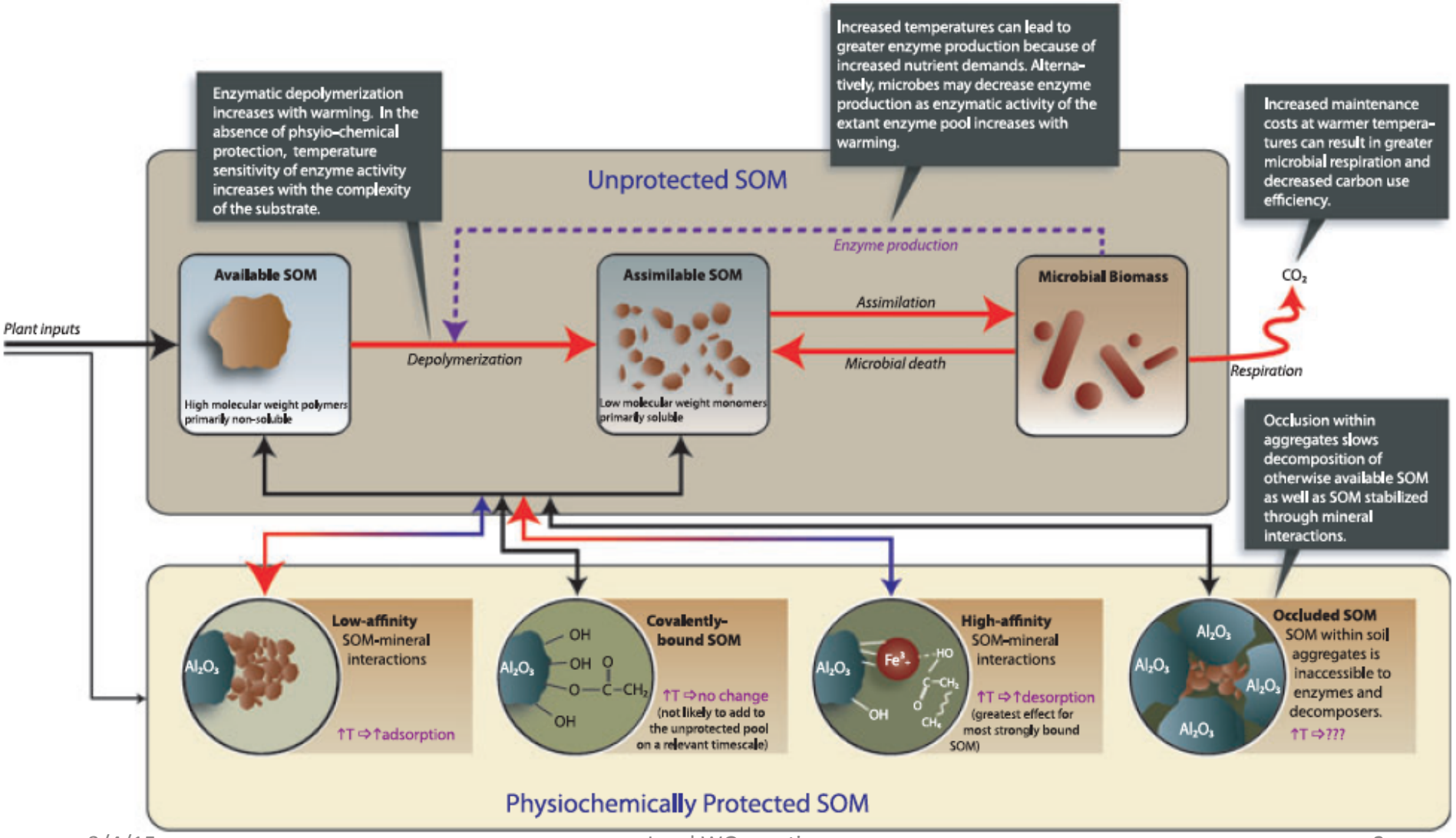
Lawrence Berkeley National Laboratory

ESD
EARTH SCIENCES DIVISION

Reactive transport module CLM BeTR-v2: description and usage for reaction-based biogeochemical modeling

