PFLOTRAN Isotope Partitioning for Kinetic and Equilibrium Processes in *GDSA Framework*

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Problem

- Certain kinetic reactions (e.g., kinetic colloid partitioning) are not yet possible for isotopes in *GDSA Framework* [1].
  - Multiple isotopes for single element presents challenge.
  - Kinetic process model should couple with equilibrium partitioning model of *GDSA Framework*.
- ***How will* GDSA Framework *include kinetic partitioning reactions for isotopes?***
  - Likely by operator splitting

Conceptual Model

- Kinetic processes simulated first at each time step
  - Decay releases daughters to aqueous phase
- Equilibrium partitioning simulated at the end of each time step using the **Isotope Partitioning Model (IPM)** of *GDSA Framework*

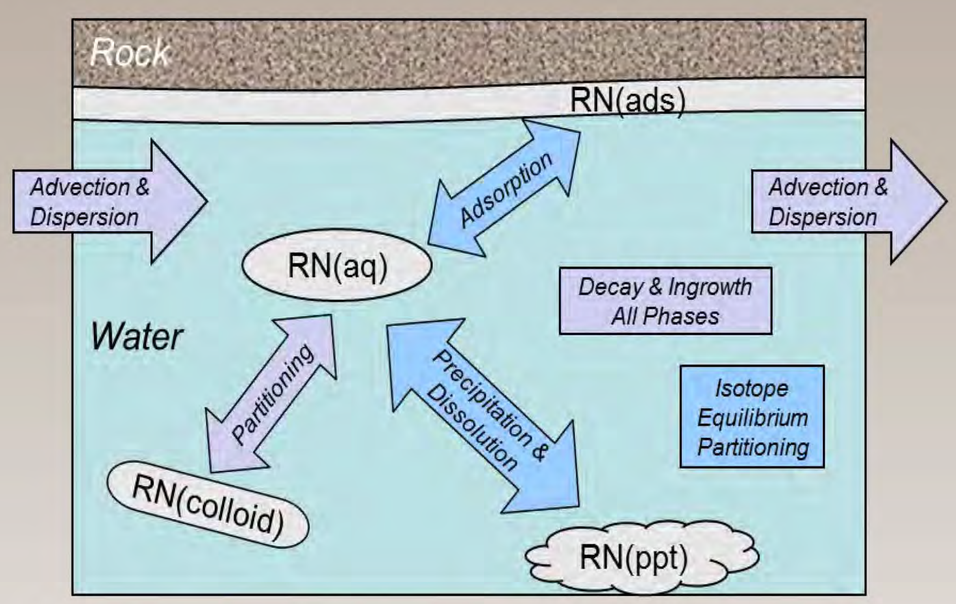

Figure 1. Conceptual model of radionuclide (RN) equilibrium partitioning processes (blue) and kinetic processes (lavender).

