THREE-DIMENSIONAL SIMULATION OF DNAPL TRANSPORT AT THE SAVANNAH RIVER SITE

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ABSTRACT

The M Area of the Savannah River Site was used for processing materials for nuclear production reactors. From 1958 through 1985, process effluent was sent to the M Area Settling Basin through a process sewer line. Because of disposal to the unlined settling basin, approximately 2.0 million pounds of chlorinated solvents were released to the subsurface in M Area. Results from ongoing groundwater and soil clean up programs indicate that relatively large amounts of DNAPL are present in the subsurface. Detailed studies have shown that a substantial fraction of the DNAPL at M Area is trapped above the water table in clays and silts and that DNAPL is present below the water table in isolated pockets and ganglia. As a DNAPL invades the saturated zone, it accumulates in coarser sediments overlying finer grained sediments such as clays. As DNAPL accumulates on top of clay layers below the water table, it can continue to flow down-dip, towards local topographic lows in the clay surface.

The geologic and hydrogeologic data were used in conjunction with generated geostatistical parameters for three lithologic units at M Area to develop a conditional model of hydrogeologic parameter distribution. This information, along with historical contaminant release profiles, was used as model input for the numerical flow simulator. The results from the initial simulations indicate that the modeling under-predicts the extent of free-phase DNAPL in comparison to what has been found in the subsurface. This is believed to be the result of element size with respect to the amount of DNAPL released. The smallest element area for the initial simulations was 100 by 100 feet. Simulations are ongoing with elements as small as 20 by 20 feet and this should improve the resolution.

1.0 INTRODUCTION

M Area was used in the past for processing uranium, lithium and other materials into fuel elements and targets for nuclear production reactors. These processes involved metallurgical and mechanical operations, and as a part of these operations, solvent cleaning and acid/caustic etching were used to prepare materials. During a period beginning in 1958, and ending in 1985, process effluent was sent to the M Area Settling Basin through a process sewer line. Because the effluent contained large amounts of chlorinated solvents, contamination of soils and groundwater occurred in this area as a result of breaks in the old process sewer line, and disposal to an unlined settling basin. It is estimated that approximately 2.0 million pounds of chlorinated solvents, mainly tetrachloroethylene (PCE) and trichloroethylene (TCE) were released.

The settling basin covers a small area of about 75,000 ft^2 (300' by 250') allowing the DNAPL emplacement to be modeled as a point source. Leaks in the process sewer line that was used to transport DNAPL to the settling basin will in actuality spread the source. The DNAPL will migrate downward through permeable zones until it accumulates on an impermeable layer, where it will then move down-dip along the surface. However, the dissolved plume is affected by ground-water movement and is carried down the hydraulic gradient with the water flow. Current maps of dissolved contaminant plumes, the subsurface structure of the "green clay" confining unit (Looney

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et al., 1992), and the water table were considered when deciding on the model boundaries (Figure 1). The dissolved plume maps indicate a west/southwesterly (SRS coordinates) migration direction, consistent with the ground-water gradient in the area. The subsurface structure of the "green clay" confining unit generally dips to the west in the model area. Based on this information, the model is positioned to center the settling basin in the eastern half of the model grid, placing the settling basin in an up-gradient and up-dip location. The model extends to the west to fully encompass the down-gradient 1 ppm contour of the dissolved TCE plume (Figure 1).

1.1 Site Geology and Hydrogeology

SRS is situated over Coastal Plain sediments comprised of interbedded sands and clays. The sediments are almost flat-lying with a gentle regional dip of about 25'/mile to the southeast, though locally dip directions are variable. The first relatively continuous confining zone at M Area is the "green clay" whose thickness ranges from 2 to 20 feet, thinning to the northeast. It underlies the water table aquifer ("M Area" Aquifer Zone) and overlies the "Lost Lake" Aquifer Zone. The vadose zone is relatively thick, ranging from 75' to 135' across the model area (about 120' at the settling basin). The thick vadose zone limits the downward migration of contaminants and captures some of the DNAPL in the clays above the water table. Only in areas where large quantities of DNAPL were disposed, such as the settling basin, has DNAPL been found as a separate phase below the water table.

