# RT-Flux-PIHM: A Coupled Hydrological, Land Surface, and Reactive Transport Model for Hydrogeochemical Processes at the Watershed Scale

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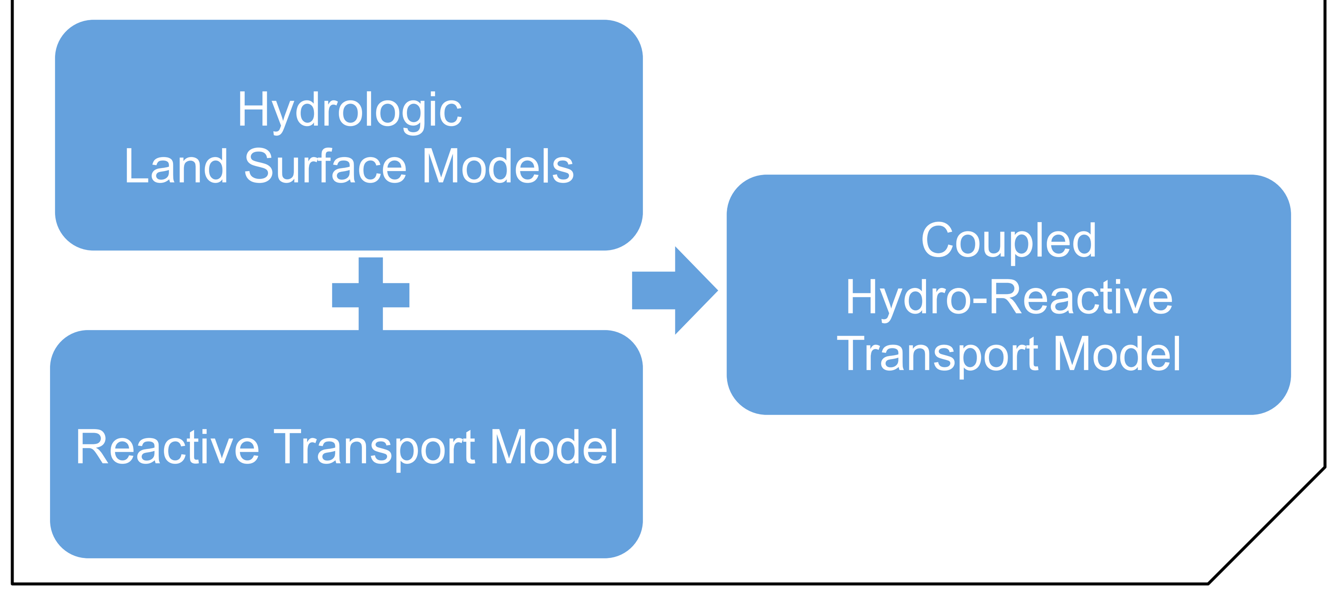
## Motivation

- ❑ Despite recent advances, interpreting complex hydro-geochemical interactions remains challenging.
- ❑ How to explain the concentration-discharge (C-Q) relationship found in many natural watersheds, especially those solutes that demonstrates "chemostatic" behaviors?
- ❑ How does the coupling of meteorological, hydrological, and (bio)geochemical processes affect clay dissolution at watershed scale?
- ❑ A numerical simulator is developed to answer these questions.




## RT-Flux-PIHM

❑ RT-Flux-PIHM couples Flux - Penn State Integrated Hydrologic Model (Flux-PIHM) (Kumar et al., 2008, Shi et al., 2013), a distributed hydrologic land surface model with a reactive transport component.

