Isotopes and Reactive Transport in CLM4: CLMiso

W. J. Riley
(Lawrence Berkeley National Laboratory)

D.C. Noone
(C.U. Boulder)
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

- Snow
- Dew
- Rivers
- Glaciers
- Urban

Riley et al. 2002, 2003
Processes Important in $\text{C}^{18}\text{OO}$ Fluxes
Goals: CLMiso Processes

• $^{18}$O and D in H$_2$O
  – 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 $\text{H}_2^{18}\text{O}$, $\text{C}^{18}\text{OO}$, and $\text{C}^{13}\text{O}_2$ 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

Evaporative Front
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

\[ \partial \left( \varepsilon t C_w \right) \frac{\partial}{\partial t} + \partial (J) \frac{\partial}{\partial t} = S \]

Aqueous Concentration
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

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

Constant top BC of \( C = 1 \)

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$_2$O$_{18}$

• 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)