2.0 MODELING METHOD

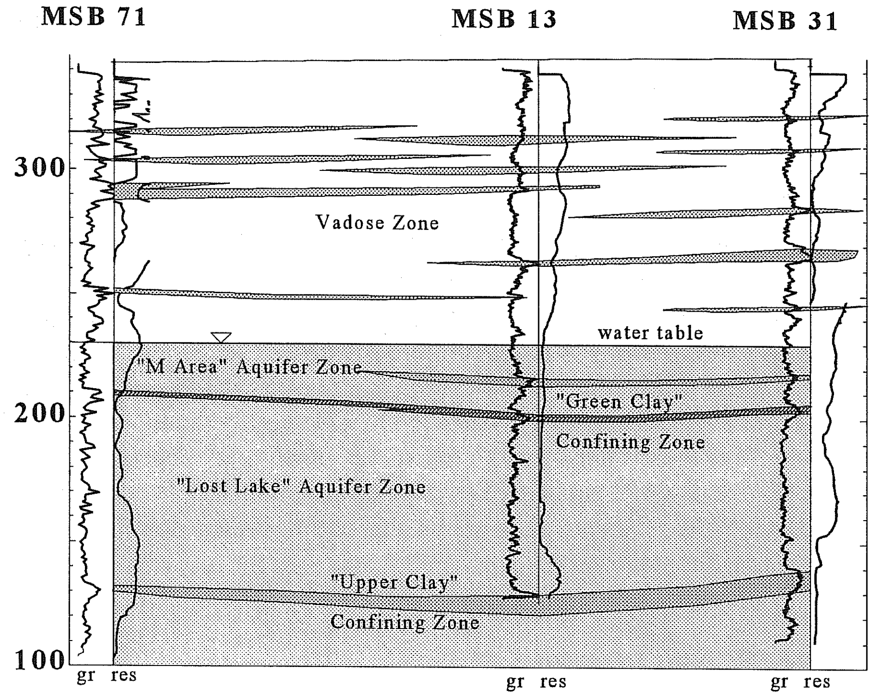
2.1 Mesh Development and Generation of Geostatistical Permeability Field

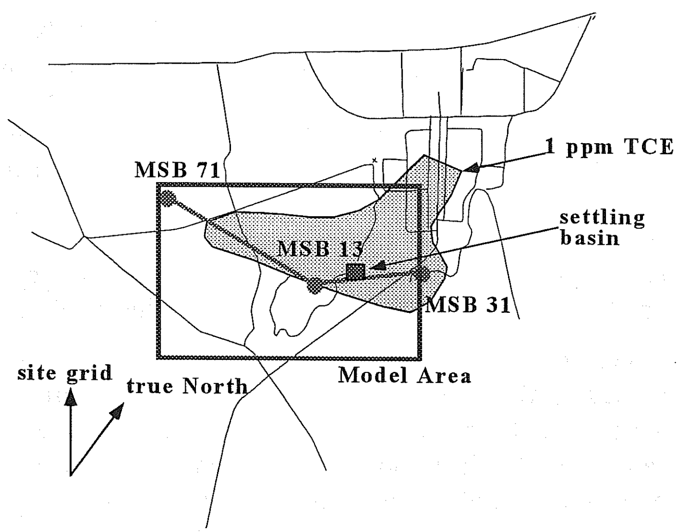
Formerly, the 3D Cartesian grid generated by T2VOC was restricted to orthogonal x, y, and z dimensions. This is limiting in an area where the primary surface (the "green clay") on which DNAPL accumulates and migrates is deformed. To perform simulations that adequately model contaminant migration in the heterogeneous subsurface, a fine mesh is required for the green clay and for several feet above the clay. To address this shortcoming, a vertically conformable mesh generator (STRAT) was developed by Stefan Finsterle while at Clemson in the spring of 1996. Using an input file with lines consisting of surface x and y coordinates along with elevations of lithologic units, STRAT generates a mesh that conforms to the topography of each lithologic unit. Each unit can be further subdivided into equal parts allowing for a fine vertical grid.