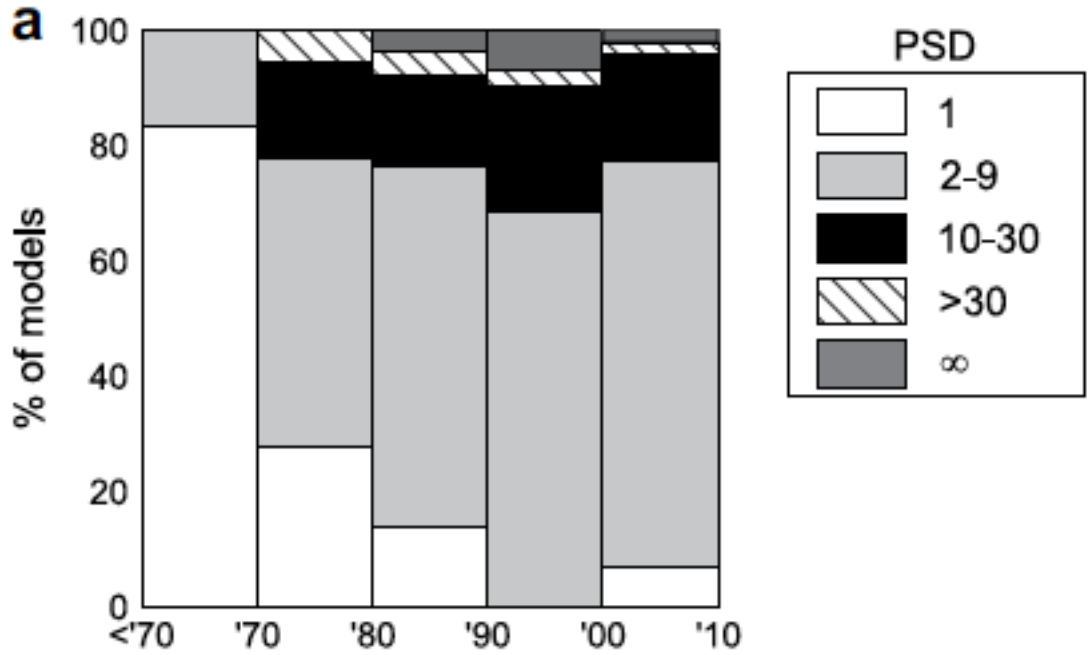
Jinyun Tang and Bill Riley

Motivation: The complex soil problem



Conant et al. 2011

Many BGC formulations



>250 models with various formulations (Manzoni and Porporato, 2009)

Which one is more plausible?

1-D mathematical representation

$$\frac{\partial}{\partial t}\left(C_v\theta_v + C_l\theta_l + C_i\theta_i\right) = \frac{\partial}{\partial z}\left[\theta_l D_l \frac{\partial C_l}{\partial z} + \theta_v D_v \frac{\partial C_v}{\partial z}\right] - \frac{\partial}{\partial z}\left(q_l C_l\right) + S$$

$v : vapor$

$l : liquid$

$i : ice$

$S : \text{sink / source}$ through runoff, transpiration, drainage

Bottom boundary condition: qcharge

Top boundary condition: net infiltration

Identical physics but variable biogeochemical formulations

CLM BeTR-v1

Geosci. Model Dev., 6, 127–140, 2013
www.geosci-model-dev.net/6/127/2013/
doi:10.5194/gmd-6-127-2013

Geoscientific Model Development

CLM4-BeTR, a generic biogeochemical transport and reaction module for CLM4: model development, evaluation, and application

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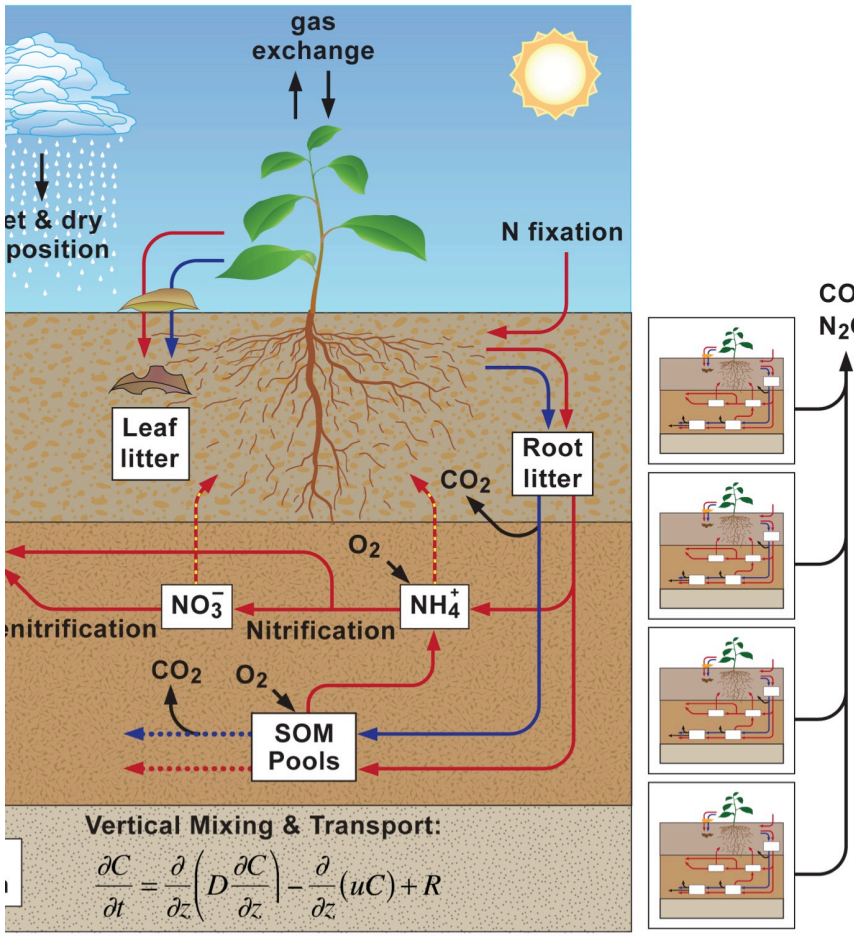
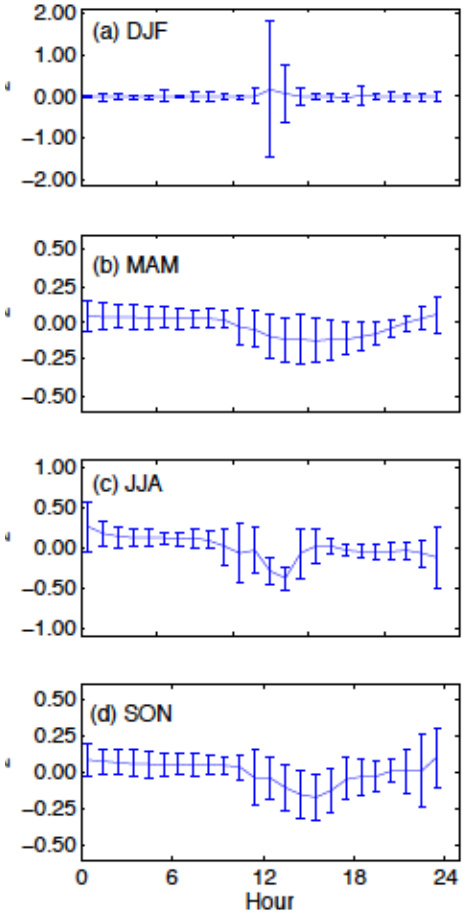
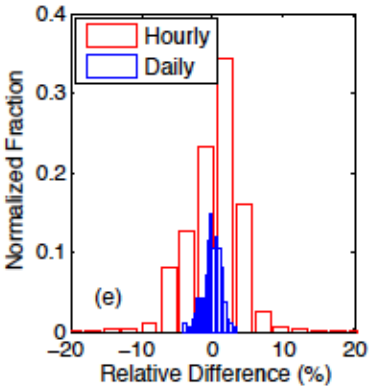
CLM BeTR-v1

