CONF-930166--1

LA-UR- 92-4053

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DE93 005446

Author(s): Bryan Travis, EES-5
Nina Rosenberg, EES-5
Kay Birdsell, EES-5

Submitted to: DOE Office of Technology Development Meeting
January 26-28, 1993

Los Alamos
NATIONAL LABORATORY

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NUMERICAL SIMULATIONS FOR THE *IN SITU* BIOREMEDIATION DEMONSTRATION AT SAVANNAH RIVER: PRESENTATION OF THE MODEL

Bryan J. Travis
Nina D. Rosenberg
Kay H. Birdsell

Geoanalysis Group, EES-5
Environmental Sciences Division
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-6384

Introduction

A series of environmental technology field tests, including *in situ* bioremediation, are being conducted at the Savannah River Integrated Demonstration (SRID) site near Aiken, South Carolina. This site is part of a larger area that was used to process fuel and target elements for use in reactors. Degreasing operations were included at several stages of the operations. Degreasers such as TCE and PCE were discharged to a seepage basin via a process sewer pipeline. In the early 1980s, inspections revealed that the process sewer line had extensive cracks, allowing solvents to leak into the subsurface environment. An *in situ* remediation technology designed to address this linear source term was tested in 1990. This technology involved air injection below the water table and vacuum extraction in the vadose zone using two horizontal wells [*Looney et al.*, 1991]. Bioremediation experiments using these same horizontal wells were begun in 1992 [*Hazen*, 1992a]. This experiment is based on the expectation that the injected air and methane will stimulate the growth of naturally occurring methanotrophs at the site and these bacteria will co-metabolize the chlorinated solvents.

Our goal is to provide support in assessing and evaluating the in situ air stripping and bioremediation demonstrations at the Savannah River Site through a combination of numerical modeling activities and cost effectiveness analysis. The goal of the modeling activities is to provide insight into the physical processes involved, support improved performance evaluations, and aid in optimizing system design. The goal of the cost effectiveness work is to provide an improved analysis of the Savannah River demonstrations using the modeling results and investigate possible reductions in the costs of technology demonstrations and characterization and monitoring activities through analysis of the value of modeling and the value of characterization and monitoring data. In this report, we describe our bioremediation model and demonstrate the capabilities of this model with simulations based on the field test at the Savannah River Integrated Demonstration (SRID) site.

The Bioremediation Model

A computational model, TRAMP, has been developed at Los Alamos National Laboratory (LANL) to support a number of field tests of *in situ* bioremediation. This model calculates the transport of air, water and dilute contaminants plus bacterial metabolism of substrates, in porous media. TRAMP, for TRAcr3d with Microbial Processes, is an extension of the TRACR3D code which simulates flow and transport of contaminants in porous media [*Travis*, 1984; *Travis and Birdsell*, 1991]. TRAMP contains two sets of equations which are solved simultaneously. The first set includes the flow equations for unsaturated/saturated flow of air and water in heterogeneous, anisotropic porous media. These are time-dependent, three-dimensional equations which are solved using a finite difference, implicit time stepping algorithm. Material properties, such as porosity and permeability, can vary in space and the model allows considerable flexibility in boundary conditions and the location of injection/extraction wells.

The second set of equations in TRAMP includes five nonlinear, coupled time-dependent transport equations, one each for oxygen, a nutrient, two substrates, and microbes. Both anaerobic and aerobic conditions are included. Monod kinetics are assumed. This coupled system is solved by an iterative finite difference algorithm. The biological activity model [*Bentley and Travis*, 1991] is similar to that described by *Widdowson et al.* [1988] and *Semprini and McCarty* [1991]. TRAMP is a general purpose code and therefore not all of its features may be needed at a specific site. For the Savannah River site, anaerobic reactions can be neglected, and the second set of equations consists of conservation equations for methane, TCE, oxygen, a nutrient, and microbes.

