18.0 Vadose Zone Remediation, Monitoring, and Characterization

D.C. Weekes

Vadose zone monitoring using leachate and soil vapor sampling occurred at three areas in the Hanford Site in calendar year (CY) 2010. Leachate and soil vapor monitoring continued at the Environmental Restoration Disposal Facility (ERDF) and the Solid Waste Landfill. Monitoring for the ERDF is discussed in Chapter 11.0, Section 11.3.4 and for the Solid Waste Landfill in Chapter 10.0, Section 10.4.1. Soil vapor monitoring at the carbon tetrachloride expedited response action site also continued during CY 2010.

The Tank Farm Vadose Zone Project installed direct-push boreholes at the C and BY Tank Farms for subsurface characterization of unplanned releases and future geophysical surveys. The Tank Farm Vadose Zone Project also completed surface geophysical exploration at Waste Management Area (WMA) S-SX and UPR-200-E-86 to map subsurface contaminant distribution. The interim surface barrier was placed over WMA TY to reduce water infiltration into the contamination area. These monitoring and characterization efforts are summarized in this chapter.

Further interpretation of data collected at the Sisson and Lu vadose zone field injection test site in the 200 East Area from the year 2000 is presented in this chapter. The spatial and temporal evolution of the observed moisture plume at the injection site was compared with simulated plumes based on three methods: (1) upscaling, (2) cokriging/artificial neural network (ANN), and (3) transition probability (TP)/ Markov chain (MC). Upscaling uses small, core-scale measurements of hydraulic properties to model large, field-scale behavior. In summary, the upscaling method captured the overall movement pattern of the injected water in terms of the first and second moments of the observed plume at the field site, but it was not able to simulate the detailed distribution of the moisture plume. The cokriging/ANN method simulated the observed moisture plume well, but the simulated vertical movement was faster than the observed vertical movement. The TP/MC method best reproduced the media heterogeneity and the contrast existing between the coarse and fine soil horizons at the Sisson and Lu site.

18.1 Carbon Tetrachloride Soil Vapor Monitoring and Remediation

E.J. Freeman

Soil vapor extraction (SVE) is used to remove carbon tetrachloride from the vadose zone in the 200 West Area. The U.S. Environmental Protection Agency and the Washington State Department of Ecology (Ecology) authorized the U.S. Department of Energy to initiate this remediation in 1992 as a *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* (CERCLA) expedited response action. This section summarizes the CY 2010 activities associated with carbon tetrachloride removal. A report containing detailed results from CY 2010 activities will be issued in CY 2011. Historic monitoring and remediation results are documented in several reports, including the following:

- SGW-44694, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Operable Unit Carbon Tetrachloride Site, Fiscal Year 2009*
- SGW-40456, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Operable Unit Carbon Tetrachloride Site, Fiscal Year 2008*
- SGW-37111, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Operable Unit Carbon Tetrachloride Site, Fiscal Year 2007*
- SGW-33746, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Operable Unit Carbon Tetrachloride Site, Fiscal Year 2006*
- WMP-30426, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Carbon Tetrachloride Site, Fiscal Year 2005*
- WMP-26178, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Carbon Tetrachloride Site, Fiscal Year 2004*
- WMP-21327, *Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Carbon Tetrachloride Site, Fiscal Year 2003*
- WMP-17869*, Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Carbon Tetrachloride Site, Fiscal Year 2002*
- BHI-00720, *Performance Evaluation Report for Soil Vapor Extraction Operations at the Carbon Tetrachloride Site, February 1992-September 2001*.

In CY 2010, two SVE systems were operating to remove carbon tetrachloride from the vadose zone. Each of the systems has an extraction capacity of 14.2 cubic meters per minute. Figure 18-1 shows the locations of the SVE wells.

One SVE system was operated at the 216-Z-1A well field and one system was operated at the 216-Z-9 well field. Each system was operated from March 1 through November 1, 2010. Temporarily suspending SVE operations at each well field during the winter allows carbon tetrachloride concentrations to recharge and be extracted more efficiently and economically when operations resume. Cyclic operation of the SVE system was implemented based on the *Rebound Study Report for the Carbon Tetrachloride Soil Vapor Extraction Site, Fiscal Year 1997* (BHI-01105). Section 18.1.1 discusses the results of the CY 2010 SVE in more detail.

Approximately 79,751 kilograms of carbon tetrachloride have been removed since extraction operations started in 1991. The mass of carbon tetrachloride removed in CY 2010 was 194 kilograms.

To track the effectiveness of the remediation effort, soil vapor concentrations of carbon tetrachloride were monitored at the inlets to the SVE systems and at individual online extraction wells during the 8-month operating period. To assess the impact of the SVE system on subsurface concentrations, soil vapor concentrations of carbon tetrachloride were monitored at offline wells and probes during the entire CY (Section 18.1.2). Remediation efforts during CY 2010 also included passive SVE (Section 18.1.3).

18.1.1 Soil Vapor Extraction

During CY 2010, SVE operations continued from March 1, 2010, through November 1, 2010, using two, 14.2 cubic meter per minute SVE systems. One system operated at the 216-Z-1A/216-Z-12/216-Z-18 well field and one system operated at the 216-Z-9 well field.

For the system at the 216-Z-1A well field, initial online wells were selected within the perimeter of the 216-Z-1A Tile Field. For the system at the 216-Z-9

well field, initial online wells were selected near the 216-Z-9 Trench. As extraction continued at both locations, additional wells in the vicinity of these two waste sites were brought online. Extraction wells open near the less-permeable Cold Creek unit (CCU), where the highest carbon tetrachloride concentrations have been detected consistently in the past, were selected at both locations to optimize mass removal of the contaminant. Extraction wells open near the groundwater were also selected for SVE or passive SVE (Section 18.1.3).

As of November 2010, ~79,751 kilograms of carbon tetrachloride had been removed from the vadose zone since extraction operations started with the pilot test in 1991 (Table 18-1). The mass of carbon tetrachloride removed in CY 2010 was 194 kilograms. The most recent performance evaluation report (SGW-44694) provides the amount of carbon tetrachloride removed per year between 1991 and 2009.

18.1.2 Monitoring of Offline Wells and Probes

During CY 2010, soil vapor concentrations of carbon tetrachloride were monitored near the ground surface, near the CCU (~40 meters below ground surface [bgs]), and near groundwater (~66 meters bgs). Soil vapor concentrations were monitored near the ground surface and groundwater to evaluate if nonoperation of the SVE system negatively affects the soil atmosphere or groundwater. The maximum concentration detected near the ground surface (between 2 and 10 meters bgs) was 5.5 parts per million by volume (ppmv). Near the groundwater (between 53 and 66 meters bgs), the maximum concentration was 12 ppmv.