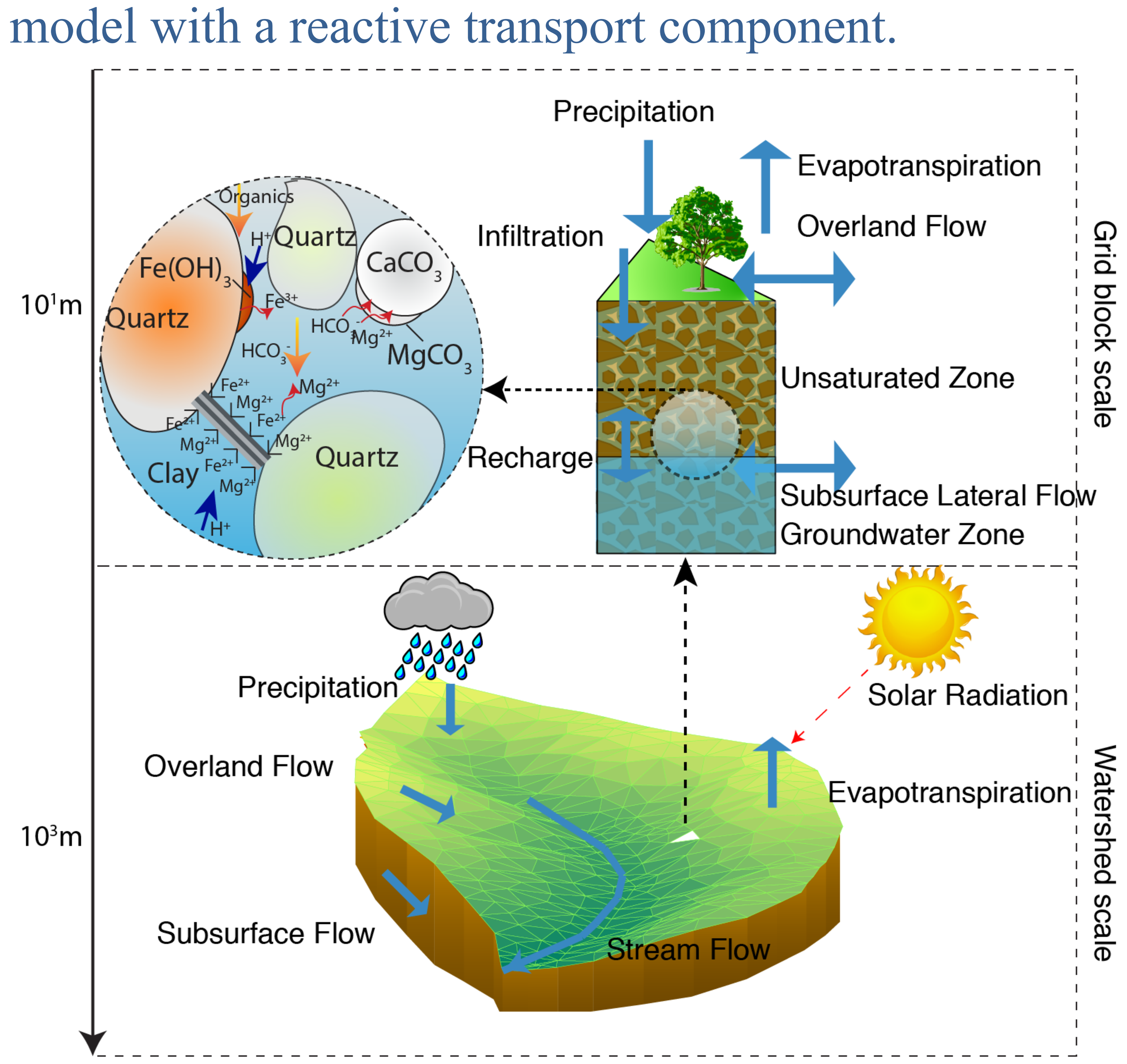



Figure1. RT-Flux-PIHM uses an unstructured mesh where hydro-geochemical processes are simulated within each grid.

## Results

*Coupling strategy*: In RT-Flux-PIHM, land surface and the hydrological processes are tightly coupled with feedbacks between processes. Based on the water distribution and flow rates predicted by Flux-PIHM, the RT module solves the ADR equation for the spatial and temporal evolution of aqueous and solid phase composition.

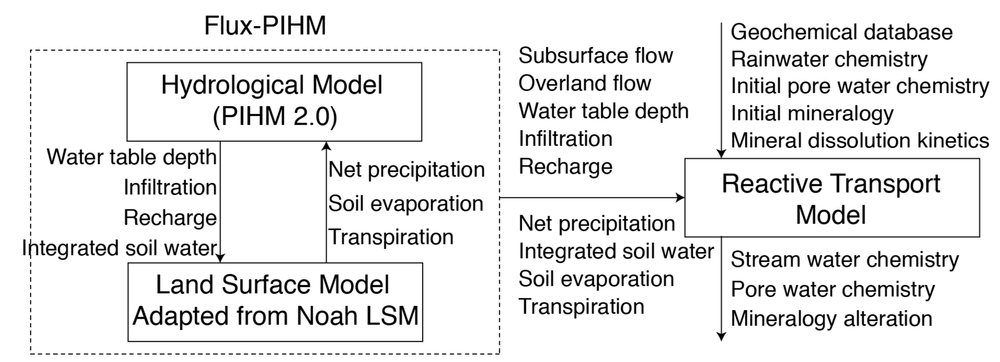



Figure 2: Data exchange between RT-Flux-PIHM components and input/output of RT

*Model verification*: The reactive transport component is benchmarked against the widely used reactive transport code CRUNCHFLOW (CF, Steefel, 2007) under a variety of flow and reaction conditions. Below we show the simulation results for a 1D column injection experiments from RT and CF.


