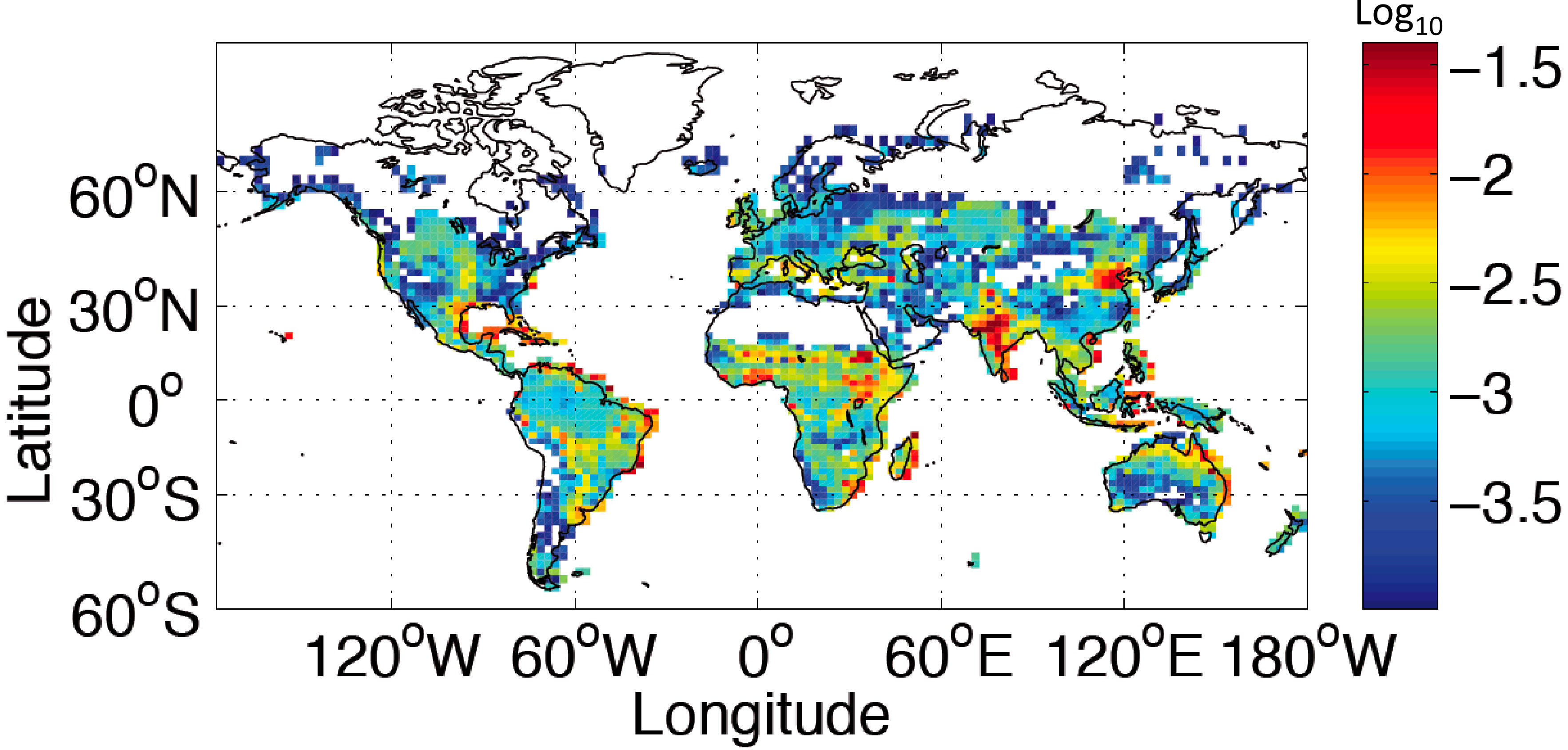


Fig. 1. Variation of the relative rate of microbial activity (f_T) with temperature using Van't Hoff (two values of Q_{10}), Arrhenius, Jenkinson (1990) ($f_T = 47.9/[1 + \exp(106/(T + 18.3))]$) and Kirschbaum (1995) ($f_T = \exp[-3.432 + 0.168T(1 - 0.5T/36.9)]$) equations.

