

Poster #21-5

Three-Dimensional OpenFOAM-PFLOTRAN Coupled Model for Mechanistic Simulation of Hydrologic Exchange Flows in Varied Hydromorphic Settings

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BER Program: SBR

Project: PNNL SBR SFA

Project Website: <https://sbrsfa.pnnl.gov/>

This element of the PNNL SFA seeks to develop three-dimensional models of coupled river hydrodynamics and subsurface fluid transport simulations in varied hydromorphic settings, for use in mechanistic reactive transport modeling and to support development of reduced-order models at system scales. Hydrologic exchange is a critical mechanism that shapes hydrobiogeochemical processes in river corridors and watersheds. Because of limitations in field accessibility, computational demand, and complexities of geomorphology and subsurface geology, three-dimensional mechanistic modeling studies to quantify hydrologic exchange flows (HEFs) have been mostly limited to local-scale applications in individual bedforms. Although it is well known that surface flow conditions, riverbed morphology, and subsurface physical properties strongly modulate hydrologic exchanges, quantitative measures of their effects on the strength and direction of such exchanges in complex hydromorphic settings are lacking. The open-source subsurface flow and reactive transport code PFLOTRAN has been used to model subsurface flow and reactive transport for hydrologic exchange studies, and commonly uses river water head as a boundary condition to drive the subsurface fluid transport, which assumes hydrostatic pressure on the river bed and neglects effects of dynamic pressure. Previous laboratory experiments and models have shown that pressure variations on the river bed induced by dynamic river flows can strongly impact hydrologic exchange. In this study, the open-source computational fluid dynamics (CFD) software OpenFOAM is used to model three-dimensional dynamic river flow and provide a more realistic pressure distribution on the river bed, through integration of the $k - \omega$ turbulence model and the volume of fluid (VOF) method. Assuming that HEFs do not affect surface water flow conditions because of their negligible magnitudes compared to the volume and velocity of river water, we developed a one-way coupled surface and subsurface water flow model that passes temporal and spatial varying pressure on the river bed derived from OpenFOAM CFD simulation to the subsurface model PFLOTRAN. The proposed three-dimensional OpenFOAM-PFLOTRAN coupled model is applied to the 7-km river section near Hanford 300A area, and used to quantitatively and systematically study the effects of river flow dynamic pressure induced on the HEFs and subsurface flow paths. Various hydromorphic settings that exist around the Hanford Reach are being classified and mapped (Hou et al. poster); the coupled model is being applied to a number of such settings to quantify the impacts of hydromorphology on HEFs and to develop information needed for reduced-order modeling at reach to watershed scales (Chen et al. poster).