Isotopes and Reactive Transport in CLM4: CLMiso

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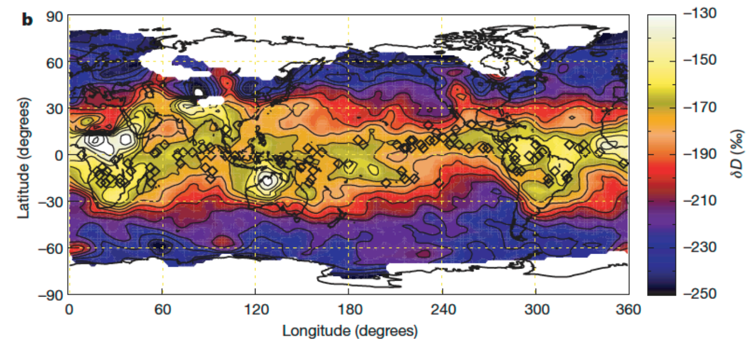
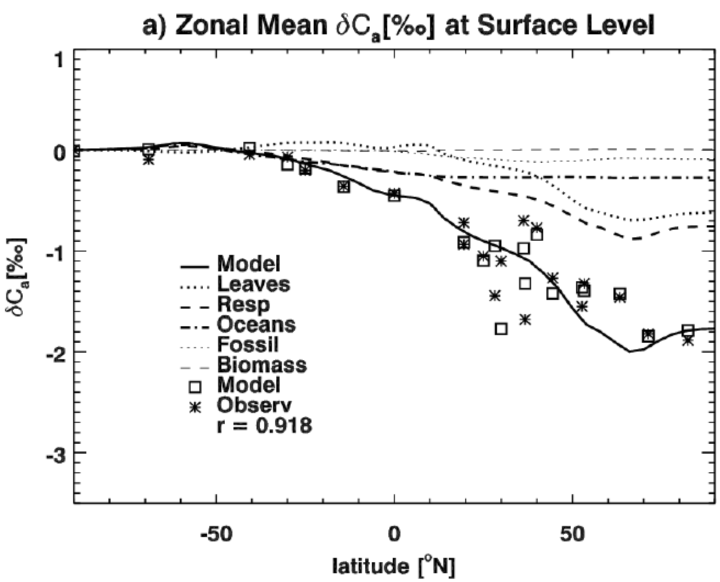
Motivation

- Isotopes as tracers of processes
  - Water flows
  - Precipitation recycling
  - Cloud water processes
  - Water and C cycle interactions
  - Etc.

