FY06 ERSP Progress Report for
"Integrated Hydrogeophysical and Hydrogeologic Driven Parameter Upscaling for Dual-Domain Transport Modeling"

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Research Objective: Our research project is motivated by the observations that conventional characterization approaches capture only a fraction of heterogeneity affecting field-scale transport, and that conventional modeling approaches, which use this sparse data, typically do not successfully predict long term plume behavior with sufficient accuracy to guide remedial strategies. Our working hypotheses are that improved prediction of contaminant transport can be achieved using a dual-domain transport approach and field-scale characterization approaches. Our overall objectives are to: (1) develop a dual-domain modeling approach using the TOUGH2 family of codes that incorporates the key interactions between mobile and immobile transport regions that are expected to play a role in long term plume behavior; (2) develop a facies-based multi-scale characterization approach that utilizes log, crosshole, and surface-based characterization information and that is guided by the parameterization needs of the dual domain modeling; and (3) evaluate the approaches by applying them to the prediction of plume behavior at the P-Area at the Savannah River Site (Figure 1). Our three-year project scope includes development of multi-scale characterization and dual-domain modeling approach and field-scale data acquisition (Year 1); Numerical simulations and field-scale characterization (Year 2); and Plume transport simulations and exploration of optimal dual-domain parameters (Year 3).

Research Progress and Implications: Our emphasis in this first half-year of the project has focused on field-scale characterization and use of numerical simulations to explore when dual-domain modeling approaches improve plume transport predictions over conventional approaches. A CPT campaign was undertaken in September 2006. CPT groundwater samples were acquired at 10 locations and over several depths; these data were used to define the vertical and horizontal extent of the P-Area TCE plume. Lithologic logs were recorded at three CPT locations, and dual-level piezometers were installed at the same locations. Headspace gas analyses were performed on sediment samples collected from both permeable and relatively impermeable intervals to define the vertical plume extent, and the distribution of contamination with respect to mobile and immobile water regions in a dual-domain conceptual model. The CPT data indicated peak TCE concentrations in the 20-30,000 ppb range in a transmissive zone that is centered at a depth of approximately 90 ft below ground surface. Comparison of lithologic and concentration data suggests that facies seem to be controlling transport in the vicinity of our study site. Based on this initial dataset, three permanent wells were installed in October along the plume center line. These wells were logged using gamma and resistivity approaches, and will be subsequently used for hydrological well tests and crosshole geophysical data acquisition.

Surface Ground Penetrating Radar (GPR), Vertical Seismic Profile (VSP), and surface electrical methods have all been tested at the site to ascertain site-specific data quality. These initial tests indicated that (100 MHz) GPR signals are unlikely to sufficiently penetrate below the water table (~15 m depth), as is needed for saturated zone characterization (Figure 2). In contrast, good data quality was observed from VSP. Key horizons exhibited distinctive signatures (Figure 3), and the preliminary data is being used to design a 2.5D campaign as part of Phase II characterization. An initial surface electrical survey to assess data quality was conducted the first week in November, 2006. Field observations suggest that electrical methods will be effective at the field site, and that the information obtained from this approach should compliment the structural information provided by the seismic approach.

In parallel to field activities, a version of iTOUGH2 using the EOS7R module was modified to enable simulation of dual-domain transport in a sedimentary system. The inverse modeling capability of iTOUGH2 will be used to optimize dual-domain parameters based on specified reference plume data. To develop and test the modeling framework, a hypothetical high-resolution heterogeneous permeability field in two-dimensions was generated. Spatial variability is represented as a distribution of two discrete facies with median permeabilities differing by 4 orders of magnitude, and continuous variability within facies (Figure 4). Solute concentration was assumed to be initially uniform throughout the 10 meter high by 100 meter long region. Solute break-through out to 4000 days was recorded. Using the high-resolution model as the reference, coarse mesh single- and dual-domain simulations were optimized using iTOUGH2. The dual-domain formulation produced excellent agreement with the reference data (Figure 5). In contrast, the single-domain model deviated significantly from heavy tail observed for the high-resolution model.