| | | | | |
|---|---|---|---|---|
| Darcian flux | m/day | 2.00 | Number of cells | 100 |
| porosity | | 0.4000 | Primary species | 6 |
| Diffusion coefficient | $cm^2/s$ | $1.0\times10^{-5}$ | Mineral | 1 |
| Dispersivity | m | 0.1 | Secondary species | 3 |
| Cementation exponent | | 1 | Ion exchange | 0 |
| Total column length | m | 10.00 | Kinetic Reactions | 1 |
| Grid size | m | 0.10 | TVD | On |

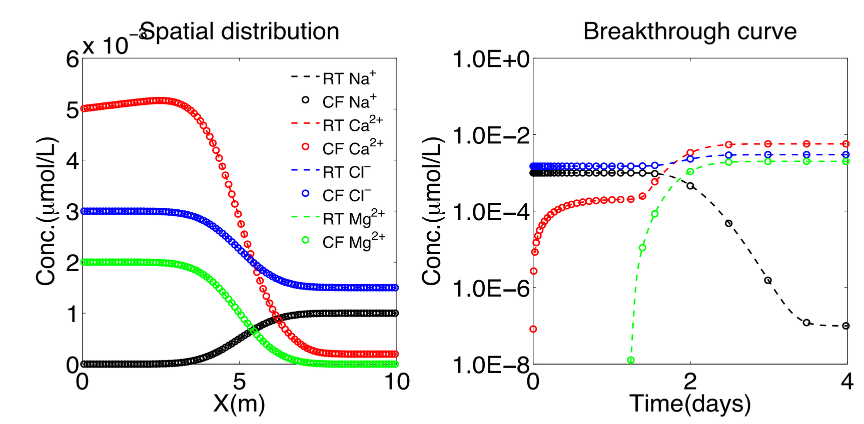



Figure 3: Identical simulation results from RT and CF

*Model validation:* RT-Flux-PIHM was implemented at the Shale Hill Critical Zone Observatory (SSHCZO, 0.08 km$^2$). The simulated field is discretized into 535 grids and 20 river segments. The non-reactive transport of chloride and reactive transport of magnsium, which is derived from clay dissolution, were simulated.