Worden et al 2004 – observations from the TES/Aura



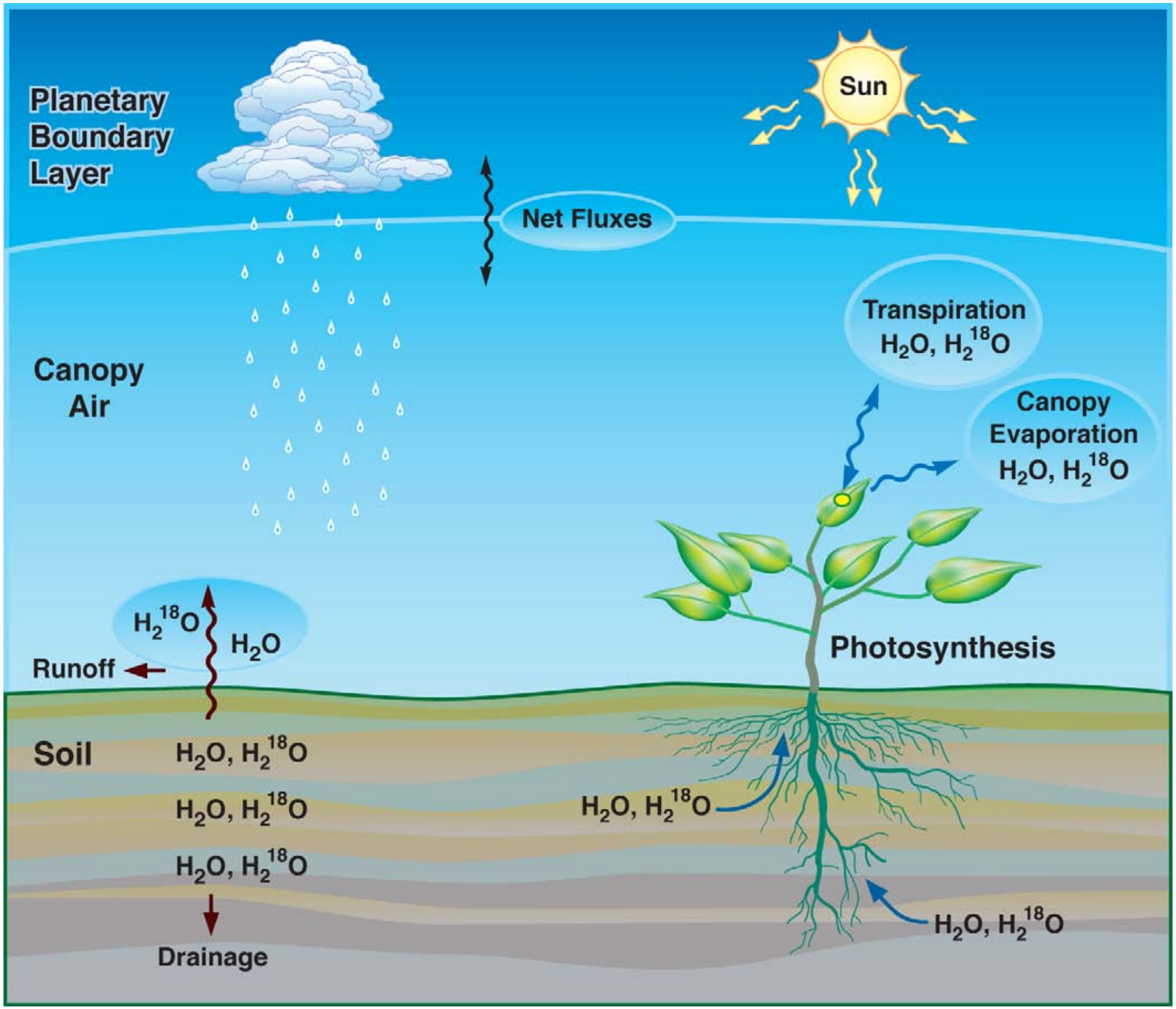


Buenning et al (submitted) - Using a coupled version of ISOLSM/CAM

Processes Important in HDO and $H_2^{18}O$ Fluxes

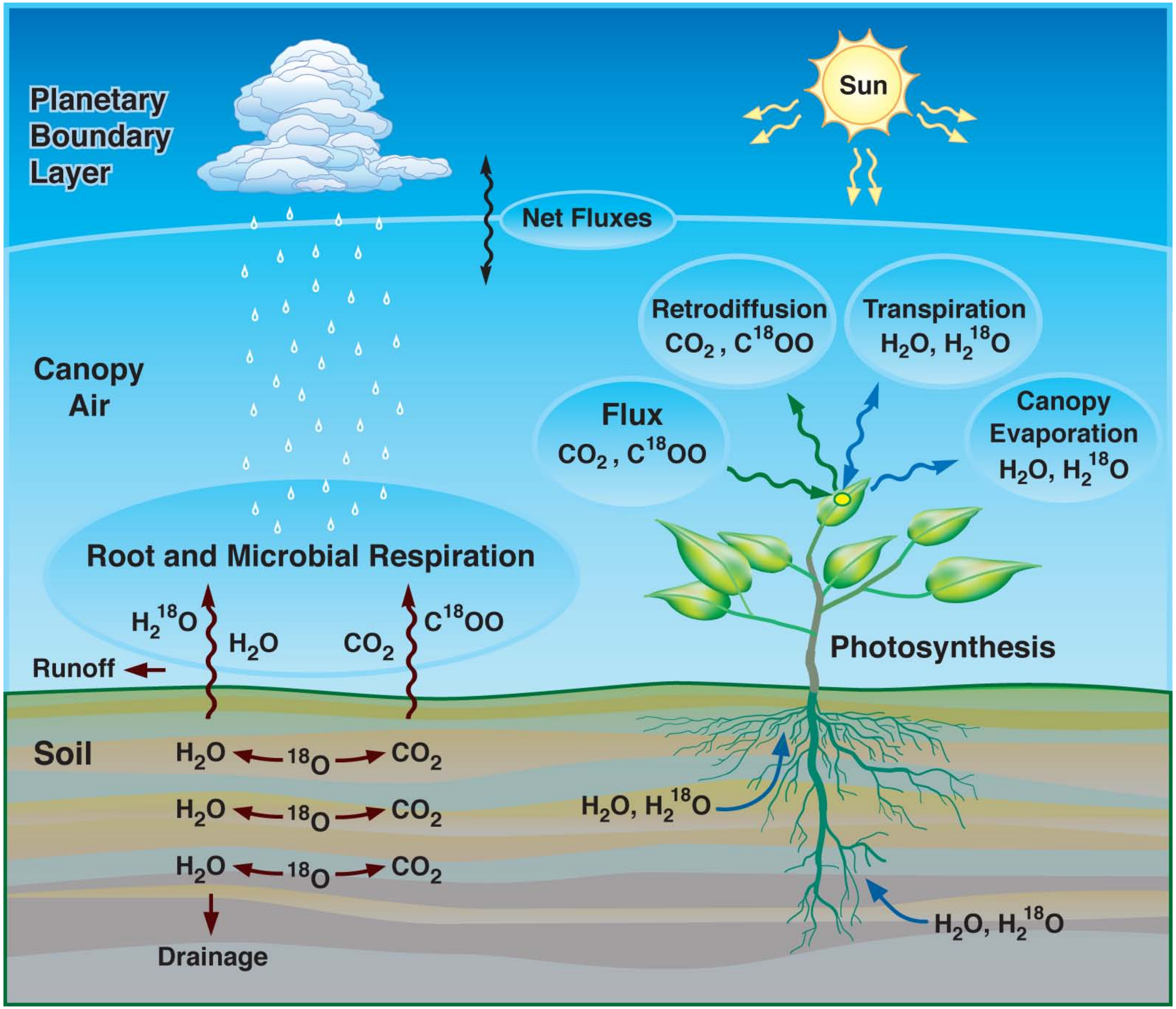
Additionally

- **Snow**
- **Dew**
- **Rivers**
- **Glaciers**
- **Urban**



Riley et al. 2002, 2003

Processes Important in $C^{18}OO$ Fluxes



Goals: CLMiso Processes

- ^{18}O and D in H_2O
  - Soil
    - Advection, diffusion, equilibrium partitioning, root uptake, interface with canopy air
  - Xylem, Leaves
- ^{18}O in CO_2
  - Equilibrium with leaf and soil water pools
- Fractionations
- Soil reactive transport multi-phase solver
  - Generic formulation