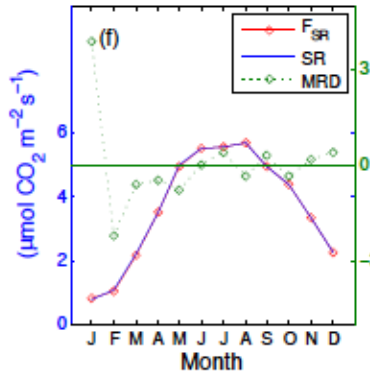


- **Uniform representation of tracer transport**
  - **multiphase diffusion**
  - **aqueous advection**
  - **gas ebullition**
  - **parenchyma transport**
- **Flexible subsurface BGC**
  - **diagnostic mode**
  - **active mode**
  - **coupling to different veg dynamics**

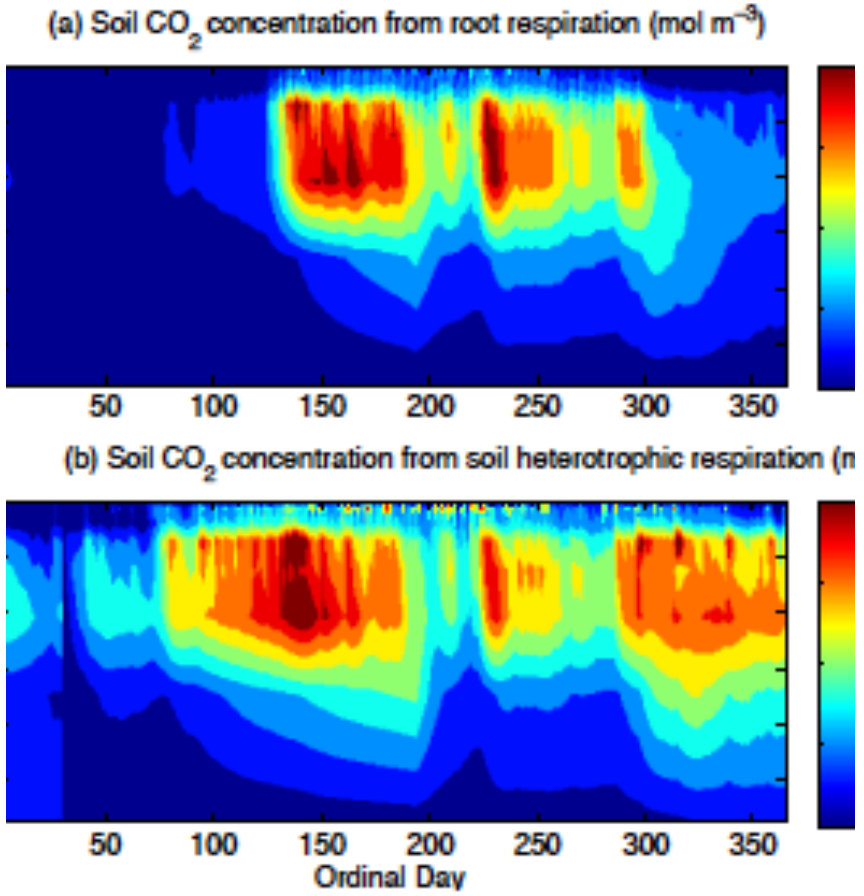
CLM BeTR-v1 applications







Produced ≠ Observed



different CO_2 tracer

Difference of BeTR v1 and v2

BeTR v2

- semi-lagrangian advection
- Implicit multiphase diffusion for any # of phase fronts
  - Tang and Riley, BG, 2014
- Dominant-gas based ebullition scheme
- OOP modular interfaces
- Unit testing of solvers

