SERDP Strategic Environmental Research and Development Program
Improving Mission Readiness Through Environmental Research

Development of Simulators for In-Situ Remediation Evaluation, Design, and Operation

Cleanup
CU-1062

RESEARCH CATEGORY: 6.2 Applied Research

LEAD AGENCY: U.S. Army

LAB: Waterways Experiment Station - Vicksburg, MS

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OBJECTIVE: The ultimate goal in remediation modeling is to minimize remediation costs and environmental and human risks while maximizing cleanup. Toward this end, the general goals of this project are: (1) to develop reliable simulators for promising technologies of interest to Department of Defense (DoD), Department of Energy (DOE), and the regulatory community, and (2) to provide efficient access to multiple remediation simulators through a common user environment amenable to multi-disciplinary cleanup teams. A common, graphical user environment has been developed for these simulators; it is the DoD Groundwater Modeling System (GMS). The GMS provides conceptualization, parameterization, visualization, and animation capabilities. Additionally, GMS extensions, either ongoing or planned, will provide capabilities for conducting remediation, uncertainty, optimization, and cost analyses. The primary technical objectives of this project are to: (1) develop/enhance state-of-the-art remediation simulators for the following technologies: in-situ bioremediation; surfactant-enhanced bioremediation; electrokinetic-enhanced bioremediation; electrokinetic-enhanced mobilization of metals; natural attenuation of petroleum hydrocarbons; natural attenuation of explosives; in-situ chemical treatment; surfactant/cosolvent flushing to recover Non-Aqueous Phase Liquids (NAPLs); soil vapor extraction and bioventing; and air sparging; and (2) verify these simulators against available laboratory and field data; and (c) incorporate these simulators into the GMS to provide DoD, DOE, and other users with the computational ability to assess the tradeoff between environmental risk (cleanup level) and cost-effectiveness for a variety of cleanup technologies prior to their implementation.

BENEFIT: The GMS-based simulators will permit efficient evaluation of multiple remediation technologies for site-specific conditions, allowing selection of effective and cheaper cleanup actions. Such simulators are needed to support advocacy for biogeochemically complex alternatives that are faster, more effective, and/or more cost-efficient than traditional methods. Simulators will improve the remedial design by permitting cleanup specialists to consider multiple scenarios that could increase cleanup effectiveness.

TECHNICAL APPROACH AND RISKS: Remediation simulator development will proceed along three paths, in order of priority: (1) utilize existing, proven remediation simulators where available and consistent with project goals, (2) modify promising groundwater codes to simulate additional technologies as appropriate, or (3) develop new codes as required for efficient simulation of innovative technologies. All simulators will be verified against available laboratory and field data. Where data permit, the simulators will be applied for National Environmental Technology Test Sites (NETTS). Results of these evaluations and the simulator codes will be documentation. Each simulator will be implemented in the GMS. This project strongly leverages technical partnering and collaboration with ongoing and proposed basic and applied research in subsurface flow, contaminant fate/transport, remedial methods, remediation simulation under heterogeneous subsurface conditions, GMS-user environment development, and high performance computing in environmental quality modeling. Technical risk issues involve: (1) uncertainty regarding key processes in complex remediation technologies; (2) the scarcity of experimental or field data for innovative technologies; and (3) the general adequacy of differing computational resources on which to run complex models efficiently. Leveraging against the new Common High-Performance Scalable Software Initiative and Army High-Performance Computing efforts will address several of the high-performance computing issues associated with simulator development and execution.

ACCOMPLISHMENTS: In FY98, the U.S. Army Waterways Experiment Station (WES) researchers have worked toward developing and verifying the various modeling codes. Corrective Action Plan Reports and Site Investigation Reports on Hill Air Force Base bioventing remediation sites, site 870, site 260 and site 280, were received. Data from all sites were reviewed, and it was decided to use site 280 as the field case for modeling bioventing processes using the NUFT3D code. Requested and received reports on Site 280 date back to 1991. Data was compiled on site characterization, soil properties, pre-and-post-remediation concentrations, respiration tests, remediation system operation, and other necessary data to begin preliminary modeling using representative input parameters. Monod kinetics were incorporated into the NUFT code. The option is very general and has the capability for multiple Monod rate laws with multiple inhibition factors. NUFT input files were then developed to include bioventing input parameters. The model has a 300 ft wide and approximately 110 ft thick cylindrical (radially symmetric) domain, centered at the bioventing injection well. The model includes multiphase, multicomponent transport with dual Monod kinetics for biodegradation of fuel hydrocarbons. Modifications to OS3D were completed in the following areas: 1)incorporation of intra-aqueous reaction kinetics into the code, while retaining the option of assuming equilibrium with respect to these reactions; 2) revision of the database routine so that the full range of possible aqueous complexation and mineral-water reactions can be included automatically; 3) modification to the OS3D input file so that it is based on keywords rather than required inputs; and 4) incorporation of additional rate laws like the Monod expressions used for microbially-mediated reactions. New data from the re-packed columns at the Dover AFB Funnel and Gate Site are being analyzed and show behavior that is more in line with other studies of zero-valent iron treatment systems. There is still indication that the efficiency of the iron reactivity is diminishing over time. Model simulations will resume following receipt of the rest of the data.

TRANSITION: The project will transition the GMS-based simulators directly to users that include DoD, DOE, EPA, and other groundwater and environmental professionals involved in hazardous waste site cleanup. Use of these remediation simulators will allow more reliable comparison between cleanup level (its duration, environmental risk level) and the cost of each level of cleanup.