History

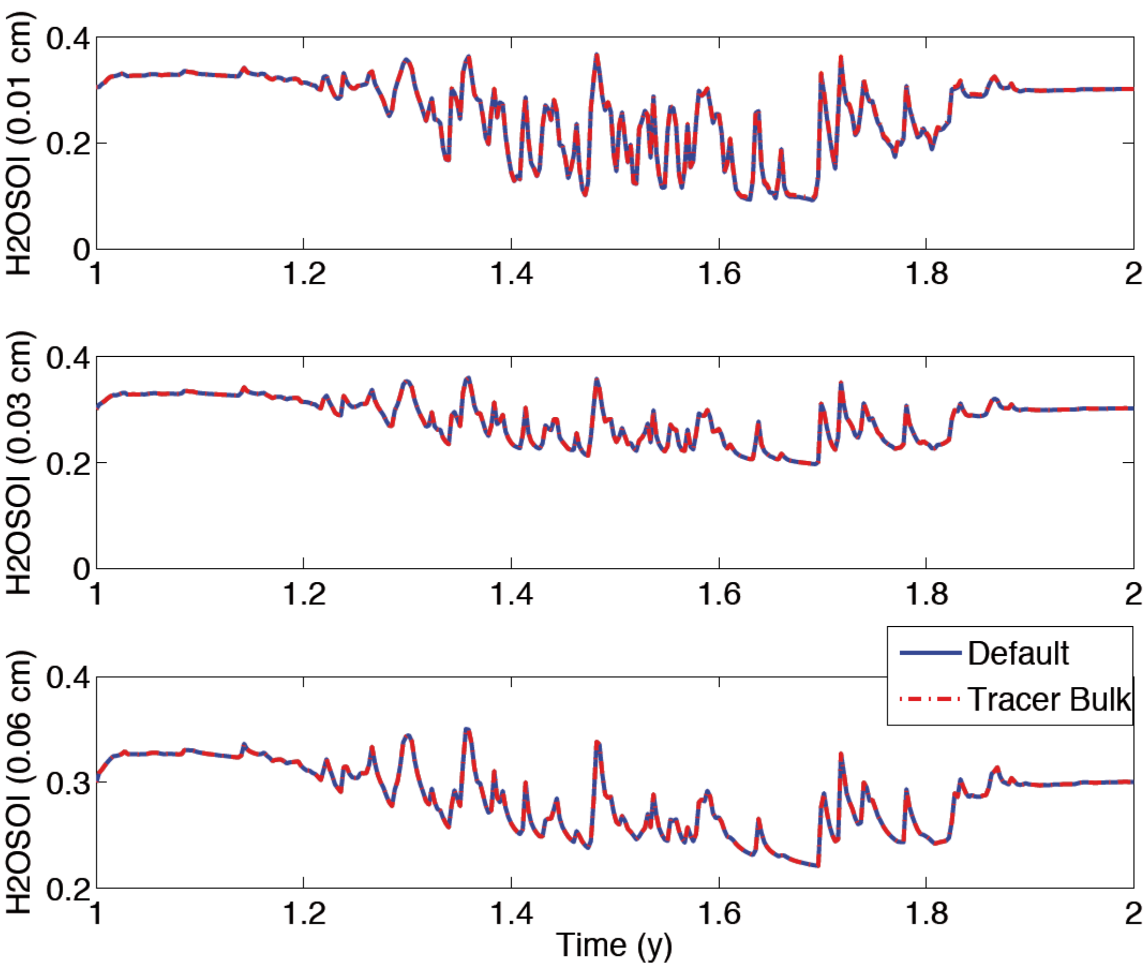
- ISOLSM (Riley et al. 2002, 2003)
  - Applied for $H_2{}^{18}O$, $C^{18}OO$, and $^{13}CO_2$ analyses
  - Site, regional, and global applications
- Coupled with CAM by David Noone
  - Buenning et al (2011)
  - Also began integration of the ISOLSM code into CLM3
- We took isotope code from CLM3 and are integrating it into CLM4
  - Some modifications and additions