BeTR v1

- 1^{st}-2^{nd} order flux limiter advection
- Crank-Nicholson diffusion for < 3 phase fronts
- Ebullition based on all gases
- Over-engaged coding style (high maintenance)

The OOP based coding in v2

- Revision 68617: /clm2/branch_tags/clm4_5_1_r085_betr_tags/clm4_5_1_r085_betr10/models/lnd/clm/src/betr

- ..
- BGCReactionsFactoryMod.F90
- BGCReactionsMockRunType.F90
- BGCReactionsMod.F90
- BeTRTracerType.F90
- BetrBGCMod.F90
- EquilibriumChemMod.F90
- KineticsMod.F90
- PlantSoilnutrientFluxType.F90
- SOMStateVarUpdateMod.F90
- TracerBalanceMod.F90
- TracerBoundaryCondType.F90
- TracerCoeffType.F90
- TracerFluxType.F90
- TracerParamsMod.F90
- TracerStateType.F90
- Tracer_varcon.F90
- TransportMod.F90
- betr_initializeMod.F90
- bgc_O18transport/
- bgc_century/
- math/

$$\frac{\partial}{\partial t}\left(C_v\theta_v + C_l\theta_l + C_i\theta_i\right) = \frac{\partial}{\partial z}\left[\theta_l D_l \frac{\partial C_l}{\partial z} + \theta_v D_v \frac{\partial C_v}{\partial z}\right] - \frac{\partial}{\partial z}\left(q_l C_l\right) + S$$