Soil vapor concentrations were also monitored above and within the CCU to provide an indication of concentrations that could be expected during restart of the SVE system. The maximum concentration detected near the CCU (between 25 and 44 meters bgs) was 229 ppmv in soil vapor probe CPT-28 (27 meters bgs), ~90 meters south of the 216-Z-9 Trench. This location may be beyond the zone of influence of the SVE system. Within the 216-Z-9 well field, the maximum carbon tetrachloride concentration detected near the CCU was 6 ppmv at well 299-W15-8U (35 meters bgs). At the 216-Z-1A well field, the maximum carbon tetrachloride concentration detected near the CCU was 70 ppmv at wells 299-W18-165 and 299-W18-167 (both about 32 meters bgs).

The maximum carbon tetrachloride concentration detected in the vadose zone overlying the CCU (between 11 and 23 meters bgs) was 68 ppmv at well CPT-21A (20 meters bgs) near the 216-Z-9 Trench.

18.1.3 Passive Soil Vapor Extraction

Passive SVE is a remediation technology that uses naturally induced pressure gradients between the subsurface and the ground surface to drive soil vapor to the surface. In general, falling atmospheric pressure causes subsurface vapor to move to the atmosphere through wells, whereas rising atmospheric pressure causes atmospheric air to move into the subsurface. Passive SVE systems are designed to use this phenomenon to remove carbon tetrachloride from the vadose zone.

Passive SVE systems were installed at the end of FY 1999 at eight wells open near the vadose/groundwater interface at the 216-Z-1A/216-Z-12/216-Z-18 well field. The passive systems have check valves that allow only soil vapor flow out of the borehole (i.e., one-way movement) and canisters holding granular activated carbon that adsorbs carbon tetrachloride upstream of the check valves before the soil vapor is vented to the atmosphere. The check valve prohibits flow of atmospheric air into the borehole during a reverse barometric pressure gradient, which tends to dilute and spread carbon tetrachloride vapors in the subsurface.

The wells are sampled periodically upstream of the granular activated carbon canisters. During CY 2010, the maximum carbon tetrachloride concentrations ranged from 12 to 15 ppmv at the three wells (299-W18-6, 299-W18-7, and 299-W18-246) near the 216-Z-1A Tile Field. The maximum carbon tetrachloride concentrations ranged from 9 to 11 ppmv at the four wells (299-W18-10, 299-W18-11, 299-W18-12, and 299-W18-247) near the 216-Z-18 Crib.

18.2 Tank Farm Vadose Zone Activities

D.A. Myers, C.L. Tabor, H.A. Sydnor, J.G. Field, and D.L. Parker

The Vadose Zone Integration Program is responsible for implementing the Tank Farm *Resource Conservation and Recovery Act of 1976* (RCRA) corrective action program through field characterization, laboratory analyses, technical analyses, risk assessment for past tank leaks, and installation of interim measures to reduce the threat from contaminants until permanent solutions can be found. In CY 2010, several direct-push boreholes were installed for soil sampling and geophysical logging in the C and BY Tank Farms (Section 18.2.1). Section 18.2.2 discusses three-dimensional applications of surface geophysical exploration of the northeast corner of the SX Tank Farm and southeast corner of the S Tank Farm (RPP-RPT-47851, *Three-Dimensional Surface Geophysical Exploration of S/SX Tank Farm*) and at UPR-200-E-86 adjacent to the C Tank Farm, and a well-to-well resistivity survey of WMA A-AX. Section 18.2.3 briefly describes geophysical logging. Section 18.2.4 describes the interim surface barrier work associated with the TY, BY and SX Tank Farms to reduce the infiltration of precipitation.

18.2.1 Direct-Push Boreholes and Sampling

The hydraulic hammer unit was deployed in three tank farms during the report period to evaluate subsurface contamination in the vadose zone. The hydraulic hammer unit was deployed in the C Tank Farm to support Phase 2 of the facility investigation. The hydraulic hammer unit was deployed in the S Tank Farm to assess the extent of contamination to support a proposed interim barrier. The sites were identified from previous investigations of subsurface resistivity (RPP-RPT-42513, *Surface Geophysical Exploration of the SX Tank Farm at the Hanford Site*). The hydraulic hammer unit was deployed at the BY Tank Farm to support a proposed interim barrier over that facility. The BY Tank Farm sites investigated were previously identified using historical release information and electrical resistivity (RPP-34690, *Surface Geophysical Exploration of B, BX, and BY Tank Farms at the Hanford Site)*.

Sample horizons were selected and agreed upon using borehole logs of gamma and moisture content. A multi-level sampler was then used at the sites to collect samples at the selected horizons for laboratory analysis. During CY 2010, installation of multiple-depth electrode strings was performed at the S, C, and BY Tank Farms. Electrodes were placed in every direct-push logging hole as the holes were decommissioned. These electrodes will be used during a future deployment of surface geophysical exploration in the tank farms. The analytical results will be used to support placement of proposed interim barriers for the BY and S Tank Farms, as necessary, and for the Phase 2 (tank farm closure) investigation of C Tank Farm. A total of 24 samples from seven boreholes were collected in the BY Tank Farm, 65 samples from seven boreholes in the C Tank Farm, and 16 samples from five boreholes in the S Tank Farm.

18.2.2 Surface Geophysical Exploration

A fully three-dimensional application of surface geophysical exploration, which is a combination of surface deployed geophysical techniques, was applied over a portion of the northeast corner of the SX Tank Farm and the southeast corner of the S Tank Farm (RPP-RPT-47851) during the report period. The primary tool applied through surface geophysical exploration is pole-pole electrical resistivity; other tools applied during CY 2010 included ground-penetrating radar. Ground-penetrating radar was used to help define locations where the direct-push sampling holes could be safely advanced. The depth to which the resistivity measurements interrogate the subsurface is determined by the distance between electrode pairs (i.e., the further apart, the deeper the interrogation). Because resistivity is an indirect measure of several subsurface phenomena (e.g., moisture distribution, saline contaminants, and soil texture), the more separated the electrode pairs, the lower the resolution of the analysis. The resistivity data are mathematically analyzed through a process known as inversion to provide a best estimate of the distribution of resistivity anomalies. Surface geophysical exploration provides a means of extrapolating direct measurements taken by sampling, logging, or other means to provide a cost-effective overview of large areas that may have been impacted by a variety of waste management practices.