Algorithm

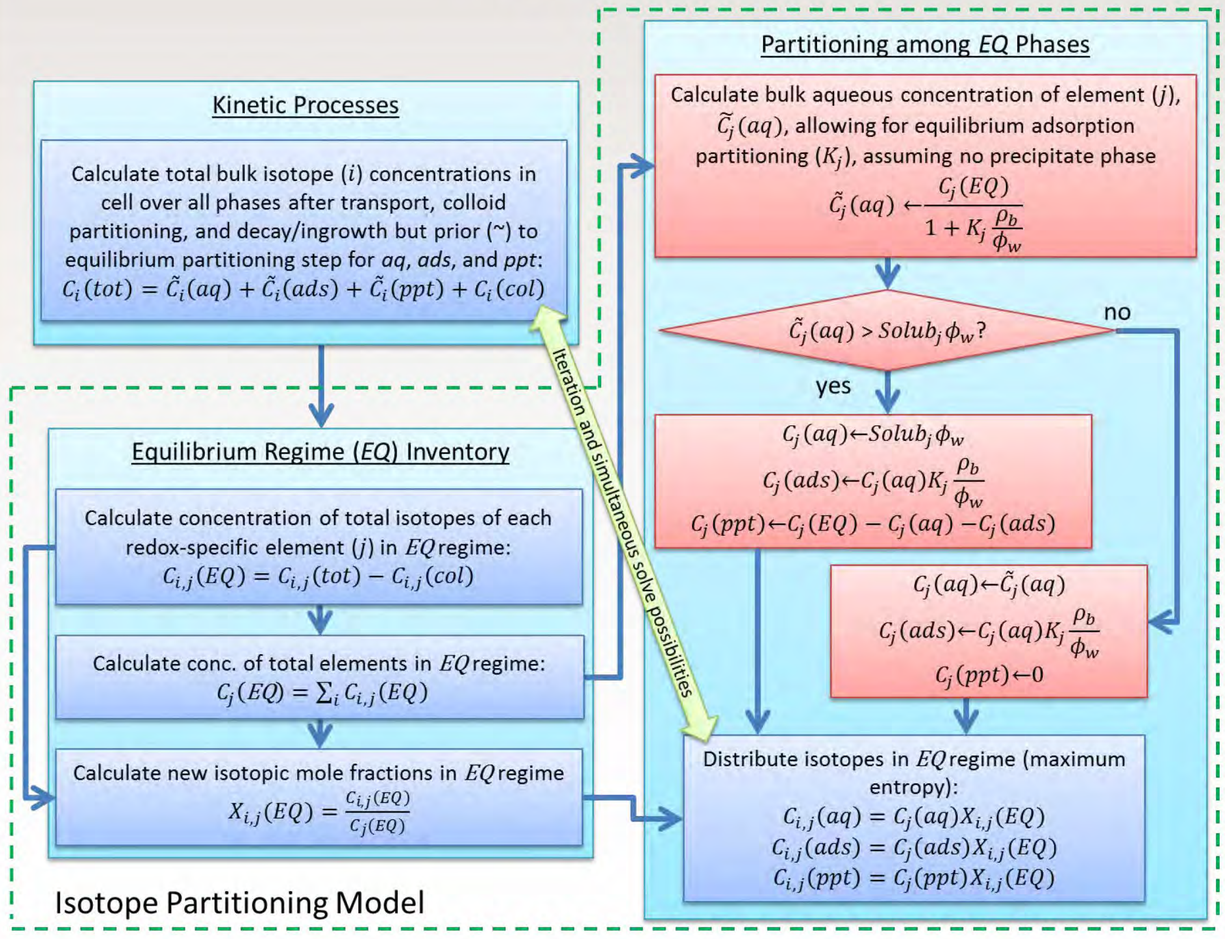

Figure 2. Proposed coupling of IPM and kinetic colloid partitioning model.

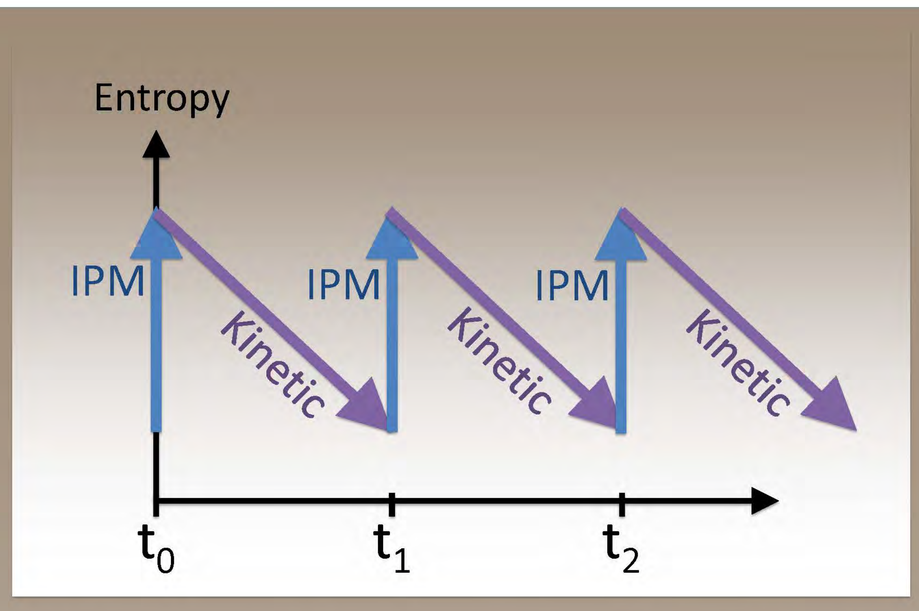

Figure 3. Operator splitting of equilibrium (IPM) and kinetic processes.