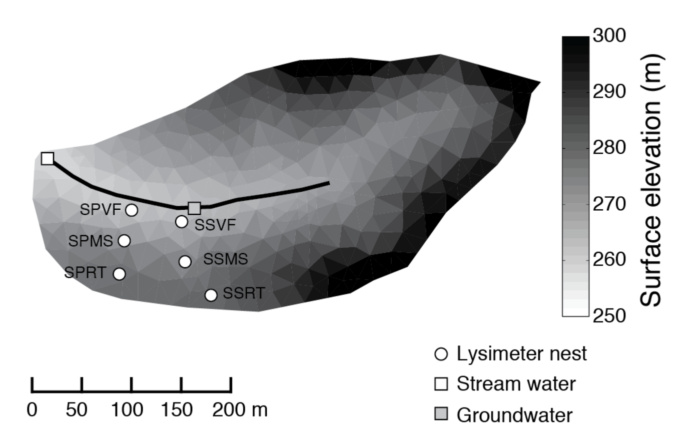
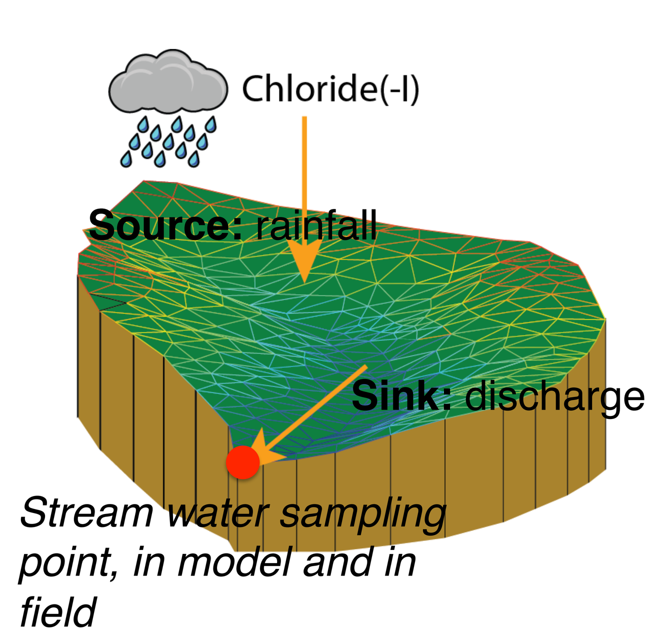
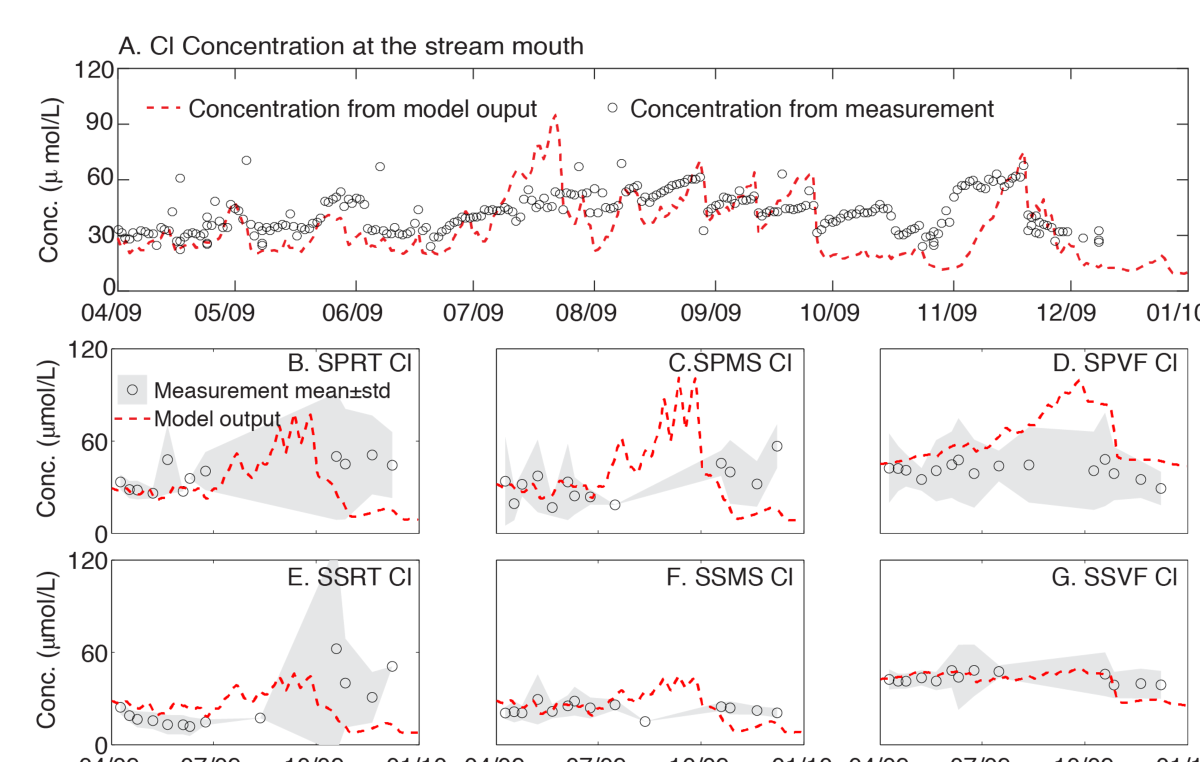



