
Contribution ID: **192**

Type: **Poster + 3 Minute Pitch**

# Direct simulation of hysteresis in upscaled reaction rates in a periodically transient river corridor using complex reactions on particles

*Monday, 14 May 2018 15:40 (2 minutes)*

Reactive transport in river corridors can be greatly complicated by fluctuations in the boundaries, which may cause changes from gaining to losing over time. The seasonal influxes of water cause wetting and drying of soils near the river, rainfall causes distributed periodic inputs to the surface, and chemical and physical heterogeneity affect the possible reaction sites. The combination of these behaviors can be computationally challenging to simulate because there is an apparent hysteresis in the reaction rates when the system is wetting versus drying. Most studies that have sought to model these behaviors in the past have used a strictly Eulerian approach. Here a hybrid Eulerian-Lagrangian method is used to investigate the differences in upscaled reaction rates under transient conditions. The simulation framework uses the Eulerian integrated model ParFlow to simulate a transient, variably saturated flow field that represents an aquifer adjacent to a fluctuating river with sparse rainfall. The pressure field is used to compute seepage velocities for a colocation based, reactive, random walk particle tracking algorithm. Complex reactions on particles are simulated by assigning multiple component masses to each particle, allowing nearby particles to exchange mass of the components, evaluating multi-component reactions on each particle independently, then moving the particles. Boundary conditions, spatially variable rate laws, interactions with solids, exposure time based reactions, and other rules are easily incorporated, allowing a high level of realism with regard to the physical processes. The approach is also unique because it separates spreading and mixing processes, which have fundamentally different impacts on reactive transport. We show that the framework is able to simulate the reaction hysteresis of wetting and drying conditions and discuss the potential applications, advantages, and limitations of this hybrid approach.

## References

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**Session Classification:** Parallel 2-A

**Track Classification:** MS 1.04: Upscaling of mixing, dispersion and reaction processes from pore to continuum scale