Progress Toward Scale-consistent Watershed Reactive Transport Models

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Project Abstract:

Most watershed-scale models focus on hydrological processes with limited capacity to represent the complex biogeochemical processes that control the efflux of greenhouse gases and the waterborne exports of carbon, nutrients, and trace metals. The IDEAS-Watersheds project in partnership with multiple watershed Science Focus Areas has been addressing that capability gap by extending parallel spatially resolved integrated surface/subsurface hydrology models to include reactive transport. The new capability addresses the central modeling challenges: coupling reactive transport across the surface and subsurface spatial domains, and tractably representing the effects of fine-scale biogeochemical phenomena without resorting to ad hoc upscaling. Those advances were enabled by software capabilities advanced by the IDEAS project including new approaches for multiphysics model coupling, mesh infrastructure that allows for multiple coupled meshes, and the application programming interface Alquimia, which provides hydrology codes access to widely used biogeochemical codes.

The Advanced Terrestrial Simulator (ATS) has been extended to couple multicomponent reactive transport across the surface water and subsurface domains (Molins et al., 2022). The integrated model has been used to investigate the response of the Copper Creek subwatershed in the East River, Colorado, Watershed over a ten-year period (Xu et al., 2022). Current modeling efforts focus on the Lower Triangle region to understand the processes affecting nitrogen exports with consideration of spatially-distributed watershed properties.

We have also developed a novel multiscale modeling approach (Jan et al. 2021) to represent the watershed-scale effects of biogeochemical transformations within small-scale biogeochemical

hotspots. We have implemented this model in ATS, used it to estimate model parameters from stream tracer tests (Rathore et al. 2021), demonstrated it on East Fork Poplar Creek Watershed and the Portage River Basin (Jan et al. 2021), and developed the workflow to build watershed-scale models from online data sources. We plan to extend the model-building workflow to improve estimates of hyporheic exchange flows using classification of hydrogeomorphic features.

These are first-of-a-kind capabilities that consider surface and subsurface reactive transport as an integrated multiscale system, thus improving representations of dynamic surface/groundwater exchanges, allowing for different reaction systems in the surface and subsurface, and avoiding *ad hoc* upscaling. We have plans to include additional watershed processes and integrate these new capabilities to provide a scale-consistent watershed reactive transport modeling tool that can be used to advance understanding of watershed hydro-biogeochemical function.

References

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