Planned Activities: The research team will concentrate on both characterization and modeling tasks during FY07. We will complete analysis of the initial geophysical surveys, and design and perform comprehensive field characterization surveys. The geophysical campaigns will include 2.5D surface seismic, 2.5D surface electrical surveys, and crosshole seismic, radar, and electrical resistivity tomographic imaging. The multi-scale characterization framework will be developed during FY07 using stochastic techniques and guided by initial field data quality. Hydrological analysis will include flowmeter and pumping tests as well as core analysis; these data will be used for initial facies analysis. An extensive set of numerical experiments will also be conducted in FY07 using the modified version of iTOUGH2 / EOS7R to determine relationships between optimal dual-domain parameter settings and site characterization information, such as facies proportions, permeability contrast / variability, spatial and temporal scales, spatial correlation and anisotropy, and head gradient relative to strata. Based on assessment of the characterization and modeling efforts, additional wells will be installed to better define plume behavior, sediment facies, vertical permeability profiles, and enhanced crosshole imaging. Figure 6 provides a timeline for FY07 activities. A project webpage is currently being developed that will enable dissemination of the project advances as well as provide a mechanism for data sharing between the three participating institutions.

Information Access: The following abstracts describe some of the progress that has been made during the first half-year of the three year project.

Cameron, A.E., C.C. Knapp, A. Addison, and M. Waddell, Applications of ground penetrating radar for hydrogeological characterization at the Savannah River Site, South Carolina, EOS. Trans.,. AGU 87(52), Fall Meet. Suppl., Abstract H31B-1411, 2006.

Flach, G.P., Integrated hydrogeophysical and hydrogeologic driven parameter upscaling for dual-domain transport modeling, Invited presentation at ERSP Fall Meeting, Oak Ridge TN, Oct. 23-25, 2006. Presentation available at http://www.lbl.gov/NABIR/generalinfo/PI_ann_mtgs.html

Hubbard, S.S., K. Williams, T. Scheibe, J. Peterson, J. Chen, S. Mukhopadhyay and E. Sonnenthal, Improved understanding of natural system processes through coupling of

geophysical characterization and numerical modeling approaches, EOS. Trans.,. AGU 87(52), Fall Meet. Suppl., Abstract H41-G-01, Invited Presentation, 2006.

Contributions of Each Institution: During FY06, Lawrence Berkeley National Laboratory co-led development of the iTOUGH2 modeling framework, and contributed to design of Phase I field activities. Savannah River National Laboratory coordinated field work at the SRS P-Area field site, lead hydrogeologic characterization (CPT, drilling/wells), and co-lead development of the modeling framework. The University of South Carolina performed surface ground penetrating radar and seismic, vertical seismic profile, and electrical surveys.

