

## Exposure-time based approach for modeling mercury transport and transformation in low-order streams

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The Mercury Science Focus Area at Oak Ridge National Laboratory recently initiated development of a new field-scale modeling framework for mercury transport and transformation in low-order streams. We describe an extensible framework that makes direct use of available field information and avoids the highly detailed site characterization that would be needed for detailed three-dimensional simulations. The approach is based on extending established travel-time based representations of watershed-scale transport to account for the time water is exposed to local biological “hot spots” for mercury methylation. In this framework, the three-dimensional concentration of mercury in various forms at any given location is controlled by the travel time of water parcels to that location from the mercury source and the exposure time, the time that water parcels are in contact with biologically active zones as they travel along their trajectories to the location of interest. In this 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, where each trajectory is characterized by travel time and exposure times. We are using the parallel, community code PFLOTRAN and are implementing a reactive transport system that includes mercury speciation in stream water, including complexation with natural organic material, sorption onto suspended solids, and diffusion-controlled exchanges between mobile water and periphyton biofilms where mercury methylation is assumed to occur (see companion Task 1 poster for details of those experiments). Potential strategies for informing the travel-time and exposure-time distributions based on field-scale tracer tests, parameter estimation, and eventually three-dimensional integrated surface-subsurface hydrology models will be summarized.