Work during CY 2010 in the S and SX Tank Farms was performed to further define anomalous features reported last year in RPP-RPT-42513. In addition, this year's survey was used to assess a variety of installation configurations for deep electrodes. The lessons learned from this assessment are being applied to ongoing surface geophysical exploration applications. Sampling of the anomalous regions showed that the anomaly was likely due to increased soil moisture; no increased levels of contamination were discovered during the sampling effort.

A fully three-dimensional surface geophysical exploration survey, including buried electrodes, was completed over UPR-200-E-86 during the reporting period. The survey covered an unplanned release site associated with a pipeline leak (RPP-RPT-41236, *Surface Geophysical Exploration of UPR 200-E-86 Near the C Tank Farm*). During this survey, 301 surface electrodes were placed over the area of the known release, including 5 electrodes placed in five direct-push holes; the entire array was then interrogated both forward and reciprocally. The results of this survey are depicted in Figure 18-2, which is an isometric view of the interpreted results. No large regions of anomalous resistivity signatures were identified; neither had significant contamination been found in the direct push derived samples from this region. This leads to a possible conclusion that the known release at this site had a much smaller volume than originally estimated.

A well-to-well resistivity survey was completed in the A and AX Tank Farms (RPP-RPT-46613, *Surface Geophysical Exploration of the A and AX Tank Farms*). The results of this application of surface geophysical exploration (Figure 18-3) generally conform to regions of previously identified releases. However, an additional anomaly to the north and east of the AX Tank Farm is indicated (this region extends beyond the bounds of the AX Tank Farm well-to-well survey). A possible reason for this anomaly is the 216-A-39 Crib.

18.2.3 Geophysical Logging

Geophysical neutron moisture logging was completed for twenty drywells in the TY Tank Farm to support interim surface barrier monitoring. Spectral gamma logging of these wells is planned for CY 2011. Spectral gamma logging was completed for 26 drywells, and neutron logging began in support of RCRA facility investigation/

corrective measures study characterization in the C Tank Farm. Additionally, in response to Ecology's concerns regarding gamma logging data, eight drywells (20-07-02 in the B Tank Farm; 21-01-01 and 21-06-05 in BX Tank Farm; 22-07-09 and 22-09-08 in the BY Tank Farm; 30-01-09 and 30-08-02 in the C Tank Farm; and 41-07-08 in the SX Tank Farm) were logged using the high-rate logging system. The CY 2010 high-rate logging system determined that cesium-137 concentrations were within a factor of three compared to previous logging results, which is well within the margin of error for the previous results and indicates little or no change in the cesium-137 distribution.

18.2.4 Interim Barriers

The *T Farm Interim Surface Barrier Demonstration: Vadose Zone FY 09 Monitoring Report* (PNNL-19123), issued January 2010, concluded that results of neutron probe, capacitance probe, and heat dissipation unit monitoring showed that the T Tank Farm interim surface barrier performed as expected. The barrier prevented meteoric water from infiltrating into the soil, resulting in the soil becoming gradually drier. The barrier also affected the soil below the barrier edge but at a reduced magnitude. Based on T Tank Farm interim surface barrier monitoring and modeling results to date, additional interim surface barriers were recommended as interim measures to slow water flux in other locations and to reduce the rate of contaminant movement toward the groundwater prior to a final remedy (RPP-RPT-47123, *Interim Surface Barrier Evaluation Report*).

During CY 2010, an interim surface barrier was constructed over the TY Tank Farm (Figure 18-4). This project altered the surface of the farm to direct runoff and placed a modified asphalt cover over all six tanks. Runoff is directed to a lined evapotranspiration basin west of the tank farm, where the water then re-enters the atmosphere. This barrier covers approximately 7,500 square meters and consists of engineered fill to create a 0.8% slope, covered by approximately 0.1 meter of modified asphalt. Monitoring of this configuration is underway to assess its performance. The evapotranspiration basin is approximately 2 meters deep and was backfilled to a depth of ~1 meter; the area of the basin is ~6,650 square meters.

The first of two interim surface barriers and an evapotranspiration basin are being designed for the SX Tank Farm to meet *Hanford Federal Facility Agreement and Consent Order* (Tri-Party Agreement) (Ecology et al., 1989) Milestone M-045-92. The first interim barrier at the SX Tank Farm, referred to as the SX south barrier, will cover the southernmost six tanks in the tank farm. The evapotranspiration basin will be located to the south of the tank farm in an existing excavation. The design for the SX Tank Farm barriers is based, in large part, on lessons learned from construction of T and TY Tank Farm barriers and will be very similar to the barrier system installed at the TY Tank Farm.

Site characterization activities are underway at the BY Tank Farm to evaluate the appropriateness of interim surface barriers over this facility. The western portion of the tank farm has been sampled as noted above and a resistivity survey has been conducted. Drilling and sampling is continuing, and a resistivity survey is planned for mid-CY 2011.

18.3 Comparison of Three Methods for Characterizing Heterogeneous Hanford Sediments

R. Khaleel

Hanford sediments are inherently heterogeneous at a variety of scales. An accurate simulation of flow and contaminant transport in heterogeneous media is often hampered by the difficulty in characterizing media heterogeneity and the variability of sediment layering structure. The difficulty partly arises due to a lack of site characterization data. In situations where data are available, the data are typically obtained from widely spaced boreholes. While the borehole data can often provide relatively adequate information of heterogeneity in the vertical direction, the data cannot provide sufficient information of heterogeneity in the lateral direction. Thus, interpolating information between boreholes is needed to characterize the lateral heterogeneity.

In order to resolve the problem of sparse characterization data, the use of multiple types of "hard" and "soft" data has often been suggested ("Heterogeneity in Sedimentary Deposits, a Review of Structure-Imitating, Process-Imitating, and Descriptive Approaches" [Koltermann and Gorelick, 1996]). Hard and soft data are, respectively, direct and indirect measurements of sediment properties. For vadose zone modeling, hard data include, for example, soil hydraulic properties and, in particular, soil moisture retention and unsaturated hydraulic conductivity measurements. Due to limits in measurement techniques, time, and/or budget, moisture retention and unsaturated hydraulic conductivity measurements are usually sparse. By contrast, it is generally easier to obtain data that contain indirect information about spatial structure and heterogeneity of the parameters. Such data may include soil moisture content, bulk density, sediment textural data, geophysical data, and other quantitative or qualitative information about a site of interest. Various inverse and forward methods have been developed to combine data of multiple types and thereby improve predictions of moisture flow in heterogeneous unsaturated media.