A. Rodrigo et al. / Ecological Modelling 102 (1997) 325–339



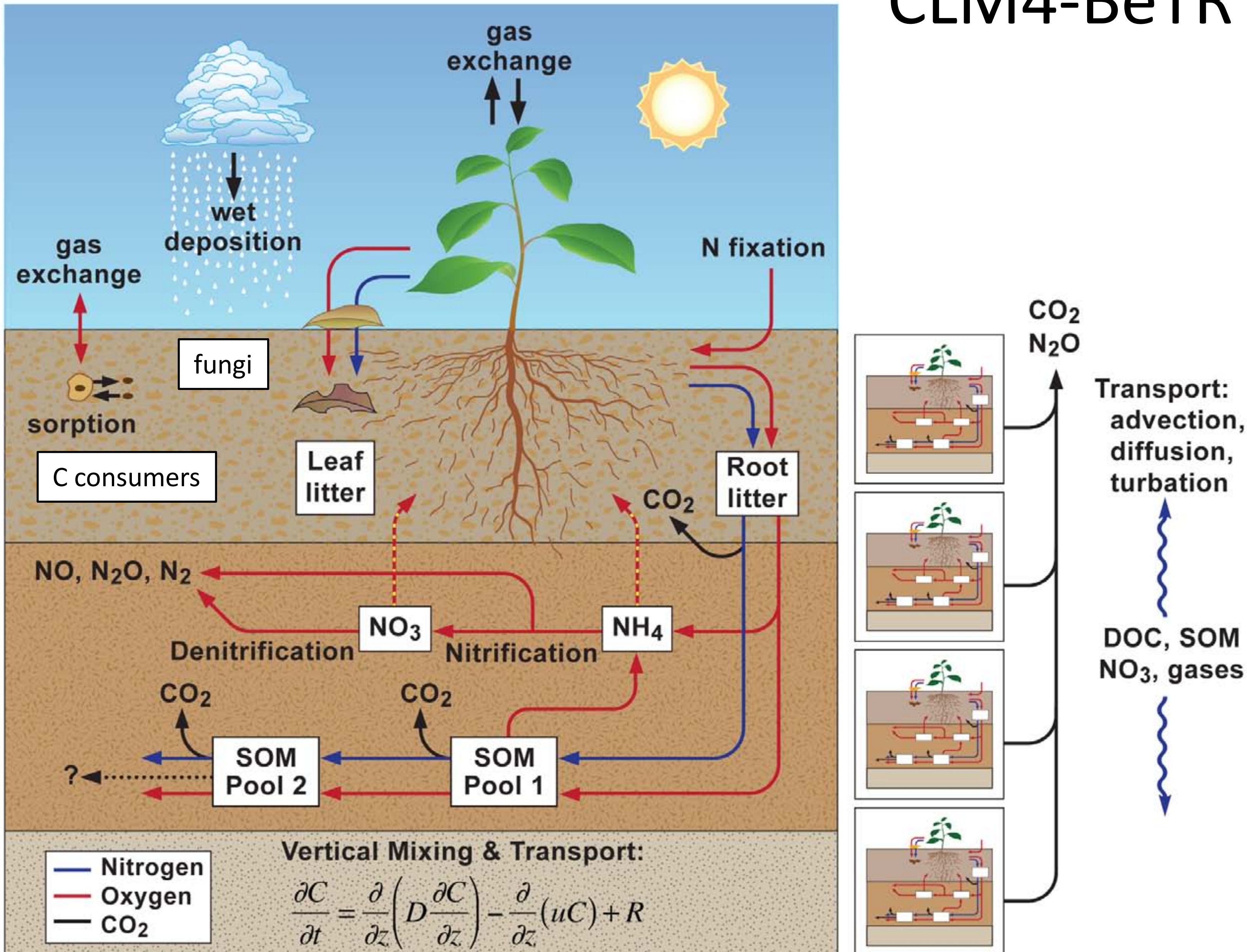
Annual Terrestrial N_2O Emission =12.6 TgN y^{-1}