$v : vapor$

$l : liquid$

$i : ice$

$S : \text{sin}k / source$ through runoff, transpiration, drainage

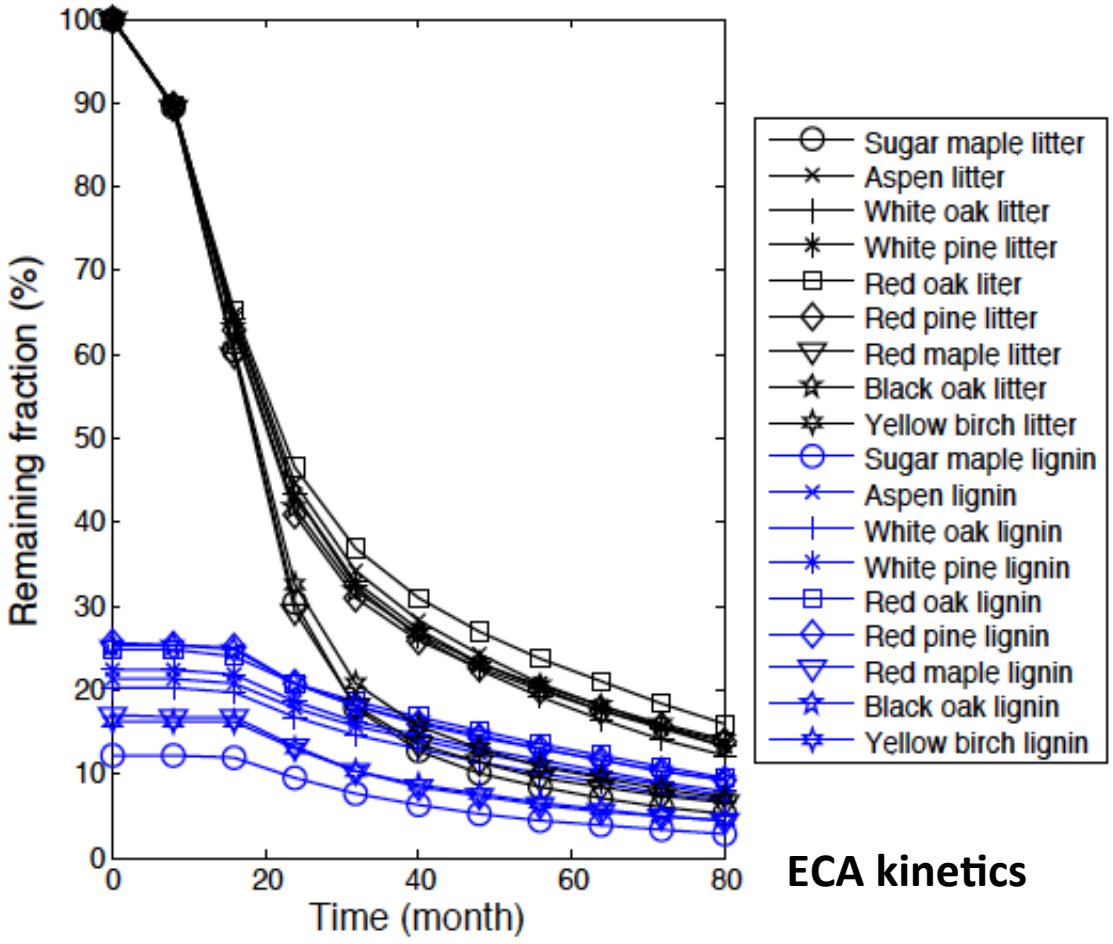
Bottom boundary condition: qcharge

Top boundary condition: net infiltration

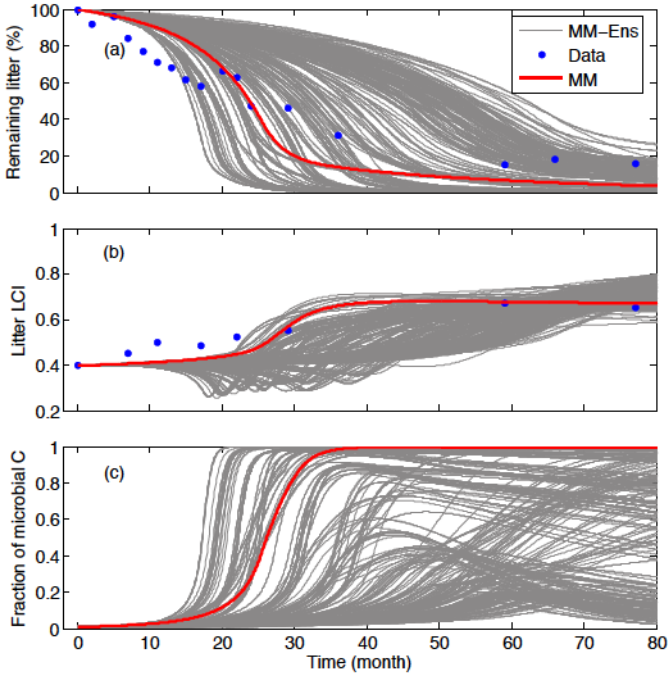
kinetics module to handle competitions

```
interface mmcomplex   !the m-m kinetics
   module procedure mmcomplex_v1s,mmcomplex_v1e, mmcomplex_m
end interface mmcomplex

interface ecacomplex  !the eca kinetics
   module procedure ecacomplex_v1s,ecacomplex_v1e, ecacomplex_m
end interface ecacomplex
```