Parameter values (e.g., substrate utilization rates) are based on a series of field experiments conducted at Moffett Field, California [*Roberts et al.*, 1990; *Semprini et al.*, 1990, 1991; *Semprini and McCarty*, 1991], laboratory tests performed by INEL on sandy soil from a contaminated region of the Snake River aquifer [*Andrews et al.*, 1991], and in cases, our own judgment and experience. These values will be replaced by values from laboratory tests conducted on soil samples from the Savannah River site when these data become available.

Brief description of the site

The Savannah River site is underlain by sediments of the Atlantic Coastal Plain. The upper few hundred feet of these sediments consist of interbedded sands and clays that were deposited in shallow marine, lagoonal and fluvial environments. The local topography is relatively flat with a surface elevation of ~360 ft above mean sea level (msl). The sediments that underlie the site are very heterogeneous. A generalized description includes a sand unit and several major clay units [*Eddy et al.*, 1991].

Two horizontal wells were used for the bioremediation demonstration [*Hazen*, 1992a; *Looney et al.*, 1991; *Kaback et al.*, 1989]. One well was installed below the water table and used for air injection. This well is ~300' long and at an elevation of ~195'. A second well was installed in the vadose zone and used for vacuum extraction. This well is ~175' long and at an elevation of ~285'. The strike of the extraction well is ~35° counterclockwise to the strike of the injection well. Both wells are screened over most of their lengths and are subhorizontal, dipping toward greater depths at their terminal ends.

The goal of the bioremediation demonstration is to stimulate naturally occurring methanotrophic bacteria at the SRID site with injection of methane and air such that significant amounts of TCE present in the subsurface will be degraded. The experiment began in late February 1992. The demonstration consisted of four phases to date. First, air was extracted from the upper horizontal well. Then, air was also injected into the lower horizontal well. Methane was then added to the injected air at a concentration of 1% methane/air. After several months, this concentration was increased to 4%. See *Hazen* [1992a, 1992b].

A Sample Simulation

The following sample simulation based on the SRID demonstration serves to illustrate the model's capabilities. The simulation is restricted to air flow only through a 2-D cross-section of the site, 100 m long by 40 m high and based on the general description of the SRID site [*Eddy et al.*, 1991]. The plane of the cross-section is approximately perpendicular to the long axis of the horizontal wells and passes through the midlength point of the extraction well.

The domain (Figure 1) is divided into ~700 rectangular grid cells and includes four different hydrogeological zones (325' clay, 300' clay, tan clay zone and a sandy material). The extraction well is represented by a single grid cell near the center of the domain. The lower boundary represents the top of the water table. The lower (injection) well is not included explicitly, but a section of the bottom boundary approximates the upward flow of air, methane and TCE that the injection well would create. The bottom boundary is impermeable to flow and dissolved materials. A source term representing the injection well, however, is included along the bottom. The top boundary is kept at constant atmospheric pressure and oxygen concentration; methane and TCE concentrations are constant at a concentration of 0. The side boundaries are also kept at a constant atmospheric pressure.

The schedule of injection/extraction from the wells mimics the experimental conditions. The extraction well is turned on and it pulls 240 SCFM and remains constant. Three weeks later, the injection well is pressurized sufficiently to inject 200 SCFM of air. This air contains TCE since it is bubbling up through the high concentration region below the water table and, of course oxygen. Five weeks later, 1% by volume of methane is added to the injection air stream. Three months later, methane is increased to 4%. The total duration of the simulation is 8 months.

Figure 2 shows contour plots of the methane, oxygen, nutrient, microbe, and TCE water concentration fields and the air pressure field at the end of the simulation. Several features are evident from these plots. The 325' layer clay is acting as a barrier in this particular example. Concentrations above this layer are basically at their initial values, and the region does not promote biodegradation. (In this simulation, the tan clay is assumed to be more permeable than the 300' clay which is assumed to be more permeable than the 325' clay).

The position of the injection well along the lower boundary is evident by the high air pressure and the high methane, oxygen, and TCE concentrations. The pressure gradient is steep in the tan clay layer along the bottom boundary but dissipates rapidly when it hits the more permeable sand layer. The methane, oxygen, and TCE contours mimic the pressure gradient near the injection well.