Approach

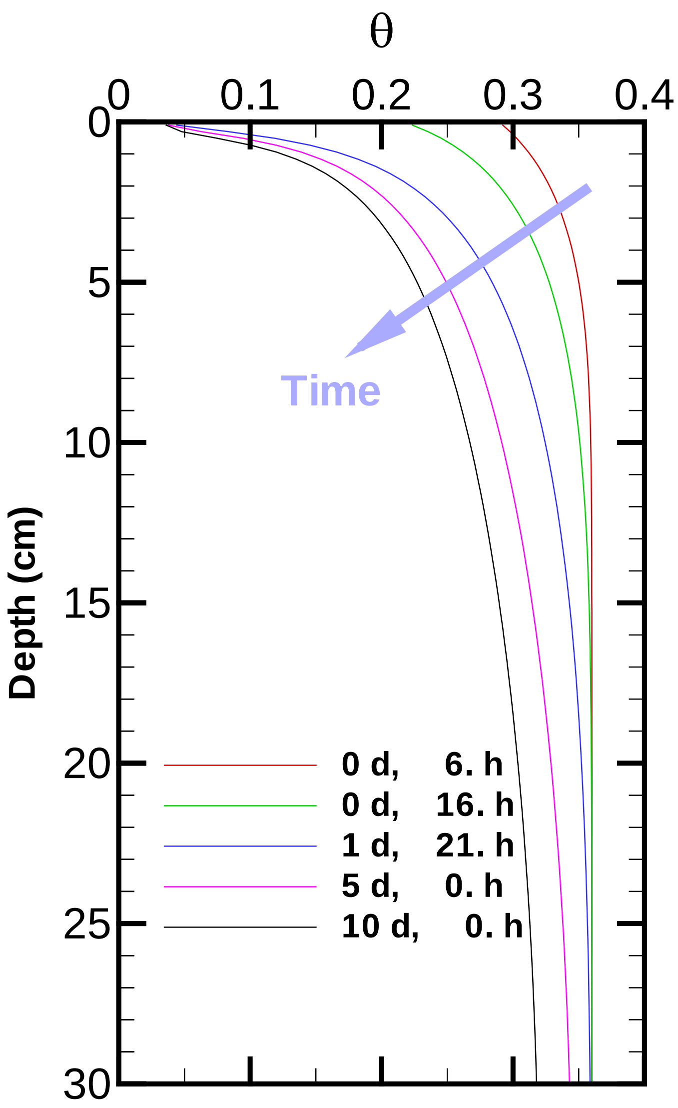
- Duplicate every water exchange in CLM4 with an tracer variable of dimension **n**
  - e.g., wtr_h2osoi_liq(c,j,**n**)
  - ~30 fluxes and stocks scattered through CLM
  - Add fractionations where applicable
- Method will facilitate change to a generic n-tracer water cycle in CLM
- Currently have only advection for water tracers, but
  - Have integrated a reactive transport model into CLM
    - Many potential applications (e.g., C & N transport and transformations)
  - Have developed a finely resolved testbed model tested against analytical solutions and observations