Kinetics are important



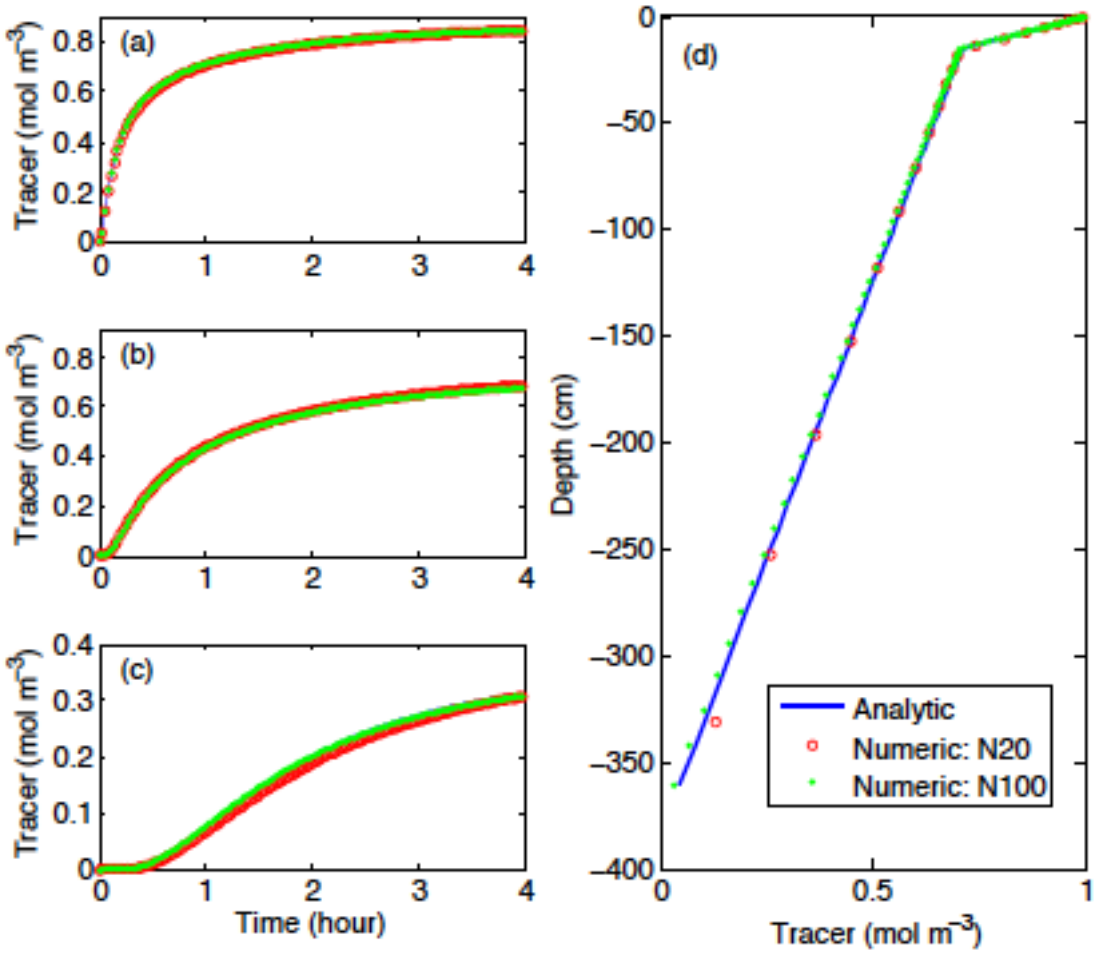
ECA kinetics

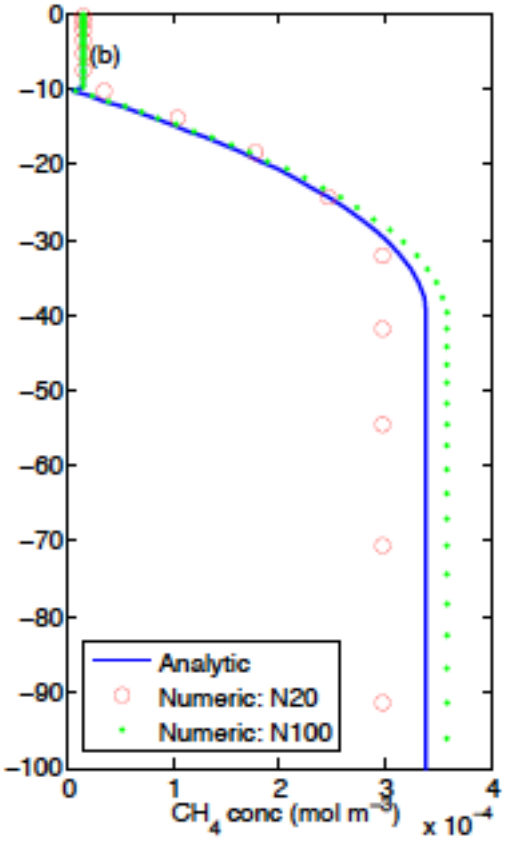


M-M kinetics doomed

Tang and Riley, Biogeosciences, 2013

Unit testing example: diffusion algorithm





Tang and Riley, Biogeosciences, 2014

The OOP based flexible BGC

$$\frac{\partial}{\partial t}\left(C_v\theta_v + C_l\theta_l + C_i\theta_i\right) = \frac{\partial}{\partial z}\left[\theta_l D_l \frac{\partial C_l}{\partial z} + \theta_v D_v \frac{\partial C_v}{\partial z}\right]$$

$$-\frac{\partial}{\partial z}\left(q_l C_l\right) + S$$

$v : vapor$

$l : liquid$

$i : ice$

$S : \sin k / source$ through runoff, transpiration, drainage

Bottom boundary condition: qcharge

Top boundary condition: net infiltration

- Polymorphism based implementation
  - diagnostic BGC
  - water isotope
  - Reaction-based bgc
  - Mock example