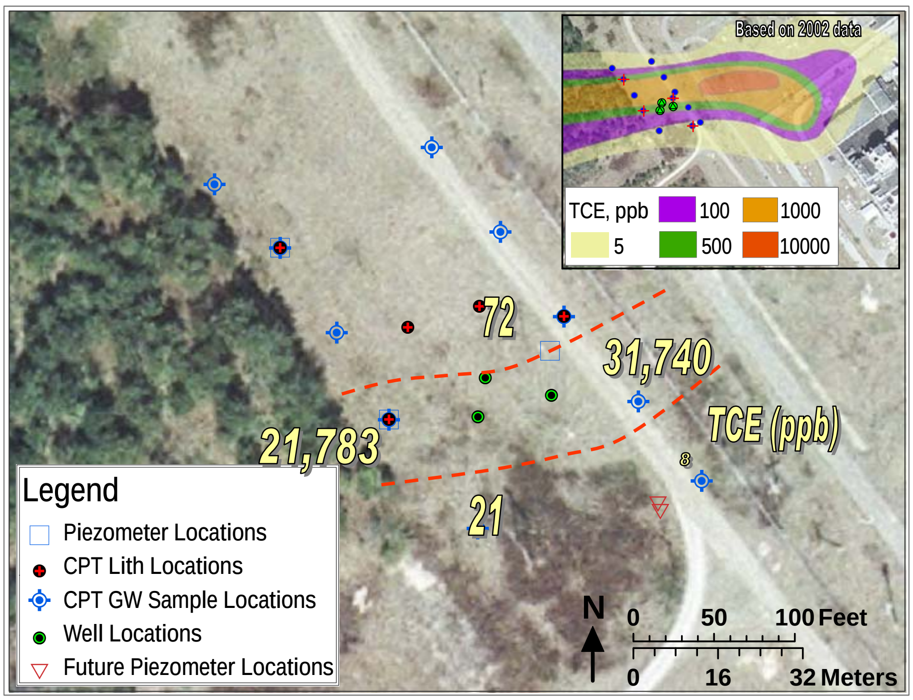


Figure 1. Field research site and TCE plume near Savannah River Site P-Reactor.

- Surface Ground Penetrating Radar (GPR)
  - 4 (50-200 m long) 50 MHz profiles
  - 4 (50-200 m long) 100 MHz profiles
  - 1 (100 m long) 200 MHz profile
  - Common mid-point GPR surveys (50, 100 MHz)
- Vertical Radar Profiles (at PGW 17B)
  - Multi-offset, 50 MHz
  - Multi-offset, 100 MHz

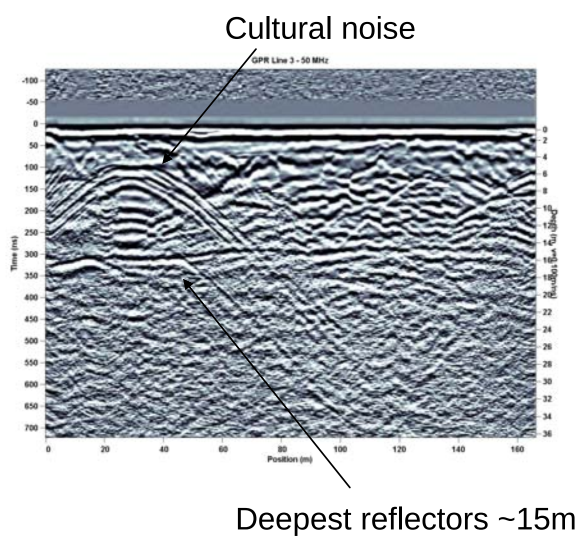


Figure 2. Results from initial surface ground penetrating radar (GPR) survey to assess data quality.