CLM4-BeTR

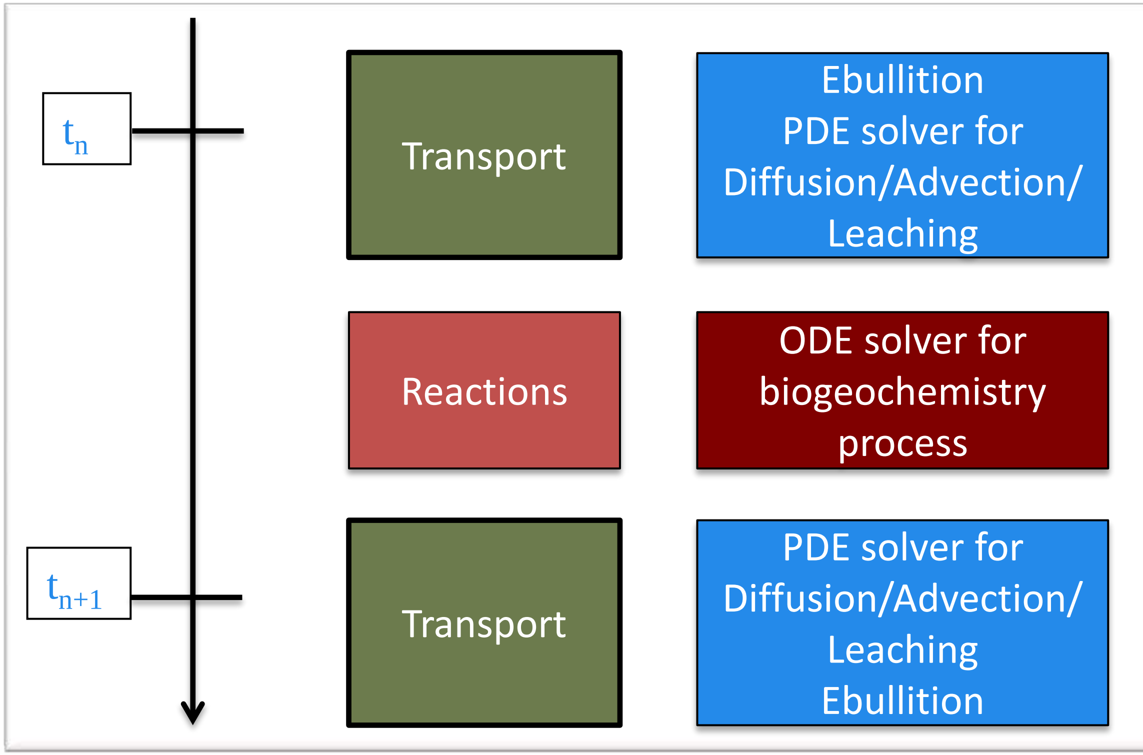
- General reactive/transport solver that includes
  - Arbitrary number of tracers
  - Aqueous, gaseous, sorbed phases
  - Vertical aqueous and gaseous and runoff fluxes
  - Transport into plants
  - Microbial dynamics
  - Isotopes
    - ^{18}O and D in water (with D Noone and T Wong)