Figure 4: Topography of SSHCZO and monitor sites

*Chloride simulation:*



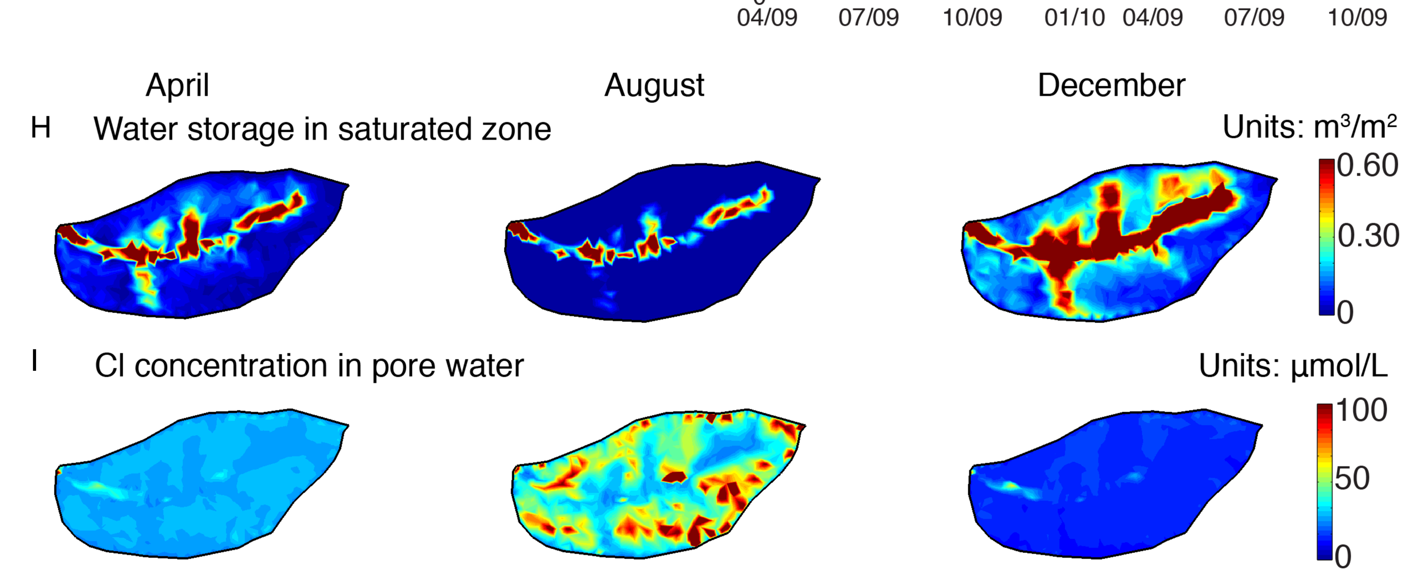
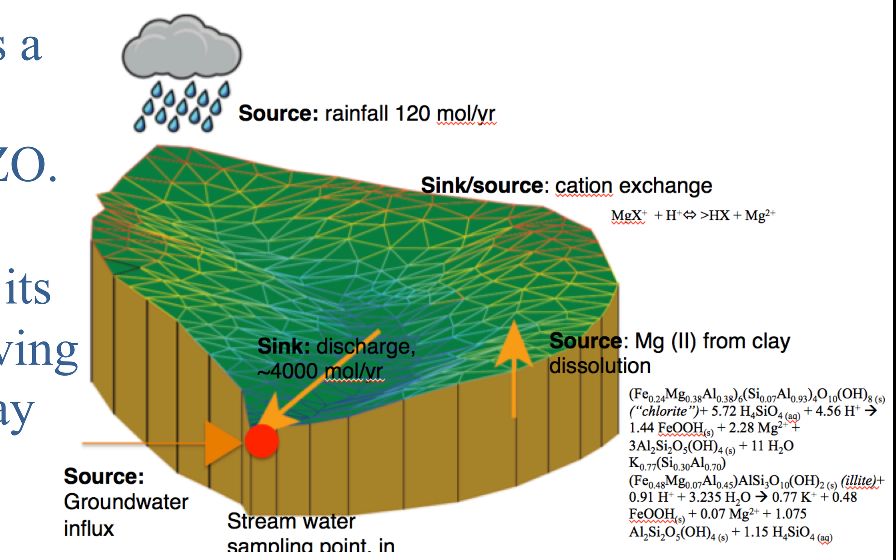




Figure 5: A~G, Cl conc. In stream water and six lysimeter sites from simulation and measurements agreed well. H~I, Spatial distribution of Cl. conc. showed opposite pattern as water storage in summer.

## Results and discussion

*Magnesium simulation:* Mg is a key indicator of the clay weathering process in SSHCZO. RT-Flux-PIHM helps to elucidates the key controls of its reactive transport process, paving ways to better quantify the clay weathering in SSHCZO.