Prior to generating the vertical component of the model grid, lithologic units must be identified and assigned a ROCK type. At M Area, three distinct vertical units were identified. The shallow-most extends from the land surface to the top of the "green clay" and is referred to as the M Area aquifer zone (MAZ). It includes both the vadose and unconfined saturated zones. The middle unit is the low permeability "green clay" confining zone (GCCZ). The lower most unit incorporated in the model is the Lost Lake aquifer zone (LLAZ).

A "fine" grid (surface elements of 100 ft by 100 ft) was designed in the vicinity of the settling basin. The x and y element dimensions were gradually increased to 500 ft by 500 ft at the model boundaries. The total number of surface elements is 780 (30 in the x direction by 26 in the y direction). The upper portion of the MAZ was divided into twelve layers with an average thickness of 12 feet. The lower 10 feet of the MAZ, where DNAPL is expected to accumulate, was divided into 5 layers, each 2 feet thick. The GCCZ was divided into 5 layers that averaged 1 feet thick. The LLAZ was divided into 5 layers that averaged nearly 14 feet in thickness. The final number of elements in the model mesh is 21,840 (28 divisions in the z-direction).

Figure 1. Cross section across the model area. The vertical extent of the model is from the surface to the "Upper Clay" Confining Zone.

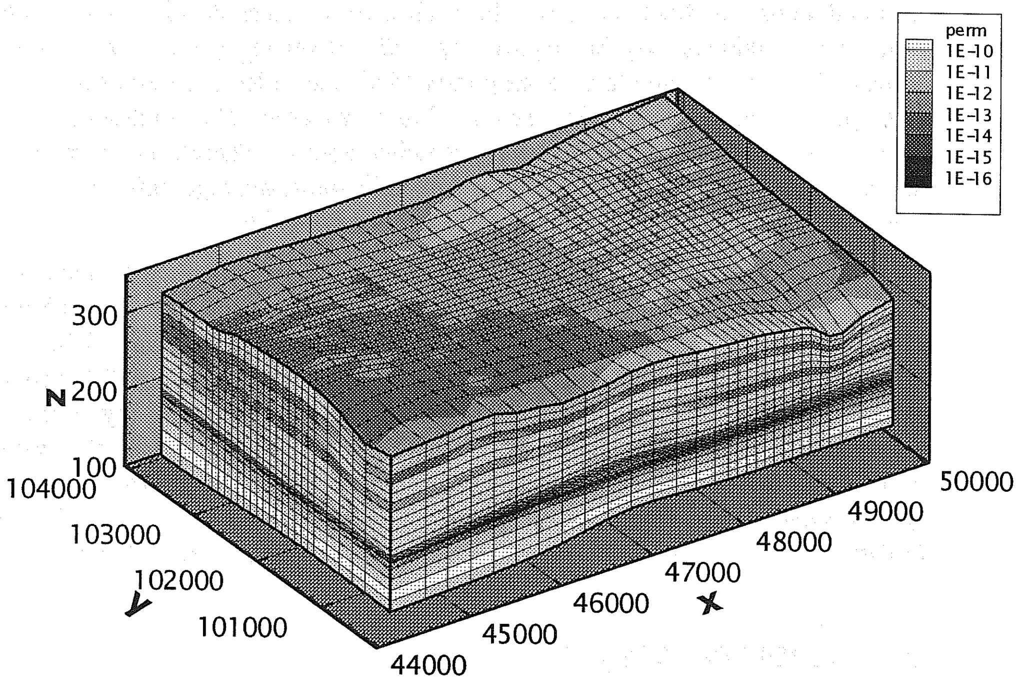




A heterogeneous permeability field is geostatistically generated for each lithologic unit. The program used was SIMAN3D, developed by Stefan Finsterle, and is based on the simulated annealing method. Within a given set of parameters, SIMAN3D will generate a spatially correlated random field based on a specified variogram. Key parameters include correlation length (x, y, and z directions), standard deviation, and a three-dimensional array of locations equivalent to the portion of the overall model mesh intended for the lithologic unit. The output file from SIMAN3D contains a permeability modifier that is added to each element in the ELEME block of the input file. The average permeability for the lithologic unit (x, y, and z directions) is specified in the ROCKS block of the T2VOC input file and can be changed without regenerating the geostatistical field. If measured permeability data at locations in the model area are available, the data can be used to condition the location of lower and higher permeability zones within the generated field.

