

# **CONTAMINANT PLUME MODELING AT OAK RIDGE INTEGRATED FIELD RESEARCH CHALLENGE SITE USING HIGH PERFORMANCE COMPUTING**

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The Oak Ridge Integrated Field Research (ORIFRC) site is located at the Y-12 National Security Complex in Bear Creek Valley (BCV) near Oak Ridge, Tennessee. Four unlined seepage pits at the site, known as the S-3 Ponds, received discharge of liquid nitric acid and uranium wastes during the operations between 1951–1983. Waste discharges to the ponds were halted in 1983 and the pond contents were treated in situ by neutralization and biodegradation; a multi-layer cap was placed over the ponds in 1988 and an asphalt parking lot was built over the top. The geology at the BCV site is complicated by dipping beds of limestone, shale and sandstone with strike N 55° E and dip 45° SE, over which is superimposed a highly porous, horizontally oriented, saprolite weathering profile. A narrow, highly permeable, transition zone lies between the saprolite zone and bedrock. Fluid flow occurs primarily through secondary porosity produced by diagenesis, fracturing and weathering of the bedrock. Groundwater flow paths are predominately parallel to geologic strike and dip.

An effort was undertaken to implement a high resolution numerical model to simulate complex coupled geochemical and hydrologic processes at the ORIFRC site using PFLTRAN, a massively parallel, variably saturated, subsurface reactive flow and transport model. To model the complex stratigraphy at the site, a 3-D grid was constructed with x-axis aligned with the strike of the geologic formation and z-axis vertical. A complex geochemical fluid with 17 primary reactive species and a number of minerals was implemented to model the contaminant discharged from the S-3 Ponds. Because the site averages 137 cm of precipitation per year, spatially and temporally variable recharge further complicates the fate and transport of the contaminants present. To better resolve the flow and transport processes at the site requires simulations at very high spatial and temporal resolution. High resolution simulations of the site using PFLTRAN were carried out using thousands of processors on Jaguar, the Cray XT5 supercomputer at Oak Ridge National Laboratory. Results from the investigations of contaminant plume processes at the site will be presented.