During CY 2010, work was completed on comparing three different methods for modeling moisture flow for the heterogeneous Hanford formation. The following discussion provides a summary of the results for application of the three methods. The methods are evaluated by comparing the simulated and observed moisture content profiles for a vadose zone field injection experiment at the Sisson and Lu site, located in the 200 East Area south of the Plutonium-Uranium Extraction Plant. This is the same field injection experiment site considered in the *Hanford Site Groundwater Monitoring and Performance Report for 2009: Volumes 1 & 2* (DOE/RL-2010-11).

18.3.1 Field Injection Experiment

The field injection site was specifically designed by Sisson and Lu (RHO-ST-46P, *Field Calibration of Computer Models for Application to Buried Liquid Discharges: A Status Report*) to understand moisture movement underneath buried discharges such as tank leaks. The Sisson and Lu site was used for a field infiltration experiment from June to July 2000 (PNNL-13679, *Vadose Zone Transport Field Study: Status Report*; PNNL-13795, *Vadose Zone Transport Field Study: Soil Water Content Distributions by Neutron Moderation*). Initial moisture content distribution was measured on May 5, 2000, at the 32 radially and symmetrically arranged cased boreholes (Figure 18-5). Injections began on June 1 (the 153rd day of the year), and

4,000 liters of water were metered into an injection point 5 meters below the land surface over a period of 6 hours. Similarly, 4,000 liters of water were injected in each subsequent injection on June 8, June 15, June 22, and June 28. During the injection period, neutron logging in 32 wells took place within a day (i.e., June 2, June 9, June 16, and June 23) following each of the first four injections. A wildfire near the field site prevented immediate logging of the moisture content (θ) distribution for the fifth injection on June 28. Three additional readings of the 32 wells were subsequently completed on July 7, July 17, and July 31. During each neutron-logging event, moisture content was recorded in each well at a depth interval of 0.3048 meters, starting from a depth of 3.9625 meters and continuing to a depth of 16.764 meters, resulting in a total of 1,376 measurements in each of the eight observation days over a 2-month period.

18.3.1.1 Upscaling Method

The upscaling method uses snapshots of the observed moisture content plume under transient flow conditions to derive a three-dimensional effective unsaturated hydraulic conductivity (K) tensor. The methodology uses the temporal evolution of spatial moments of observed moisture content (θ) plumes. Thus, unlike stochastic methods which rely on the spatial statistics of small-scale hydraulic properties, this method derives directly the effective properties using observed responses, specifically, the spatial and temporal changes in θ within the vadose zone. Additional details are provided in "Estimation of Effective Unsaturated Hydraulic Conductivity Tensor Using Spatial Moments of Observed Moisture Plume" (Yeh et al., 2005), which are briefly outlined below:

- The method estimates the upscaled unsaturated hydraulic conductivity based on spatial moments of the initial moisture content measurements.
- Unsaturated hydraulic conductivity in the vertical direction (K_z) is first estimated using the first-order moment in the z direction.
- The lateral to vertical unsaturated hydraulic conductivity ratios (K_x/K_z and K_y/K_z) are estimated next using the second-order moments in the respective x and y directions.

Numerical results based on the upscaling method are compared with laboratory-measured unsaturated media properties at the site (WHC-EP-0883, *Variability and Scaling of Hydraulic Properties for 200 Area Soils, Hanford Site*; "Evaluation of van Genuchten-Mualem Relationships to Estimate Unsaturated Conductivity at Low Water Contents" [Khaleel et al., 1995]); PNNL-14284, *Laboratory Measurements of the Unsaturated Hydraulic Properties at the Vadose Zone Transport Field Study Site*). Subsequently, using the derived effective hydraulic properties, the evolution of the three-dimensional moisture plume is simulated during to the injection experiment. The results are then compared with the observed moisture plume.

18.3.1.2 Cokriging/Artificial Neural Network Method

This methodology integrates data that can be easily obtained (e.g., initial moisture content, θ_i, bulk density, and soil texture) with data on soil hydraulic properties via cokriging and ANN-based pedotransfer functions. Details on the technique are presented in "Simulation of Field Injection Experiments in Heterogeneous Unsaturated Media using Cokriging and Artificial Neural Network" (Ye et al., 2007). Briefly, the cokriging/ANN method directly estimates the heterogeneous soil hydraulic properties in two steps:

1. Cokriging is first used to estimate heterogeneous fields of pedotransfer variables (the primary variables) using the database on initial moisture content (θ_i) as the secondary variable.
2. Heterogeneous soil hydraulic parameters are estimated next using ANN, which uses the heterogeneous pedotransfer variables as inputs.

Using the cokriging/ANN-based parameter estimates, the evolution of the three-dimensional moisture plume is simulated for the Sisson and Lu site. The results are then compared with the observed moisture plume.

18.3.1.3. Transition Probability/Markov Chain Method

By applying the TP-based MC model to sediment textural classes, the TP/MC method leverages use of "soft" data for characterizing the media heterogeneity and sediment layering structure. The TP/MC method is used for characterizing media heterogeneity by describing spatial variability of the geometry of soil textural classes. Details of the TP/MC method are presented in "A Markov Chain Model for Characterizing Medium Heterogeneity and Sediment Layering Structure" (Ye and Khaleel, 2008), which can be briefly summarized as follows:

- The TP/MC method characterizes the heterogeneity of soil classes, each of which is associated with a set of soil hydraulic parameters.
- The observed initial moisture contents are transferred into soil classes using a log score type of transform method.
- The transferred soil classes are used to estimate the Markov chain model and conditioning data for generating heterogeneous soil classes.

The TP/MC method is evaluated by simulating the moisture movement at the Sisson and Lu site, where the stratigraphy consists of imperfectly stratified layers.

18.3.2 Comparison of Observed and Simulated Moisture Plume

The spatial and temporal evolution of the observed moisture plume at the Sisson and Lu injection site was compared with simulated plumes based on the three methods: (1) upscaling, (2) cokriging/ANN, and (3) TP/MC. The comparison results are presented only for July 31, 2000 (Figure 18-6, panels [a] through [d]).

As is typically the case, soil hydraulic parameter measurements are sparse at the site; sixty measurements are from boreholes S-1, S-2, and S-3 (see Figure 18-5 for borehole locations) (PNNL-14284) and seventeen measurements are from boreholes A-7, E-1, and E-7 (WHC-EP-0883). An extensive data set exists, however, for initial water content, θ_i, which carry signature about site heterogeneity, particularly, the sediment layering structure. The θ_i observations are distributed uniformly over the site and are used as a surrogate for describing the site heterogeneity. All three methods use the observed initial moisture content as secondary information for characterizing heterogeneity of soil hydraulic parameters.

