## **Poster #187**

## Modeling Solute Transport and Coupled Biogeochemical Transformations in Low-order Streams Using a Stochastic Travel-time Approach

Scott L Painter<sup>1</sup> and Scott Brooks<sup>1</sup>

<sup>1</sup> Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: Scott L Painter [paintersl@ornl.gov]

The transport and transformation of carbon, nutrients, and trace metals in low-order streams are controlled to a large degree by contact time with hyporheic and transient surface storage zones that act as local biological "hot spots" for transformation processes. Travel-time based representations provide an alternative to detailed threedimensional simulations for those multiscale reactive transport processes. In the Lagrangian travel-time conceptualization, computationally demanding three-dimensional reactive transport simulations are replaced with one-dimensional reactive transport simulations on an ensemble of trajectories through the stream channel, transient surface storage zones, and hyporheic zones. The approach is particularly appealing for broad-scope sensitivity analyses. We use mercury as a use case, and consider a simplified model for mercury methylation in low-velocity hyporheic zones and stagnant zones that are diffusively coupled to advective flow paths, accounting for transport of dissolved organic carbon, oxygen, nitrate, sulfate, inorganic mercury, and methylmercury. Growth and decay of biomass is modeled explicitly in low-velocity hyporheic transport pathways, assuming limits on biomass carrying capacity of the sediments and dual-Monod kinetics with phenomenological inhibition functions to suppress activity of nitrate- and sulfate-reducing bacteria when more energetically favorable reactions are possible. Mercury methylation is assumed to be a byproduct of the activity of sulfate-reducing bacteria. The relationships between the travel-time distributions and reach-scale methylation rates are analyzed, addressing both shallow hyporheic flows and horizontal hyporheic flows driven by planimetric variations such as meander bends. Biomass dynamics are not addressed explicitly in the scenarios that consider methylation in biofilms that are diffusively coupled to advective pathways. Instead, the focus is on identifying how that small-scale process manifests at reach scales, specifically how the effect of those small-scale heterogeneities can be represented in reach-scale models by upscaling the reaction inhibition functions.