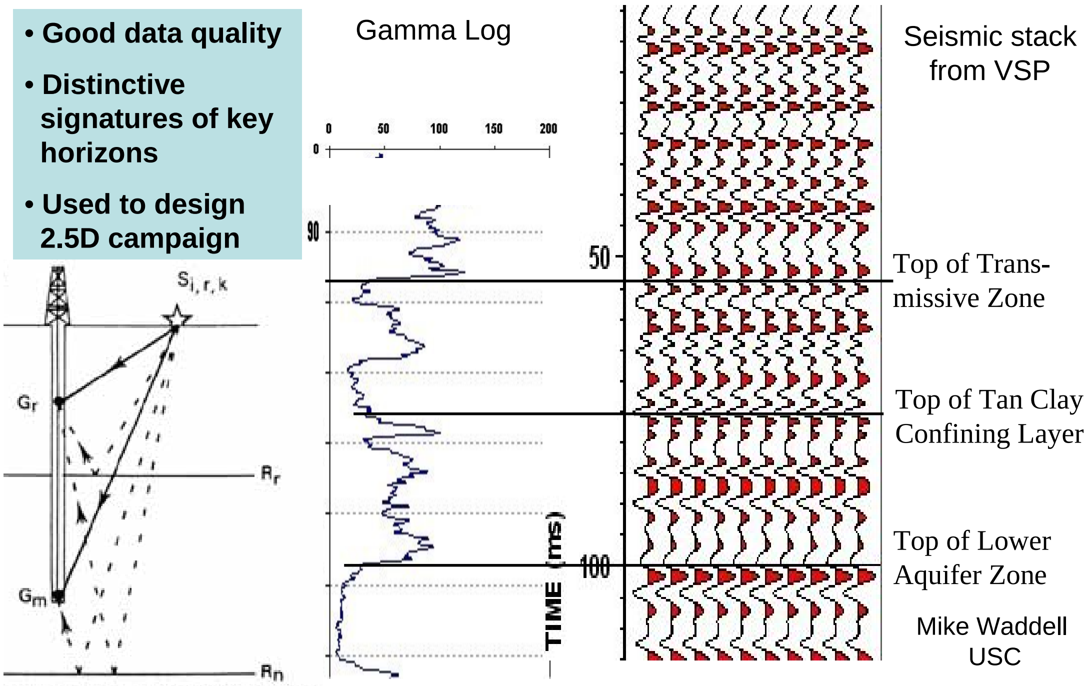
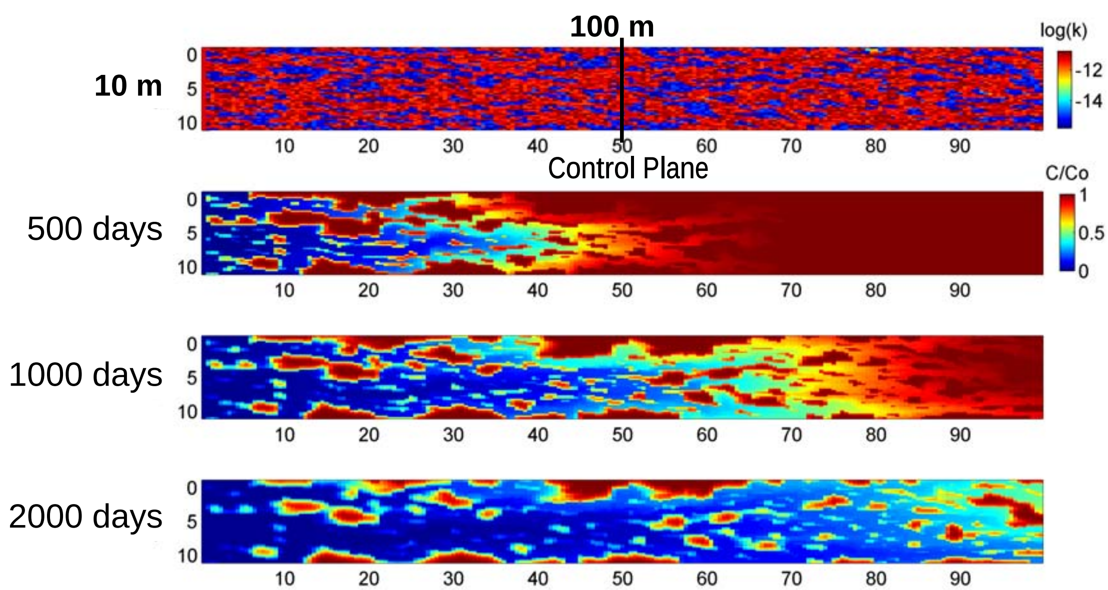
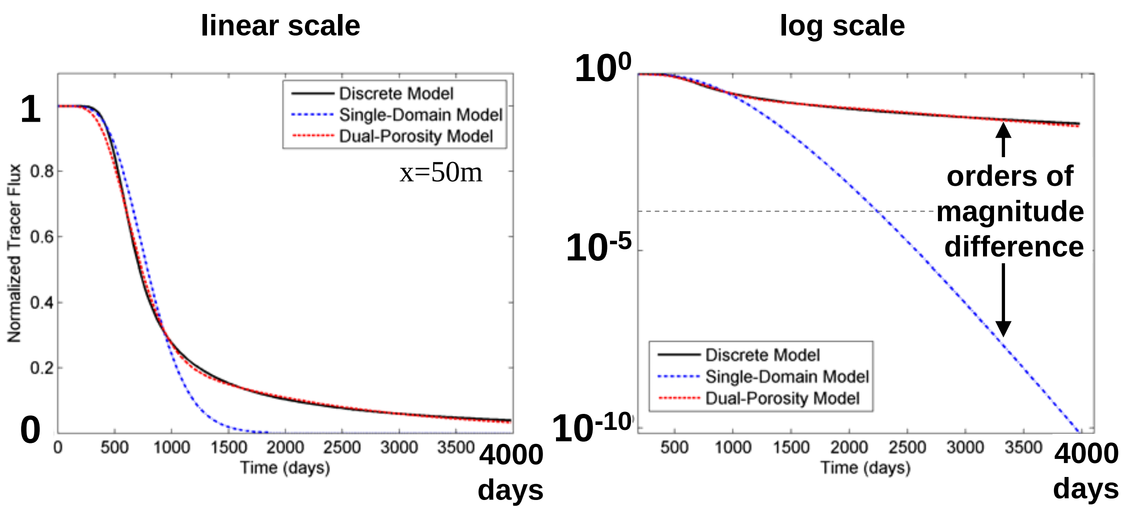