The effective hydraulic conductivities, based on the upscaling approach, compared well (not shown here) with the laboratory-measured conductivities for core samples (Yeh et al., 2005). Furthermore, spatial moments of the simulated plume based on the effective hydraulic conductivities were in good agreement with those for the observed plume. The upscaling method not only provided a new way to estimate effective K but also allowed the previously developed moisture-dependent anisotropy concept to be quantitatively evaluated (Yeh et al., 2005). The overall good agreement of conductivities derived from laboratory measurements and the good comparison

between the numerically simulated plume and the observed plume demonstrate that moisture-dependent anisotropy is a valid, reproducible phenomenon in the field. The macroscopic anisotropy does indeed vary with decreasing moisture content of the unsaturated medium. For the Sisson and Lu field site, the effective hydraulic properties of an equivalent homogeneous medium can yield a similar temporal evolution of spatial moment of the observed moisture plume. The simulated moisture plume, based on the effective hydraulic conductivities of an equivalent homogeneous medium, however, does not necessarily resemble the observed distribution (Figure 18-6[b]). Nonetheless, in spite of the inherent limitation of the effective property approach, the upscaling method is a useful, practical tool for estimating effective unsaturated hydraulic conductivities based on snapshots of moisture movement in a large-scale vadose zone.

For the cokriging/ANN method, the overall shape and local variation of the observed moisture plumes were simulated well (Figure 18-6[c]) when compared to the upscaling method. In particular, the effects of imperfectly stratified layering structure on moisture movement were captured well. At the Sisson and Lu site, the injected water spreads in the top layer of fine material at an elevation of ~9 meters; the vertical movement of the injected water is retarded by the bottom layer of fine material at an elevation of ~5 meters. Between these two layers of fine materials is a layer of coarse material where the plume splits. Such a separation of the plume beneath the top layer of fine material, as well as the observed eastward movement of the injected water above the bottom layer of fine material, was well represented in the simulation (Figure 18-6[c]). Unlike in cokriging/ANN, the upscaling method conceptualized the heterogeneous medium at the Sisson and Lu site as an equivalent homogeneous medium. Thus, the upscaling numerical simulations essentially captured the ensemble mean behavior and did not capture the highly variable, single realization behavior of the observed moisture plume and its splitting within the coarse-textured layer that is between two fine-textured layers. Nonetheless, while the cokriging/ANN method simulated the split in the moisture plume well, the simulated vertical movement was faster than the observed vertical movement (Ye et al., 2007).

Among the three methods, the TP/MC method provided a superior match of the observed plume behavior (Figure 18-6[d]). An evaluation of the root-mean-squared error and correlation coefficient suggested that the overall pattern of the moisture movement and the spatial variability of observed moisture content are captured better by the TP/MC method (Ye and Khaleel, 2008). The heterogeneous geometry of soil classes generated by the TP/MC method is the cornerstone of successful simulation of the injection experiments at the Sisson and Lu site. The θ_i measurements, when transitioned into soil classes, were indispensable for depicting the sediment layering structure prevalent at the site. Multiple conditional realizations of the soil classes were generated to represent uncertainty in characterizing geometry of the soil classes (Ye and Khaleel, 2008). A Monte Carlo simulation showed that the simulated mean moisture contents were in agreement with corresponding field observations, whose spatial variability was sufficiently captured by the 95% confidence intervals calculated from the Monte Carlo simulations. This was achieved by treating soil hydraulic parameters of each soil class deterministically and estimating them from core samples. The TP/MC method adequately simulated the observed flow patterns, including the splitting of the moisture plume in the coarse layer which is between the two fine layers, the southeastward movement of the plume, and the near-zero fluid flux below the bottom fine layer (Ye and Khaleel, 2008).

In summary, the upscaling method captured the overall movement pattern of the injected water in terms of the first and second moments of the observed plume at the Sisson and Lu site but was not able to simulate the detailed distribution of the moisture plume. The cokriging/ANN method simulated well the observed moisture plume, but the simulated vertical movement was faster than the observed vertical movement. The TP/MC method reproduced best the media heterogeneity and the contrast existing between the coarse and fine soil horizons at the Sisson and Lu site. The TP/MC method used the soft data in the most direct way and yielded a superior comparison of observed and simulated moisture movement. Spatial variability of the observed moisture contents was well simulated by considering uncertainty in the soil class geometry. This suggests that uncertainty in geometry of soil classes is more important than uncertainty of the soil hydraulic parameters. In other words, if soil types and their textural distribution are important aspects for an accurate simulation of unsaturated flow, additional focus should be placed on collecting such data.

Table 18-1. Carbon Tetrachloride Inventory Removed by Vapor Extraction from Primary Disposal Sites

Well Field	Mass Removed Using SVE, March 2010 to November 2010 (kg)	Mass Removed Using SVE, 1991 to November 2010 (kg)
216-Z-1A	93*	24,938*
216-Z-18		
216-Z-9	101	54,812
Totals	**194***	**79,751***

* Total due to rounding.

Figure 18-1. Locations of Carbon Tetrachloride Soil Vapor Extraction Wells at 216-Z-1A/216-Z-12/216-Z-18 and 216-Z-9 Well Fields