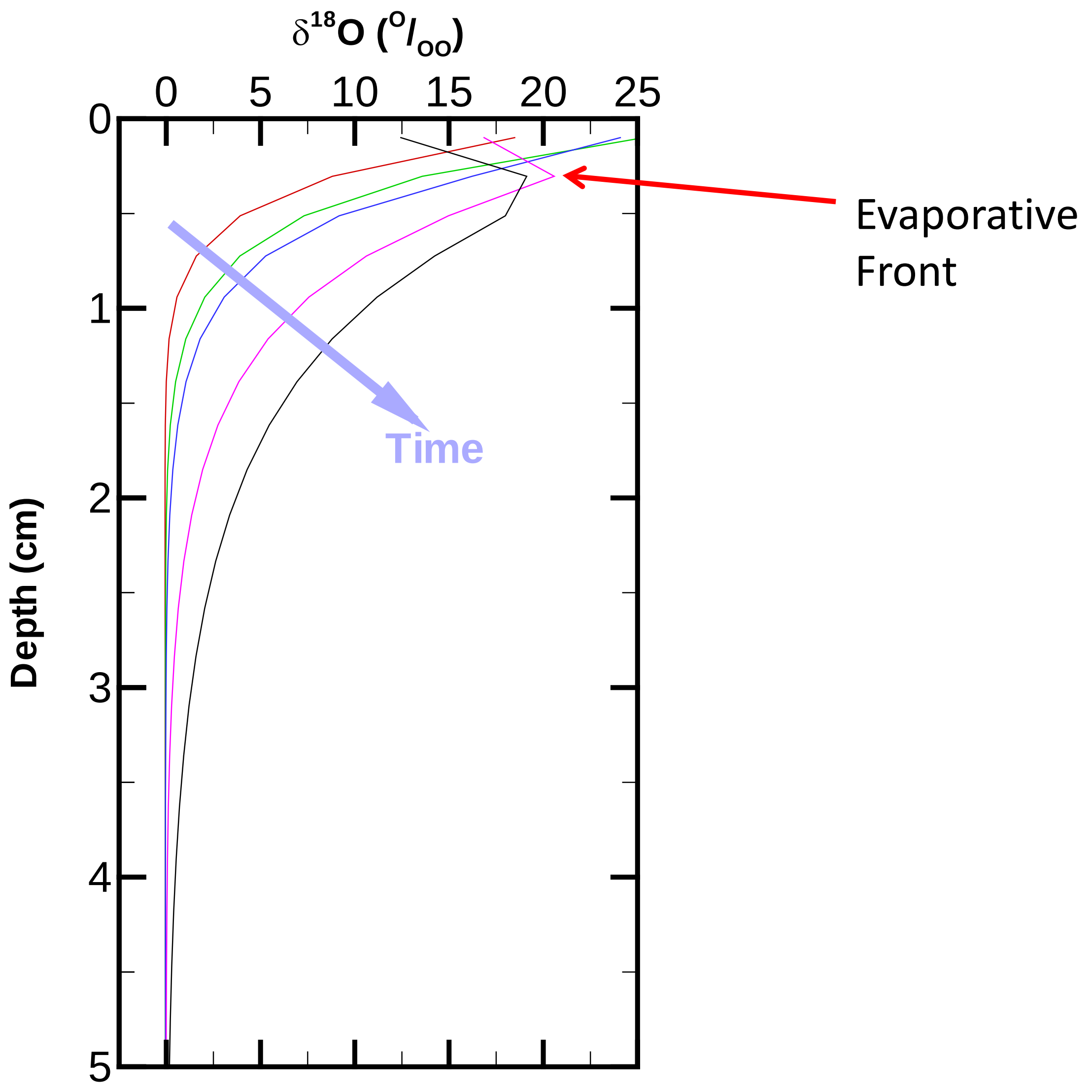
Progress on CLMiso

- Bulk water appears to be working, except for some cases with dew and snow



Example: 10-Day Soil Drying





Multi-Phase Reactive Transport Solver in CLM4

- Applications: C&N cycling, isotopes, contaminants
- Mass Balance Equation:

$$\frac{\partial(\varepsilon_t C_w)}{\partial t} + \frac{\partial(J)}{\partial t} = S$$

Multi-Phase Reactive Transport Solver in CLM4

- Mass Balance Equation

Aqueous Concentration

$$\frac{\partial(\varepsilon_t C_w)}{\partial t} + \frac{\partial(J)}{\partial t} = S$$

Multi-Phase Reactive Transport Solver in CLM4

- Mass Balance Equation

$$\frac{\partial(\varepsilon_t C_w)}{\partial t} + \frac{\partial(J)}{\partial t} = S$$

Source

Multi-Phase Reactive Transport Solver in CLM4

- Mass Balance Equation

aqueous, gaseous, sorbed

Phase partitioning: $\varepsilon_t = \varepsilon_w + \frac{\varepsilon_a}{K_H} + \rho_b K_d$

$$\frac{\partial(\varepsilon_t C_w)}{\partial t} + \frac{\partial(J)}{\partial t} = S$$