The permeability distribution for the initial simulations at M Area was generated "randomly" using the average statistics of each rock unit to control the spatial correlation within the unit. This resulted in a permeability distribution similar to M Area, high and low permeability bodies approximately the same size, but randomly situated within each rock type. Average horizontal and vertical permeabilities used were 1 and 0.1 darcys for the MAZ, 0.0005 and 0.00001 darcys for the GCCZ, and 10 and 1 darcys for the LLAZ.

Figure 2. Heterogeneous permeability field used for modeling.



2.2 Multiphase Flow Simulations

Once a T2VOC mesh file has been designed and assigned permeability modifiers, a set of initial conditions for each element is generated under gravity-capillary equilibrium conditions. All elements are filled with water (assigned a gas saturation (Sg) of 0.0) and allowed to drain in a two-phase simulation until equilibrium is achieved. An infiltration rate of 6"/year (Aadland, 1995) was included in the simulations at M Area.

Waste effluent was sent to the settling basin over a period of about 27 years, from 1958 to 1985. From 1958 to 1971 trichloroethene (TCE) was the primary cleaning solvent. In 1971 tetrachloroethene (PCE) was substituted for TCE and there was a marked increase of waste solvent sent to the settling basin. The quantity of effluent sent to the settling basin sharply declined in 1977. Based on the actual yearly estimated release history, the simulated spill began with a rate of 25,000 pounds per year and continued for 12 years. The rate was increased to 100,000 pounds per year for 5 years. The last spill rate was 300,000 pounds per year for 4 years, after which no more DNAPL was released. After 21 years of simulated DNAPL release (2.0 million pounds), from 1958 to 1979, and an additional 15 years for redistribution, the NAPL phase was limited in extent, and did not reach the water table.