The position of the extraction well can be seen as the light circle in the air pressure plot above and to the right of the injection well. The extraction well has swept TCE from above the 300' clay layer and to the right of the well. In this simulation, the extraction well appears to act as a barrier, keeping the injected methane, oxygen, and TCE from reaching this region. A lower microbe population and higher nutrient concentration also occurs in this region, presumably because the microbes prefer to grow where the methane and oxygen concentrations are higher and the extraction well removes the microbes' substrate supply. In this simulation, the most effective biodegradation occurs between the injection and extraction wells.

Figure 3 shows a time history plot of the microbe concentration at a position in the sand just above the tan clay zone, and to the left of the source region. The microbes grow slowly during the first five weeks when no methane is injected. Their population increases during the injection of the 1% methane (5 weeks to 5 months) then again during the injection of the 4% methane (5 months to 8 months). Toward the end of the simulation, however, their growth rate slows and begins to decrease slightly, possibly due to nutrient limitations.

Conclusions

This preliminary simulation illustrates the fact that biodegradation only occurs in zones with the right mix of microbes, oxygen, methane, TCE and nutrient (see *Andrews et al.* 1992). Assessing and evaluating bioremediation requires a model such as TRAMP that combines microbial processes with flow and transport processes. Additional simulations are in progress. This work includes study of the effectiveness of bioremediation compared to in situ air stripping alone, possible improvements to system design, and assessment of how this technology might perform at other sites.

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Acknowledgements

This work has been supported by the Office of Technology Development in the U.S. Department of Energy's Office of Environmental Restoration and Waste Management.

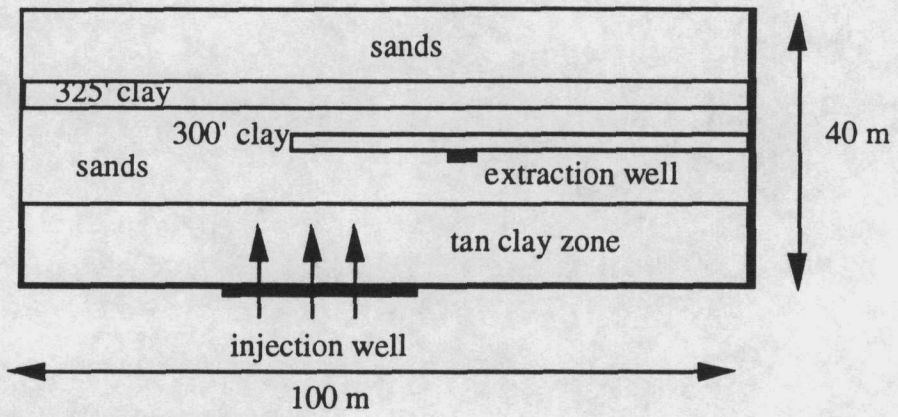

Figure 1. Domain used in simulation.

