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Simulation of Soil Vapor Extraction at Building 518 Lawrence Livermore National Laboratory Livermore Site

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Summary

Computer modeling was used to evaluate the feasibility and guide the design of a soil vapor extraction (SVE) system near Building 518 at Lawrence Livermore National Laboratory's Livermore Site. A SVE system was proposed to remediate unsaturated soil containing volatile organic compounds (VOCs), primarily trichloroethylene (TCE).

To solve the problem of active fluid and gas flow under unsaturated and saturated conditions, a numerical multiphase, multicomponent computer code, NUFT (Nonisothermal Unsaturated-Saturated Flow and Transport) was used. NUFT is capable of simulating the non-isothermal flow and transport of multiple phases and contaminants in three-dimensions using an integrated finite-difference discretization with cartesian or cylindrical coordinates. The code is a valuable tool to guide the design of remediation systems that apply technologies such as SVE, air sparging, steam injection, and ground water pump-and-treat.

The main objectives of the conceptual model calibrations and simulations at Building 518 were to forecast potential impacts of TCE in soil on the underlying ground water as a result of migration processes, which are usually dominated by gaseous diffusion in the natural state, and to estimate the efficiency and long-term performance of the proposed single-well SVE system under heterogeneous site conditions. Site-specific soil cleanup goals were developed based on the modeling results.

The model results showed that incremental TCE concentrations in ground water are likely to drop below the Maximum Contaminant Level of 5 parts per billion after approximately five to six years of continuous SVE. Maximum soil VOC concentrations after five years of continuous SVE were estimated to be in the range of 0.02 to 0.03 parts per million. The proposed single-well SVE system was predicted to effectively remove the bulk of the VOCs located at shallow depths. However, due to the heterogeneous nature of the alluvial sediments at Building 518, VOCs located at greater depths near the water table are likely to be removed at a much slower rate.

The modeling results stressed the importance of including soil heterogeneities in the analysis. Rapid mass removal rates proved to be strongly correlated with high air flow velocities and flushing rates, which are generally associated with high-permeability soil strata. While field measurements of the pressure gradient are commonly used to estimate the zone of influence of a SVE system, modeling of flow velocities provides a unique tool to evaluate channeling effects and better predict system efficiency under heterogeneous site conditions.

1. Introduction

Analyses conducted in 1990 indicated that volatile organic compounds (VOCs) in unsaturated soil beneath the Building 518 Area at Lawrence Livermore National Laboratory (LLNL) Livermore Site (Figs. 1 through 3), if left unremediated, may result in VOCs migrating to ground water in concentrations above Maximum Contaminant Levels (MCLs) (Isherwood et al., 1990). To mitigate the effects of this potential source of VOCs on ground water, a soil vapor extraction (SVE) system was proposed, and a two-day treatability test was performed to evaluate the feasibility of the proposed system (Berg et al., 1994). In addition to the treatability test, conceptual and mathematical modeling was conducted to evaluate the feasibility of the proposed SVE system, estimate the long-term performance of the system, evaluate the potential incremental impact of vadose zone VOCs on ground water, and to better understand vadose zone VOC migration processes at the site.

A multiphase, multicomponent flow and transport code, NUFT (Nonisothermal Unsaturated Flow and Transport) developed at LLNL (Nitao, 1995), was used to simulate and evaluate the feasibility of the proposed SVE system. The code consists of a suite of multiphase, multicomponent modules for mathematical solution of nonisothermal flow and transport in porous media. NUFT can simulate the coupled transport of heat, fluids, and chemical components, including VOCs. For this application, a single-phase, two-component, isothermal module was used to simulate vadose zone transport of trichloroethylene (TCE), the primary VOC of concern in the Building 518 subsurface.

2. Site Description

The Building 518 Area geology, hydrogeology, and VOC distribution are summarized in Berg et al. (1994), and this section. Details of the Livermore Site hydrogeology and contaminant distribution can be found in the Remedial Investigation report (Thorpe et al., 1990).

The Building 518 Area is located in the southeast corner of the Livermore Site (Fig. 2). Historically, this area was used to store drums containing solvents and hydrocarbons. It is likely that over the last 20 to 30 years, small spills and/or leaking drums were the sources of VOCs in the vadose zone in the Building 518 Area. (Thorpe et al., 1990; Dreicer, 1985).