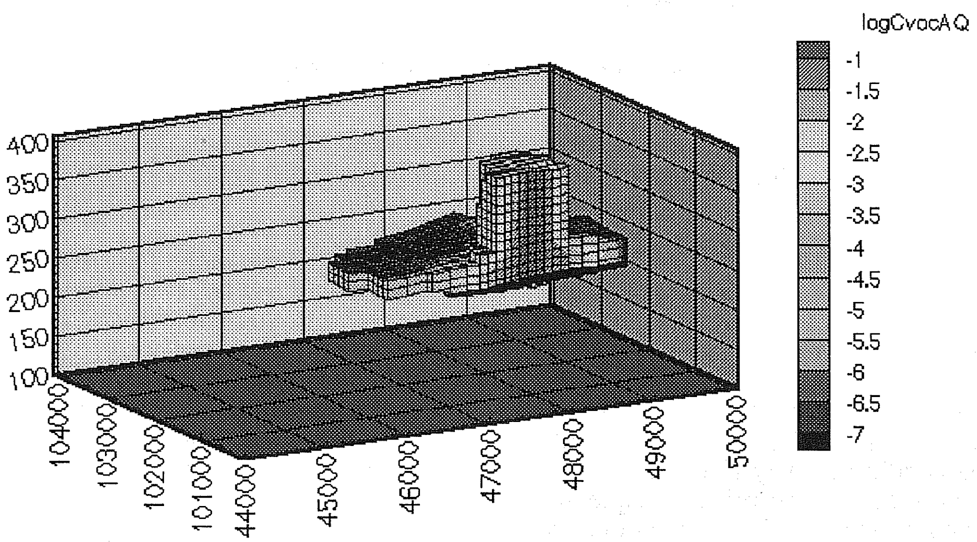
As DNAPL migrates through a thick vadose zone, significant amounts will remain as residual NAPL saturation (Snr). A normal average Snr is about 10%, depending on the relative permeability and capillary pressure of the sediments. However, since DNAPL forms preferential pathways, a 10% Snr for elements the size of the model mesh (the smallest are 100 by 100 by 12 feet) is unrealistic. Therefore, the Snr was set at 1% (possibly still too high without a much finer mesh) in the ROCKS block of the T2VOC input file. Also, the release point for DNAPL was only one 100' by 100' grid block while the settling basin is roughly 300 by 250 feet. The aquifers (MAZ and LLAZ) were given a porosity of 30% and the GCCZ was given a porosity of 40% for all simulations. A finer mesh will be needed to simulate detailed NAPL migration and special numerical techniques may be required as well. Reducing the Snr in consideration of the mesh element size is considered to be a temporary "fix" and reflects the fact that handling sub-grid block scale physics need to be addressed in future research. No conditioning points were used to preferentially locate high and low permeability zones. Therefore, the model results are only a generality, though lithologic unit elevations, spill rates, average unit permeabilities, and the static ground-water flow field were matched as closely as possible.

Modifications were made to the T2VOC code to improve the modeling of heterogeneous media. Previously, T2VOC used a single three phase capillary pressure (Pcap) function for each ROCK type with no adjustments for a heterogeneous permeability field. The Pcap for each element in a rock unit is now varied from the average Pcap function of that rock unit by the square root of the ratio of the average unit permeability to the cell permeability $(\text{avg k} / \text{cell k})^{1/2}$ providing more realistic simulations for heterogeneous media. T2VOC was also modified to write key parameters (such as pressure, NAPL saturation, concentration of NAPL in the aqueous phase) for each element to files formatted for graphical display (using the commercially available program, TECPLOT) at user specified times during a simulation and at the end of the simulation.

3.0 MODELING RESULTS

We believe that the initial model greatly under-predicts both the lateral and vertical extents of the DNAPL distribution in the M-Area. An interesting aspect of the simulation is the size of the dissolved DNAPL plume above and below the water table. The simulation suggests that high concentrations in the dissolved plume can travel relatively far from the NAPL phase by these mechanisms. Figure 3 shows the plume in 1994 (these plots have a cutoff of 1 ppm). A top view of the PCE plume for 1994 is qualitatively similar to the mapped TCE plume shown in Figure 3.

Figure 3. Simulated dissolved contaminant plume in 1994, 1 ppm cut off, cut away view [log g/l].



3.1 Ongoing Models

To begin addressing the problem of residual NAPL saturation in relatively large elements, the model volume has been re-gridded to create a finer mesh. The number of elements was increased from 780 (30 x 26) to 980 (35 x 28) per layer. The number of vertical layers was also increased, from 28 to 32. This increased the number of total elements from 21,840 to 31,360. The elements beneath the settling basin are 20 by 20 by 8, significantly smaller than the original 100 by 100 by 14 elements.

In order to more closely match the geology, the M Area Aquifer Zone is being subdivided into four lithologic units (MAZ1 through MAZ4). Additionally, 721 conditioning points are being used to condition the permeability distribution to be more representative of the true distribution at M Area. Estimated mud fractions from foot by foot core descriptions were converted to conductivities based on a function from Hydrogeologic Inc (1996). Of the 721 conditioning points, 130 are in the MAZ1, 123 in the MAZ2, 103 in the MAZ3, 184 in the MAZ4, 88 in the GCCZ, and 93 in the LLAZ.

5.0 REFERENCES

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