The polymorphism implementation for flexible subsurface BGC

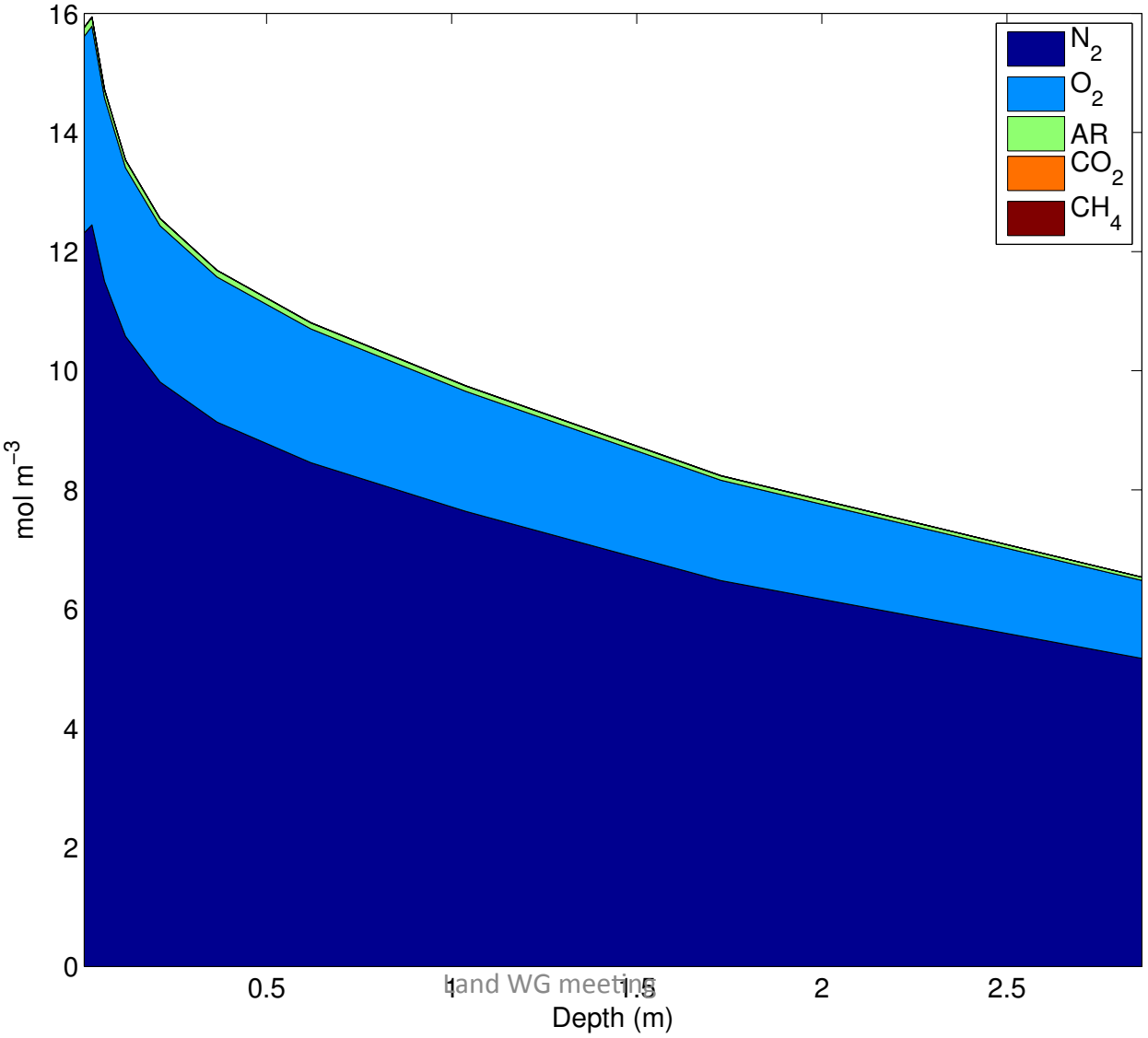
```
module BGCReactionsMod
!
! module doing bgc reaction
! created by Jinyun Tang
! This is dirty version just to make sure the model is running
! Eventually, I want to introduce polymorphism to make it
! consistent with other developments in soil hydrology and the clm4.5/clm5 bgc

implicit none
  save
  private
  public ::  bgc_reaction_type

  type, abstract :: bgc_reaction_type
      private
    contains
      !initialize betr bgc
      procedure(Init_betrbgc_interface)                , deferred :: Init_betrbgc
      !doing bgc reaction
      procedure(calc_bgc_reaction_interface)           , deferred :: calc_bgc_reaction

      !set boundary condition for related tracer transport
      procedure(set_boundary_conditions_interface)     , deferred :: set_boundary_conditions

      procedure(init_boundary_condition_type_interface) , deferred :: init_boundary_condition_type

      !do equilibrium tracer chemistry
      procedure(do_tracer_equilibration_interface )    , deferred :: do_tracer_equilibration

      !do cold initialization of different tracers
      procedure(initCold_interface)                    , deferred :: initCold
  end type bgc_reaction_type

  abstract interface
```