2.1. Hydrogeology

The Building 518 Area is underlain by the Plio-Pleistocene Livermore Formation. In the Livermore Site vicinity, the Livermore Formation is subdivided into Upper and Lower members (Thorpe et al., 1990). In the Building 518 Area, the depth of investigation includes both the Upper and the top of the Lower members of the Livermore Formation. Data from 25 boreholes drilled in the Building 518 Area (Fig. 3) indicate that five of the six hydrostratigraphic units described in other areas of the Livermore Site (Berg et al., 1994) are also present in the Building 518 Area. Figure 4 is a hydrogeochemical cross section through the Building 518 Area showing interbedded alluvial sediments that range from low-permeability silty clay to high-permeability gravelly sand. The water table is about 115 ft (35 m) below ground surface (bgs). The general direction of ground water flow in this area is from northeast to southwest with an average horizontal hydraulic gradient component of about 0.012 ft/ft, and a ground water velocity of about 3 ft/y (1 m/y).

2.2. VOC Distribution

Data from soil samples in the Building 518 Area indicate that the vadose zone contains low to moderate concentrations of VOCs, primarily TCE. Although VOCs are present from 5 ft below the ground surface to the water table, the maximum VOC concentrations are found in two distinct depth intervals (Figs. 3 and 4).

- The shallower interval is located at an elevation of 580 ft (177 m) to 650 ft (198 m) above mean sea level (MSL). Maximum VOC concentrations are at elevations above 610 ft (186 m) above MSL. The highest reported total VOC concentration (6.35 parts per million [ppm]) was in a sample collected from borehole SIB-518-001 at 630 ft (192 m) above MSL (Fig. 4). TCE concentrations above 1 ppm extend about 30 ft (9.1 m) in the northwest-southeast direction and about 120 ft (36.6 m) in the northeast-southwest direction. Most of the TCE mass in vadose zone soil in the Building 518 Area is found in this shallower interval.
- A deeper interval containing elevated concentrations of TCE is found between 565 ft (172 m) above MSL and the water table at 535 ft (163 m) above MSL (Fig. 4). VOC concentrations in this zone are much lower than in the upper zone and generally do not exceed 0.1 ppm.

Both intervals of elevated TCE concentration are composed of moderate- to high-permeability sediments separated by low-permeability silt and clay. Available geological data indicate that the low-permeability sediments appear to be horizontally continuous throughout the Building 518 Area.

Ground water in the Building 518 Area contains VOCs in concentrations above MCLs. Although it is likely that most of the VOCs in ground water in this area originate from upgradient sources rather than from soil in the Building 518 Area (Thorpe et al., 1990), the potential exists for VOCs in the Building 518 Area to migrate through the vadose zone and impact ground water in the future. The purpose of the modeling described in this report is to evaluate whether a proposed vapor extraction and treatment system can prevent VOCs in the vadose zone from impacting ground water, resulting in concentrations of VOCs above MCLs.

3. Conceptual Model

Based on field observations and measurements described above, a conceptual model of subsurface conditions and contaminant migration was developed for the Building 518 Area

(Fig. 5). The conceptual model summarizes site conditions, the major contaminant transport processes, and is the basis for building a mathematical representation of the site (i.e., a mathematical model).

Because the objective of this study is to evaluate the potential *incremental* impact of vadose zone TCE in the Building 518 Area on ground water, the existing background TCE concentrations in ground water were not taken into account.

The physical processes that may result in TCE migration within the vadose zone are:

- Aqueous advection, diffusion, and dispersion (i.e., migration of TCE dissolved in soil moisture), and
- Gaseous advection, diffusion, and dispersion (i.e., migration of TCE vapor contained in soil gas).

The importance of each of these processes in affecting vadose zone VOC migration varies with soil properties (e.g., intrinsic permeability, water saturation, temperature) and environmental parameters (e.g., precipitation and remediation-induced stress from pumping). The following section describes previous work that qualitatively analyzed and ranked contaminant transport processes in the Building 518 Area.

4. Previous Work

Results of previous analytical modeling and treatability testing are summarized below.

4.1. Analytical Modeling

A preliminary analysis was performed to evaluate the potential impact of vadose zone VOCs on ground water south of Building 518 and southeast of Building 511 (Fig. 2). Analytical models were applied to evaluate the importance of several physical processes affecting VOC migration through the vadose zone. This preliminary analysis provided estimates of VOC migration and estimated future VOC concentrations in ground water (Isherwood et al., 1990).

The vadose zone characteristics beneath Building 511 are similar to those in the Building 518 Area. The vadose zone in both areas is approximately 110 ft (33.5 m) thick and consists of a heterogeneous distribution of silt, clay, sand, and some clayey to sandy gravel. However, the vadose zone beneath Building 511 has generally lower concentrations of TCE compared to the Building 518 Area. A maximum 1,2-dichloroethylene (1,2-DCE) concentration in soil of 0.98 ppm was measured at 9.8 ft (3 m) bgs in the Building 511 Area in 1989.