Test

- Batch reactor with initial concentrations of ^{237}Np, ^{233}U, ^{229}Th, and ^{230}Th equilibrated among aqueous (aq), adsorbed (ads), and precipitated (ppt) phases.
- Isotopes decay (^{233}U and ^{229}Th will also ingrow):

$^{237}Np \rightarrow {}^{233}U \rightarrow {}^{229}Th \rightarrow$ and $^{230}Th \rightarrow$

- Add a colloidal (col) phase with ^{229}Th and ^{230}Th *irreversibly* adsorbed at initial bulk concentrations of 10^{-10} mol L^{-1}.
- Simulate over time, allowing decay and ingrowth to change the total isotope concentrations and equilibrium partitioning.

Results

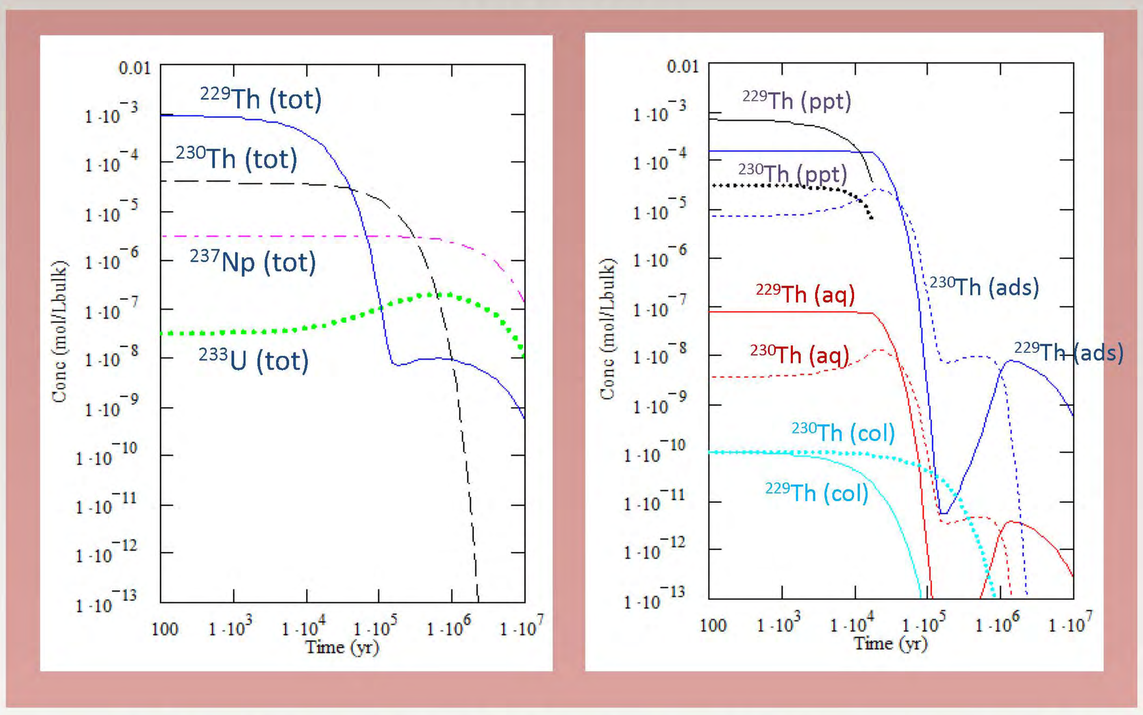

Figure 4. Simulation results showing effects of decay, ingrowth, and equilibrium isotope partitioning between aq., ads., and ppt. phases.

Conclusions

- Constitutive relationships are maintained.
- Proposed algorithm for integrating kinetic partitioning reactions with the Isotope Partitioning Model (IPM) of *GDSA Framework* [1] is ready for implementation.

Reference

1. SNL (2017). *GDSA Framework*: A Geologic Disposal Safety Assessment Modeling Capability. Open Source. Available from: pa.sandia.gov.

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