Figure 3. Results from vertical seismic profile survey using existing SRS P-Area wells.



<log(k1)> = -11.3, <log(k2)> = -15.3, $\sigma_{k1} = \sigma_{k2} = 0.29$, V1/(V1+V2) = 0.7
Spherical semivariograms: range = 0.5 m, anisotropy = 5, angle = 5^o

Figure 4. High resolution permeability field and solute transport simulations.



Single-Domain Parameters
log(k)=-11.72, ϕ=0.39

Dual-Porosity Parameters
log(k_1)=-11.72, ϕ_1=0.34, ϕ_2=0.42, A_{12}=0.0052

Figure 5. **Comparison of coarse-mesh single- and dual-domain break-through curves to high-resolution transport simulation.**

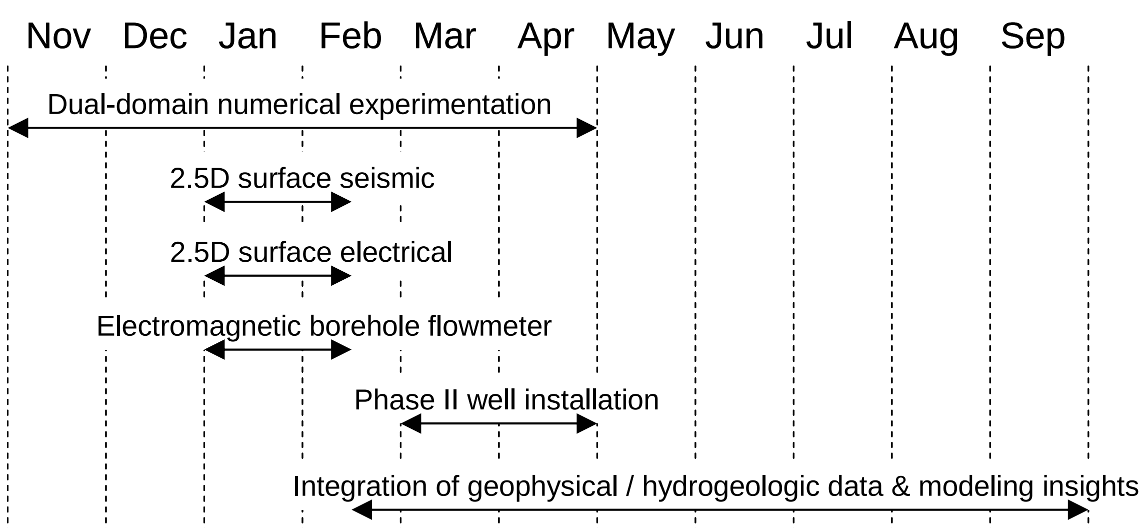


Figure 6. **FY07 project timeline.**