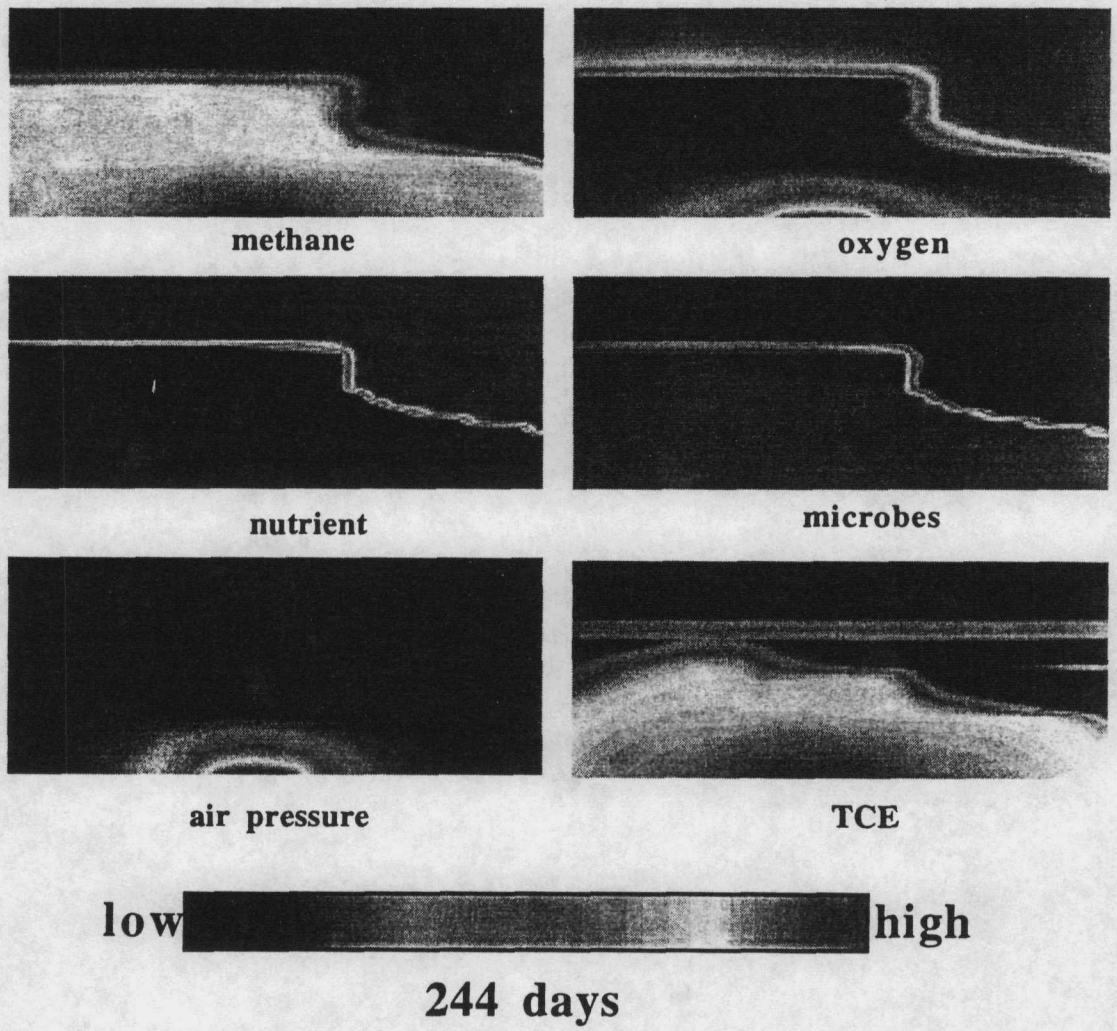

Figure 2. Field plots at end of simulation.

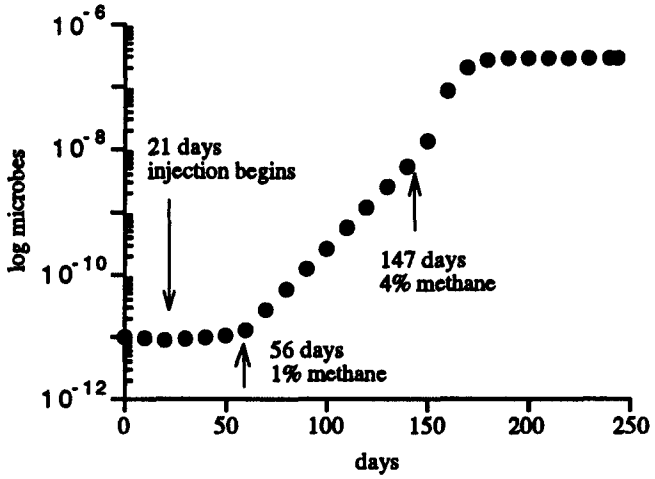

Figure 3. Simulated time history plot of methanotroph population at a point above the tan clay zone and to the left of the extraction well.