Multi-Phase Reactive Transport Solver in CLM4

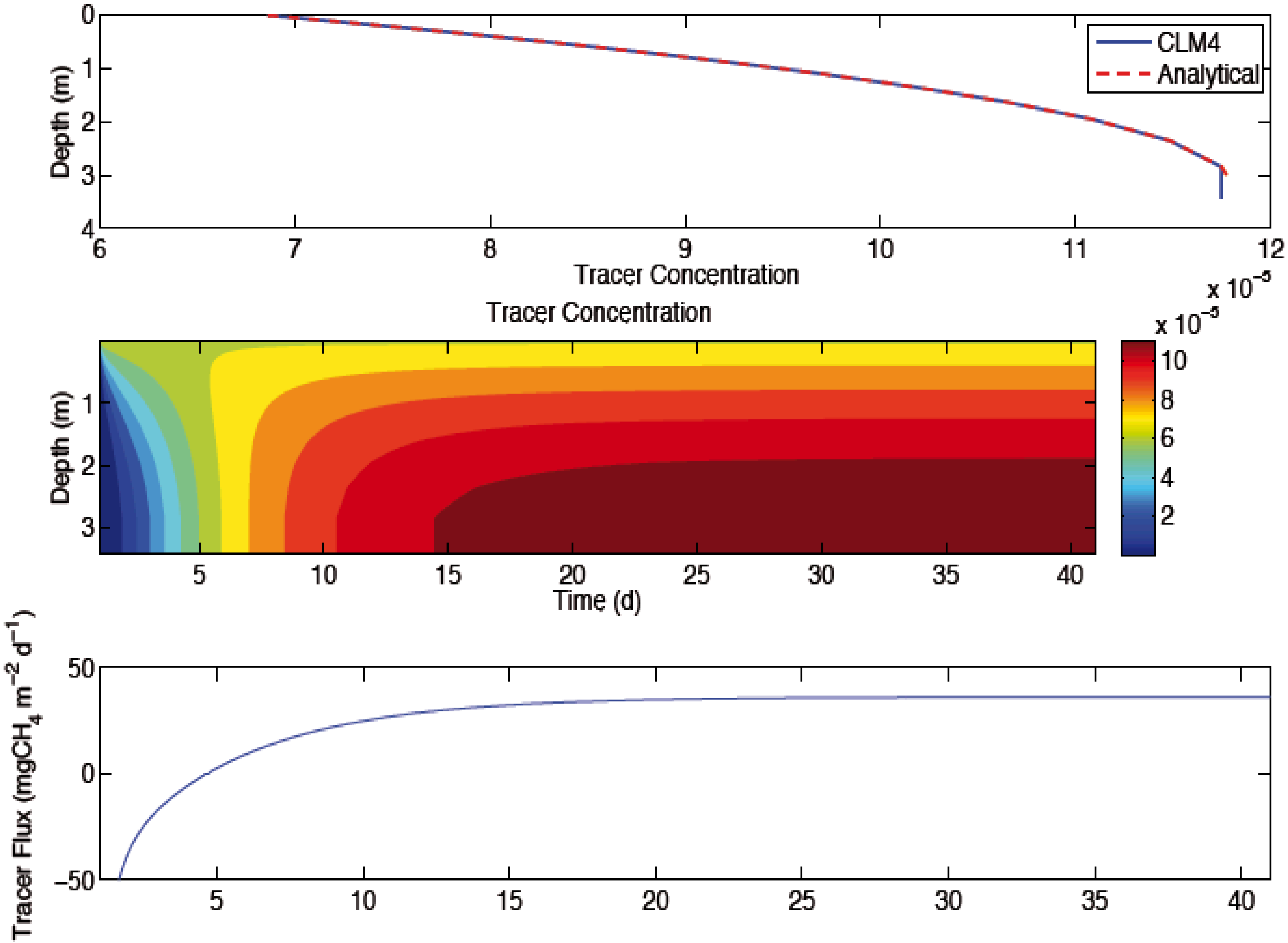
- Mass Balance Equation

$$\frac{\partial(\varepsilon_t C_w)}{\partial t} + \frac{\partial(J)}{\partial t} = S$$

