Impacts of Designed Nano-materials and Nano-scale Processes on the Fate and Transport of Contaminants in Groundwater

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A major area of research at PNNL involves controlling or predicting the fate and transport of a wide variety of environmental contaminants in groundwater. Molecular and nanoscale processes often control the migration and ultimate disposition of contaminants. We have both a robust research program and have developed an important set of research tools that are available to researchers from around the world as part of the Environmental Molecular Sciences Laboratory (EMSL) a US Department of Energy User Facility Located at PNNL. Significant research areas include: i) the design, synthesis, characterization and property measurements of nano-structured materials for contaminant removal; ii) molecular and nanoscale measurements on model and natural systems related to contaminant migration and transformation; iii) design and measurements on model systems that guide and verify the development of predictive models of contaminant transport. Examples of materials to remove environmental contaminants include iron metal-core oxide-shell nanoparticles for reduction of chlorinated hydrocarbons and other organics, the formation and functionalization of nano-porous silica for heavy metal contaminant removal and the functionalized metal nanoparticles designed for removal or radionuclide contaminants. High spatial resolution or surface sensitive tools are useful for examining the location of nano-sized regions of contaminant concentration in natural and model systems. This information is critical for understanding how contaminants such as U interact with mineral phases in the environment. Both meso-scale and micro-scale flow systems have been designed that allow observation of fluid flow, contaminant reduction and reactive transport processes that can be modeled by increasingly sophisticated computer codes. Appropriate inclusion of the nano- and molecular-scale processes is essential for accurate transport model development.

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