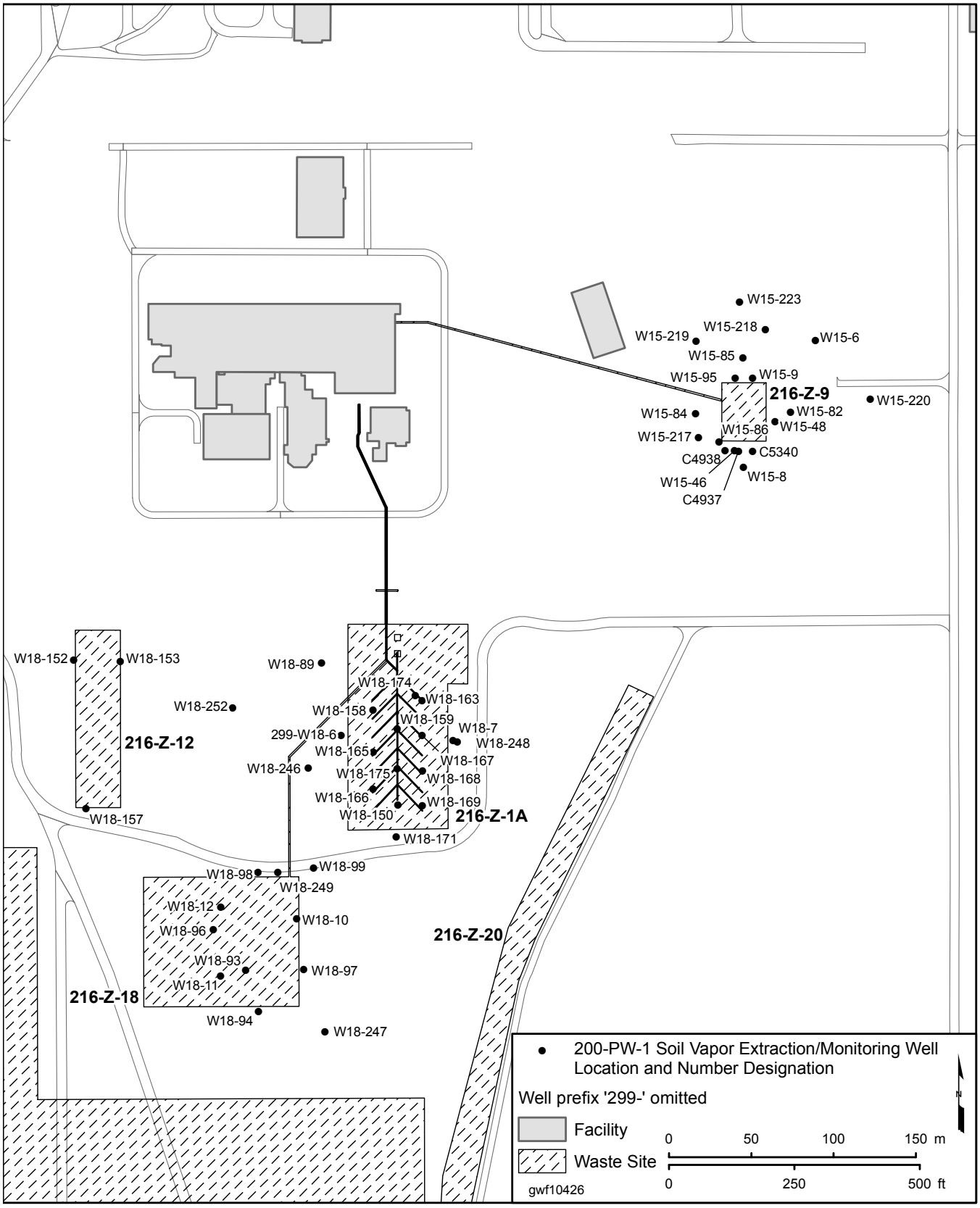


Figure 18-2. Results of Three-Dimensional Resistivity Survey of UPR-200-E-86

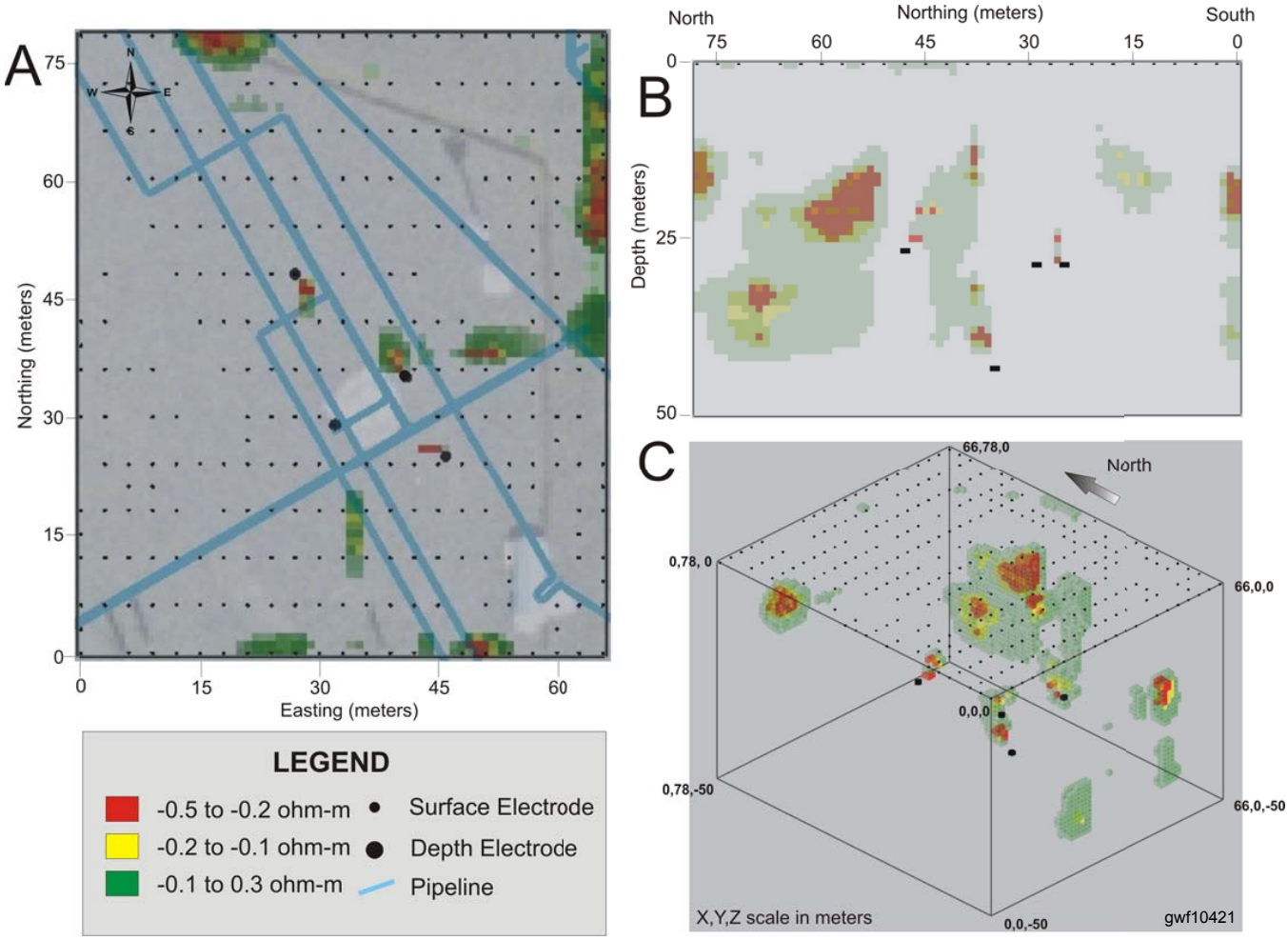
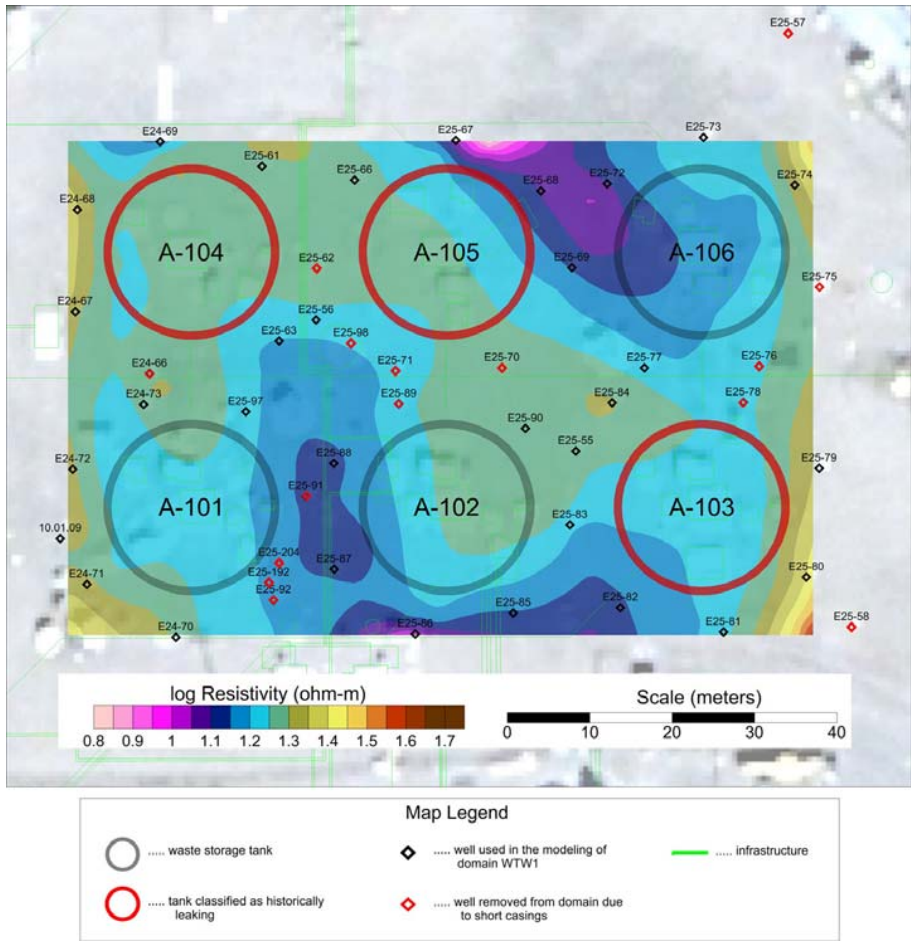