CLM4-BeTR

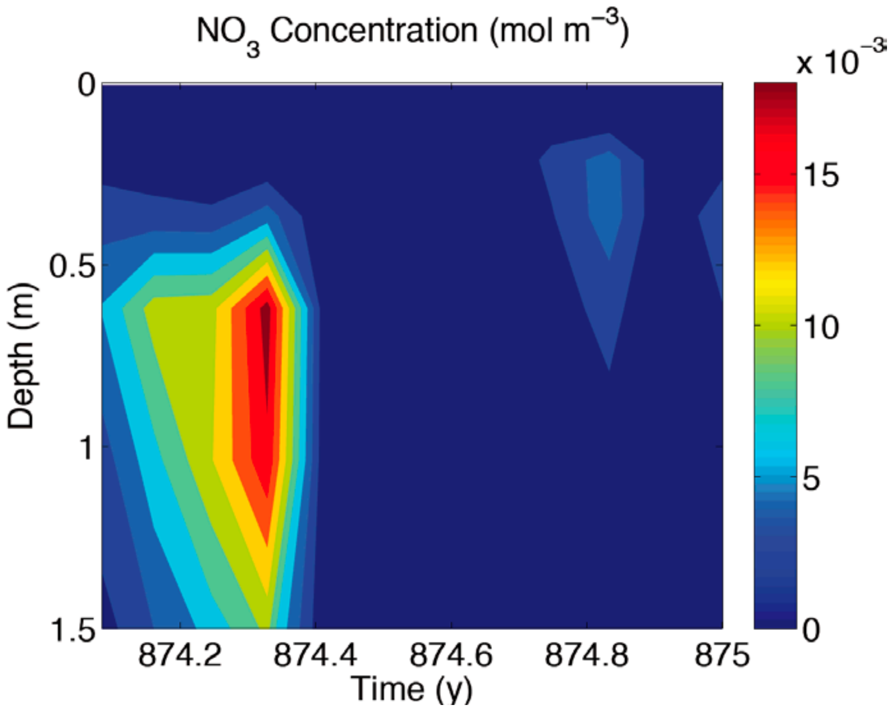

gas exchange
wet deposition
gas exchange
N fixation
fungi
sorption
C consumers
Leaf litter
Root litter
CO_2
NO, N_2O, N_2
NO_3
NH_4
Denitrification
Nitrification
CO_2
CO_2
SOM Pool 2
SOM Pool 1
?
Nitrogen
Oxygen
CO_2
Vertical Mixing & Transport:
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right) - \frac{\partial}{\partial z}(uC) + R$$
CO_2
N_2O
Transport: advection, diffusion, turbation
DOC, SOM
NO_3, gases

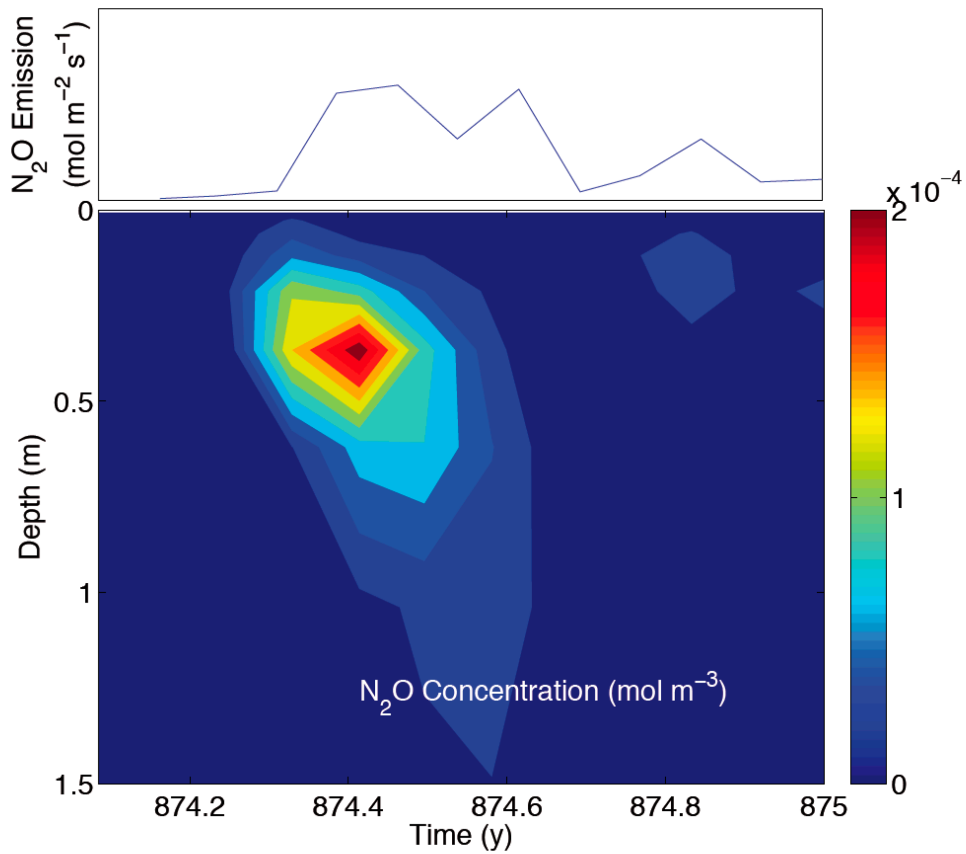
CLM4-BeTR Numerical Scheme

- **Processes evolve at different time scales**
- **Solved with standard numerical solvers at different internal time steps**
- **Mass conservation maintained at each sub-step**
- **Diffusion solved with a Crank-Nicolson finite-volume method**
- **Advection solved with 1st order upstream or 2nd order flux-limited scheme**
- **Biogeochemical processes solved with a standard ODE solver**