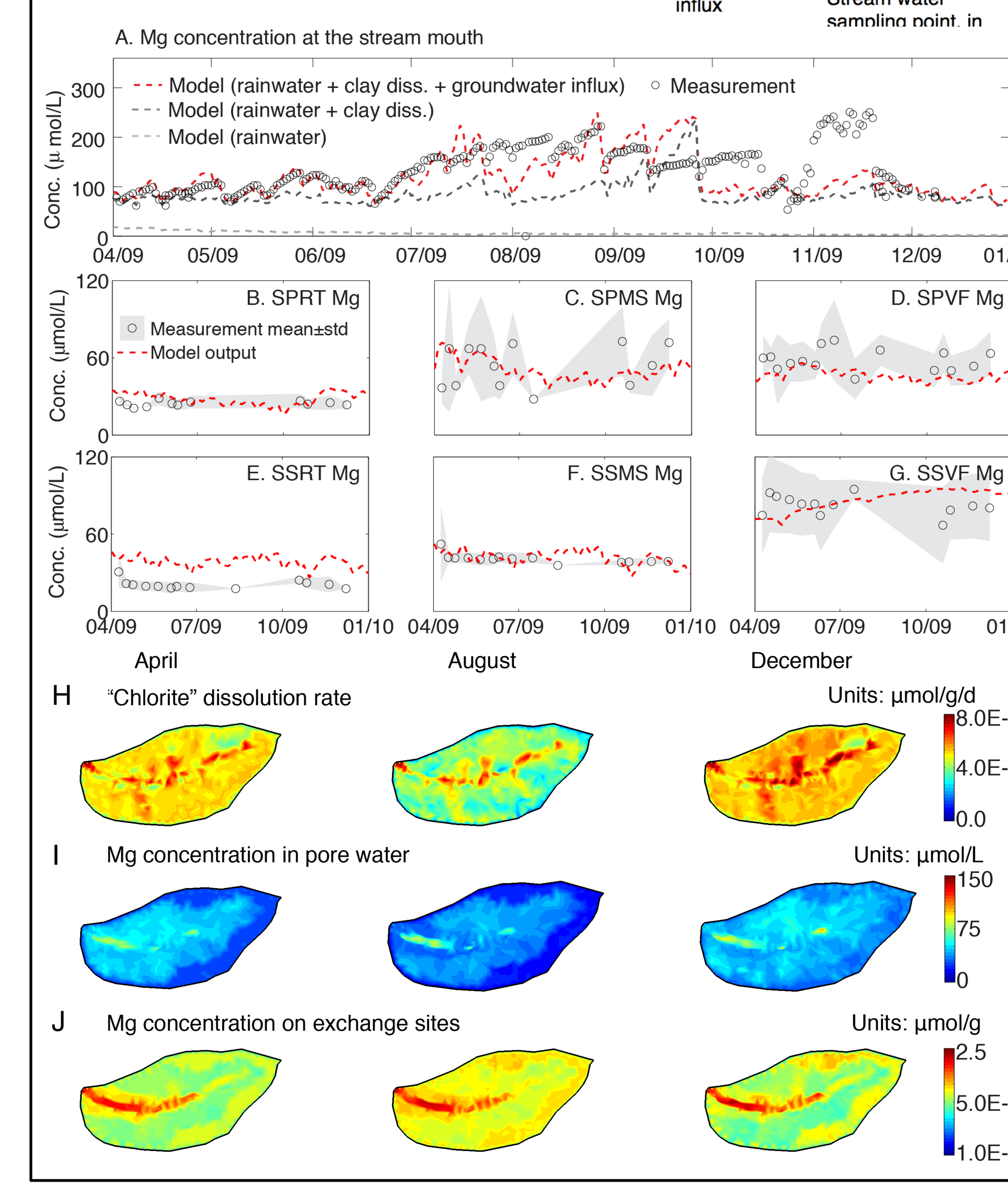




Figure 6: A~G, Mg conc. In stream water and six lysimeter sites from simulation and measurements agreed well. H: "chlorite" dissolution releases Mg. Its dissolution rate is water storage in RT-Flux-PIHM. I: Mg conc. did not increase from spring to summer, unlike Cl. Because cation exchange reactions control Mg concentration in pore water. J: Mg conc. on cation exchange sites. It increased in summer. Mg on exchange sites is enriched in convergent flow regions: swales and valley floors, which agrees with measurements.

## Conclusions

- ❑ RT-Flux-PIHM offers a unique interface to explore hydrologic and geochemical interactions at the watershed scale.
- ❑ Non reactive tracer Cl concentration is negatively correlated to water storage in SSHCZO.
- ❑ Reactive transport of Mg is more likely controlled by the balance between its source (clay dissolution) and sink (discharge), and is buffered by cation exchange

## Acknowledgement

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