Figure 18-3. Results of Well-to-Well Resistivity Survey of Waste Management Area A-AX



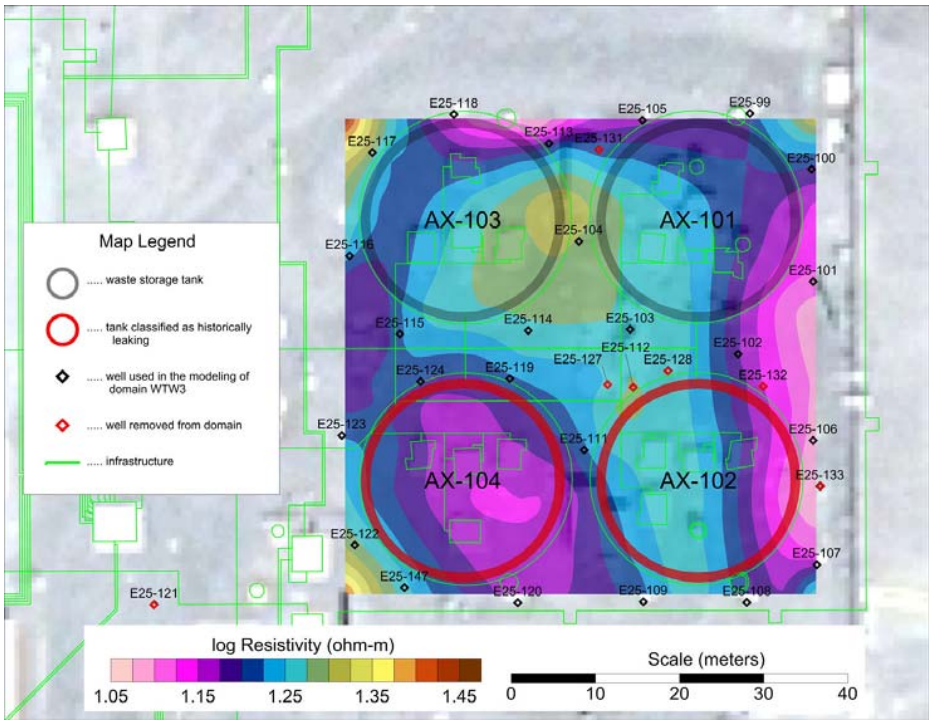


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Figure 18-4. Aerial Photograph of Interim Surface Barrier and Evapotranspiration Basin, TY Tank Farm

Figure 18-5. Plan View of the Sisson and Lu Injection Site and the Well Numbering Scheme