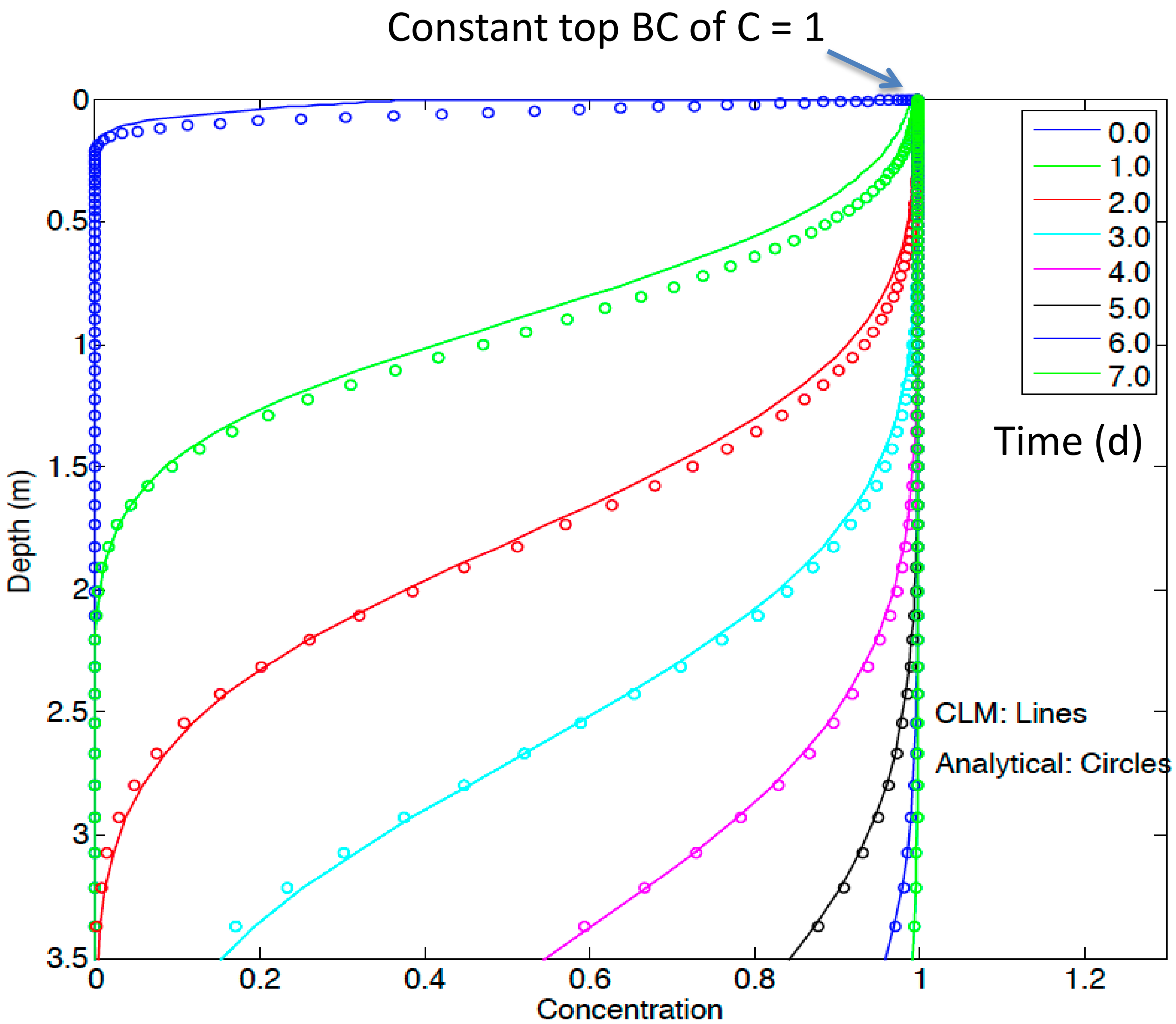
Sum of aqueous and gaseous fluxes:

$$J = u_w C_w - D_w \frac{\partial C_w}{\partial z} + u_g C_g - D_g \frac{\partial C_g}{\partial z}$$

Steady-State, Constant-Source Comparison with Analytical Solutions



Transient Diffusion & Advection Comparison to Analytical Solution



Remaining Issues:

- **Spatial resolution**
- **Temporal resolution**
- **Testing needed for multi-phase solutions**

Next Steps

- Remaining fixes to code for isotopes
  - Dew, snow, ice
  - Urban, glaciers
- Integrate water isotopes with full transport solver including diffusion
- Integrate CO_2 transport and equilibration with $H_2{}^{18}O$
- Integrate with atmosphere and ocean components
- Do some isotope science in CESM!

Extras

Multi-Phase HDO and $H_2^{18}O$ Model

Bulk Water :

$$\frac{\partial\left\{\rho\theta + h\rho^{s}(p-\theta)\right\}}{\partial t} + \frac{\partial f^{lm}}{\partial z} + \frac{\partial f^{\lg}}{\partial z} + \frac{\partial f^{v\theta}}{\partial z} + \frac{\partial f^{vT}}{\partial z} = 0$$

Isotopes :

$$\frac{\partial\left\{\rho\theta R^{L} + h\rho^{s}(p-\theta)R^{v}\right\}}{\partial t} + \frac{\partial f_{*}^{lm}}{\partial z} + \frac{\partial f_{*}^{\lg}}{\partial z} + \frac{\partial f_{*}^{ld}}{\partial z} + \frac{\partial f_{*}^{vT}}{\partial z} + \frac{\partial f_{*}^{vd}}{\partial z} = 0$$

- Built a ‘model testbed’
  - Based on Barnes and Allison, Barnes et al. (1980’s) and Mathieu and Bariac (1996)