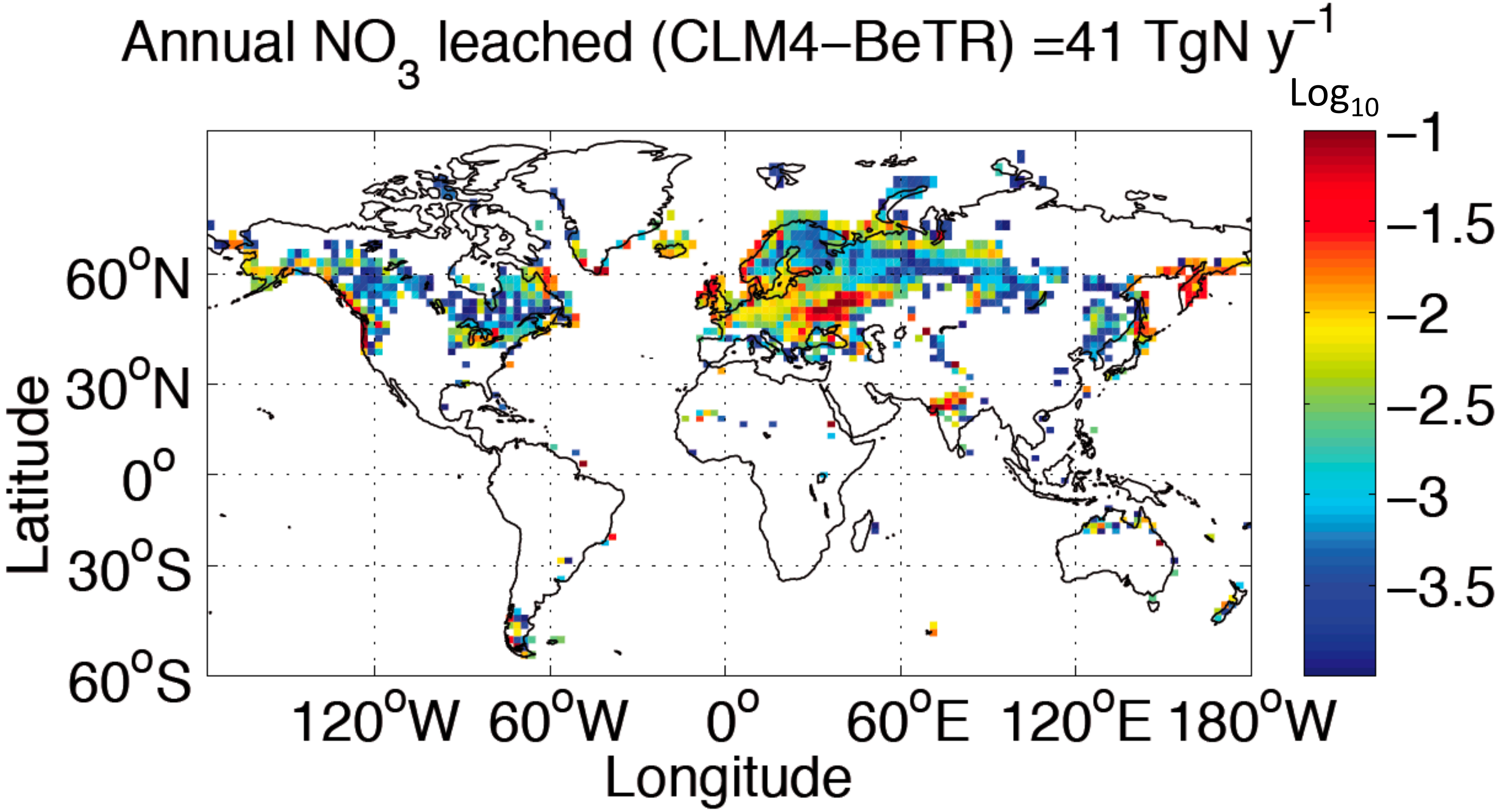


CLM4-BeTR N Cycle Simulations





NO_3 Leaching



Next Steps

- Model development
  - Integrate microbial processes and evaluate impacts
  - Crop model with fertilization
  - Integration of CH_4 dynamics (CLM4-Me)
- Model testing
  - Existing N experiments and controls
  - Sorption and stabilization mechanisms for C
  - Regional and global N_2O emission predictions against inversions and other estimates
- Model applications
  - Coupled C & N simulations; characterizing atmospheric interactions and feedbacks
  - Priming
  - C stabilization and potential destabilization under climate change
  - …