Mock example

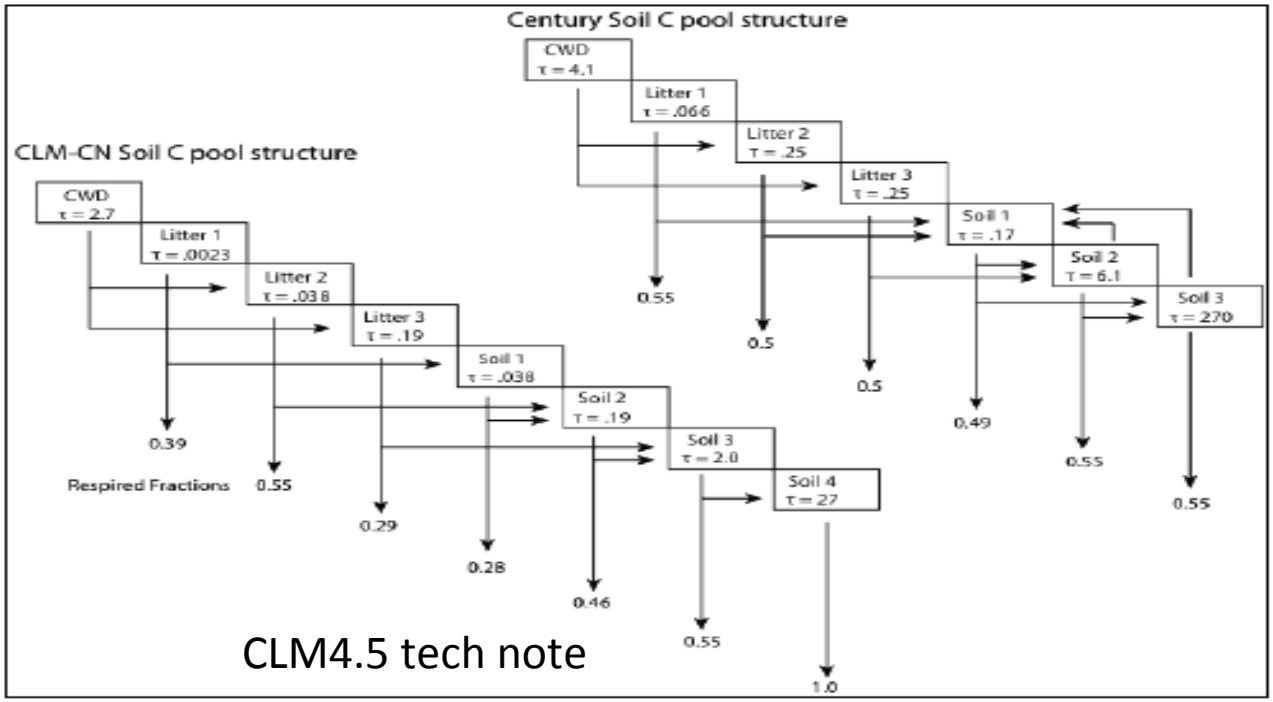
```
! !PUBLIC TYPES:
public :: bgc_reaction_mock_run_type

type, extends(bgc_reaction_type) :: &
   bgc_reaction_mock_run_type
   private
 contains
   procedure :: Init_betrbgc                    ! initialize betr bgc
   procedure :: set_boundary_conditions         ! set top/bottom boundary conditions for various tracers
   procedure :: calc_bgc_reaction               ! doing bgc calculation
   procedure :: init_boundary_condition_type    ! initialize type of top boundary conditions
   procedure :: do_tracer_equilibration         ! do equilibrium tracer chemistry
   procedure :: InitCold                        ! do cold initialization
 end type bgc_reaction_mock_run_type

 interface bgc_reaction_mock_run_type
   module procedure constructor

 end interface bgc_reaction_mock_run_type
```

```
betrtracer_vars%tracernames(betrtracer_vars%id_trc_n2)='N2'
betrtracer_vars%tracernames(betrtracer_vars%id_trc_o2)='O2'
betrtracer_vars%tracernames(betrtracer_vars%id_trc_ar)='AR'
betrtracer_vars%tracernames(betrtracer_vars%id_trc_co2x)='CO2x'
betrtracer_vars%tracernames(betrtracer_vars%id_trc_ch4)='CH4'

betrtracer_vars%is_volatile(betrtracer_vars%id_trc_n2)=.true.
betrtracer_vars%is_volatile(betrtracer_vars%id_trc_o2)=.true.
betrtracer_vars%is_volatile(betrtracer_vars%id_trc_ar)=.true.
betrtracer_vars%is_volatile(betrtracer_vars%id_trc_co2x)=.true.
betrtracer_vars%is_volatile(betrtracer_vars%id_trc_ch4)=.true.
```

Example tracer profiles



Reaction-based subsurface BGC (in ACME)



$1\ \text{lit1} + \gamma O_2 \rightarrow \gamma CO_2 + (1-\gamma)SOM_1 + f_{CN}\ NH_4 + f_{CP}\ P(\text{mineral})$

$X=[\text{lit1}, O_2, CO_2, SOM_1, NH_4, P]^T$

$dX/dt= [-1,-\gamma, \gamma, 1-\gamma, f_{CN}, f_{CP}]^T R$

Reaction based BGC

$$lit1 + a_1 O_2 + a_2 NH_4 + a_3 NO_3 \rightarrow a_1 CO_2 + (1 - a_1) SOM1$$

$$lit2 + \ldots$$

$$lit3 + \ldots$$

...

$$NH_4^+ + (2 - f) O_2 + (2 - f) OH^- \rightarrow (1 - f) NO_3^- + \frac{f}{2} N_2 O + \left(3 - \frac{f}{2}\right) H_2 O$$

$$\frac{dx}{dt} = [C] r$$

x : state variable,

r: kinetics based reaction rates

- **Stoichiometric based mass balance**
- **Consistent treatment of substrate competition**
- **Easy extension to new processes**

Reaction based BGC

$$lit1 + a_1 O_2 + a_2 NH_4 + a_3 NO_3 \rightarrow a_1 CO_2 + (1 - a_1) SOM1$$

$$lit2 + \ldots$$

$$lit3 + \ldots$$

...

$$NH_4^+ + (2 - f) O_2 + (2 - f) OH^- \rightarrow (1 - f) NO_3^- + \frac{f}{2} N_2O + \left(3 - \frac{f}{2}\right) H_2O$$

$$\frac{dx}{dt} = [C] r$$

x : state variable,

r: kinetics based reaction rates

```
subroutine one_box_century_bgc(ystate, dtime, time, nprimvars, nstvars, dydt)
```

Using standard solvers

```
call ode_adapt_mbbks1(one_box_century_bgc, y0(:,c,j), centurybgc_vars%nprimvars,centurybgc_vars%nstvars, time, dtime, yf(:,c,j))
```

Summary

CLM-BeTR provides opportunities to do more advanced BGC modeling

Acknowledgement

- Funding support from DOE sponsored projects: NGEE-Arctic, BGC-Feedback and ACME.