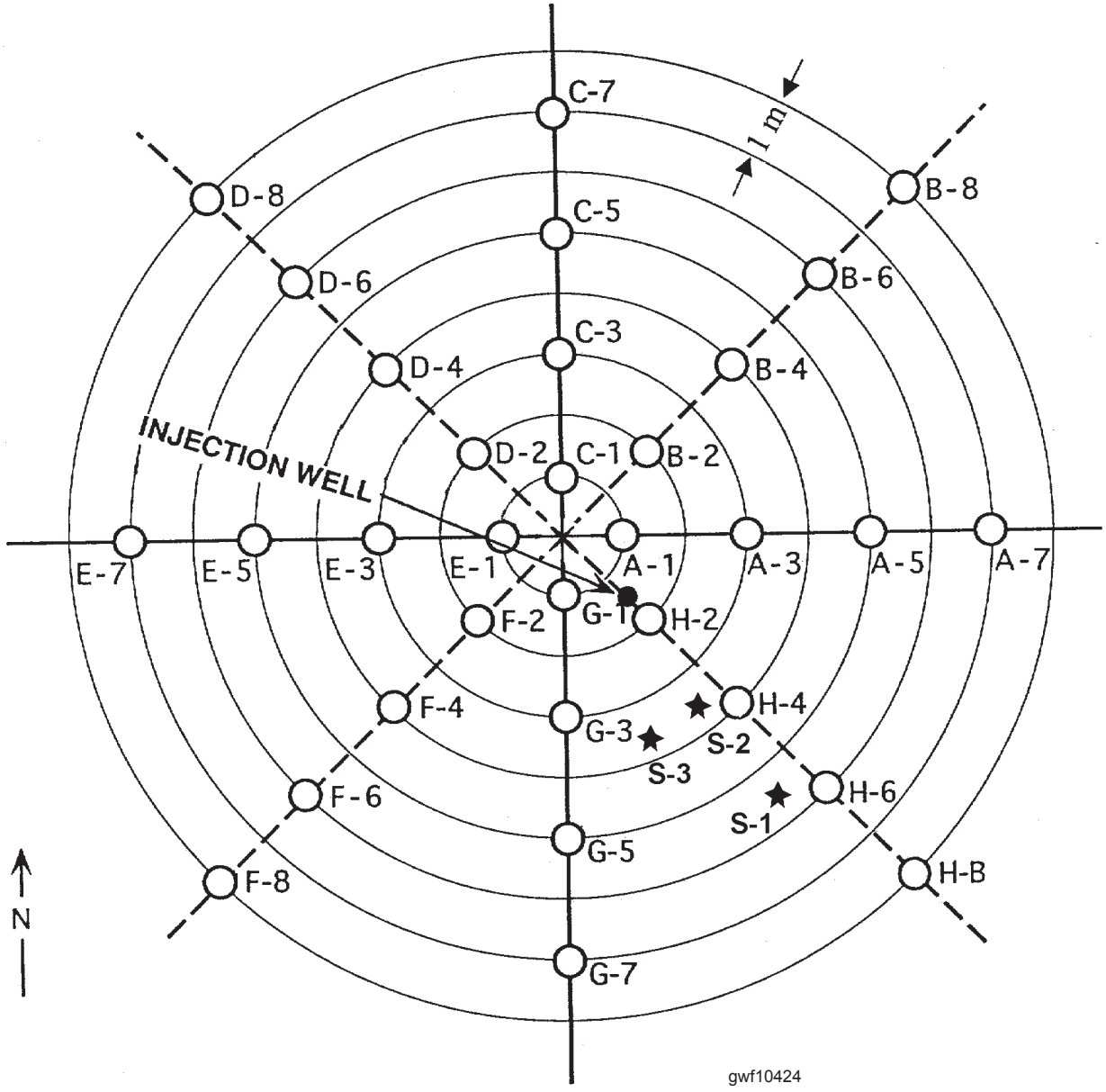
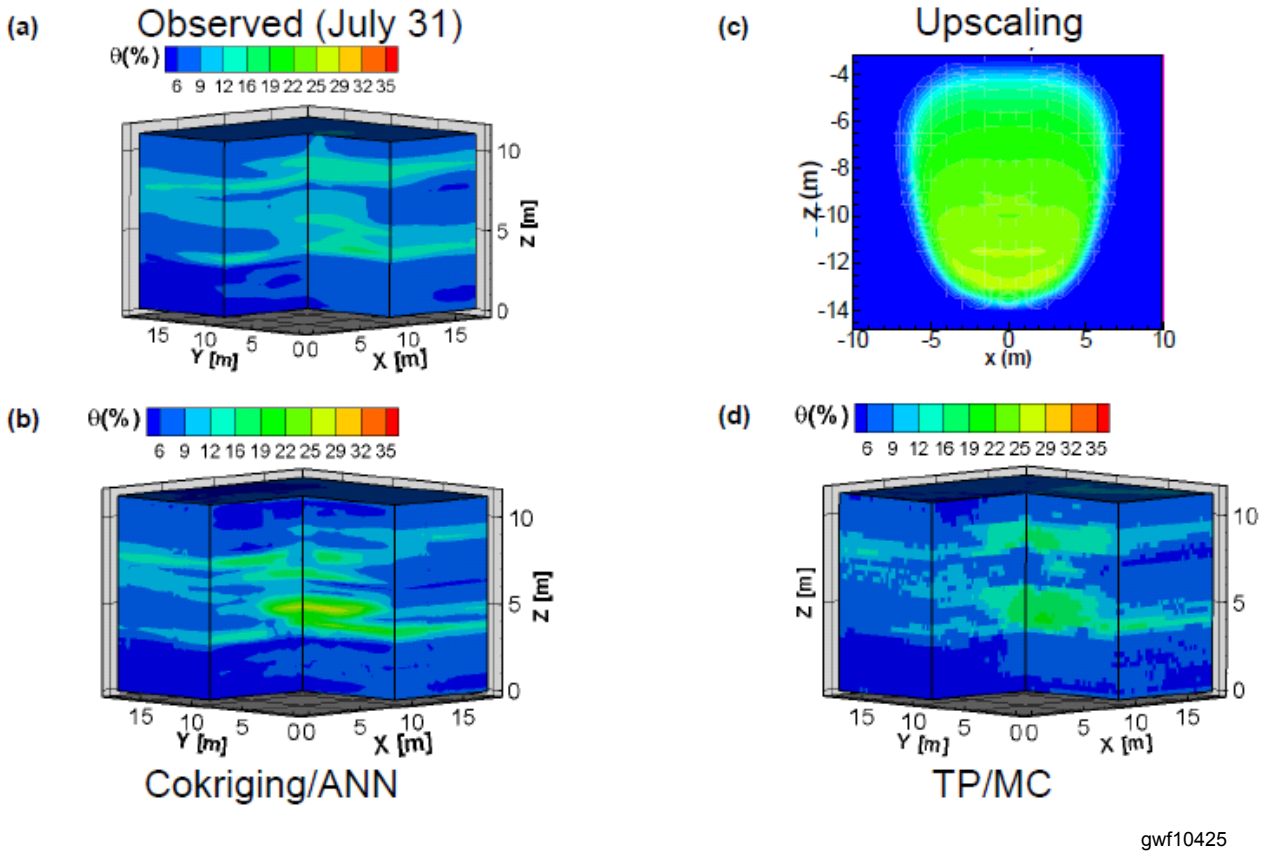
Figure 18-6. (a) Observed Moisture Plume at the Sisson and Lu Injection Site on July 31, 2000; (b) Upscaling Method Based Simulated Moisture Plume at the Sisson and Lu Field Injection Site on July 31, 2000; (c) Cokriging/Artificial Neural Network (ANN) Method Based Simulated Moisture Plume at the Sisson and Lu Field Injection Site on July 31, 2000; and (d) Transition Probability (TP)/Markov Chain (MC) Method Based Simulated Moisture Plume at the Sisson and Lu Field Injection Site on July 31, 2000