4.1.1. Qualitative Evaluation of Transport Processes in the Vadose Zone

In general, VOCs in the vadose zone may partition between four phases:

- A free VOC phase (free product in pore space),
- An aqueous phase (VOCs dissolved in pore water),
- A gaseous phase (VOC vapors in soil gas), and

- An adsorbed phase (VOCs adsorbed onto soil particles).

VOC migration through the vadose zone may occur by:

- Free-phase advection,
- Aqueous advection,
- Gaseous advection,
- Aqueous diffusion and dispersion, and/or
- Gaseous diffusion and dispersion.

In the 1990 qualitative analysis, each of these five transport processes was evaluated with respect to its potential importance in vadose zone VOC migration. For each process, site-specific input parameters were used to find an analytical solution to the process-specific governing transport equation.

Isherwood et al. (1990) concluded that in the dry climate of the Livermore Valley, gaseous diffusion is likely to be the dominant vadose zone VOC transport mechanism. Depending on precipitation patterns and/or infiltration from sources such as creeks and artificial surface water bodies, aqueous advection was considered to be the second most important transport mechanism. Other potential vadose zone transport processes (free-phase advection, gaseous advection, aqueous diffusion) were judged to be insignificant under the natural conditions prevailing in the Building 518 Area before remediation.

4.1.2. Preliminary Quantitative Evaluation of TCE Transport

Isherwood et al. (1990) quantified VOC transport through the vadose zone by gaseous diffusion only. TCE and 1,2-DCE were selected as representative compounds because they occur in the highest concentrations in the Building 518 Area (TCE at 6.1 ppm) and Building 511 Area (1,2-DCE at 0.98 ppm), respectively. These VOCs were probably released during spills dating back to the early 1970s (Thorpe et al., 1990).

An analytical model based on Fick's law of diffusion was applied to estimate vadose zone chemical transport solely by gaseous diffusion. The model was found to be most sensitive to the initial VOC mass distribution, degradation half-life, and intrinsic permeability. Intrinsic permeability is a function of the soil matrix and is not dependent upon the properties of the fluid. The saturated hydraulic conductivity is proportional to the intrinsic permeability and is dependent upon the density and viscosity of the fluid.

If no remediation is assumed, TCE concentrations in ground water beneath the Building 518 Area were estimated to increase by 17 parts per billion (ppb) after 55 years as a result of gaseous diffusion of TCE through the vadose zone. The predicted maximum concentration increase of 1,2-DCE in the Building 511 Area was only 0.04 ppb in ground water after 75 years.

4.1.3. Conclusions from Analytical Modeling

The qualitative analytical evaluation of vadose zone VOC transport at Buildings 518 and 511 identified gaseous diffusion as the likely dominant transport process. Given the distribution of TCE in the vadose zone in the Building 518 Area, the preliminary analyses indicated that TCE may migrate to ground water in concentrations above its 5 ppb MCL. In the Building 511 Area, qualitative analyses indicate that 1,2-DCE may also reach ground water, but in concentrations well below its 6 ppb MCL (Isherwood et al., 1990).

4.2. Treatability Test

To evaluate the applicability and effectiveness of SVE as a remediation technique, and to provide preliminary design parameters for the SVE system, a vapor extraction treatability test was conducted in the Building 518 Area from June 2 through 4, 1993. The treatability test and the test results that were used to calibrate the vadose zone model used in this study are briefly summarized below. A detailed description of the treatability test is presented in Berg et al. (1994).

Soil vapor boring SVB-518-201 (Fig. 3), completed as a soil-vapor extraction well in March 1993, was used to conduct the treatability test. This well is screened between 34 and 50 ft (10.4 and 15.2 m) bgs in silty gravel interfingered with clayey silt. The treatability test consisted of extracting vapor from SVB-518-201 and monitoring the effects in nearby piezometer SIP-518-101, located about 50 ft (15.2 m) east of the extraction well (Fig. 4). SIP-518-101 is screened from 55 to 61 ft (16.8 to 18.6 m) bgs in 1 to 2 ft (0.3 to 0.6 m) of sandy gravel that is embedded in sandy and clayey silt. The extracted vapor was treated by two granular activated carbon (GAC) canisters in series prior to atmospheric discharge.

The test was performed in two steps:

- On June 2, 1993, soil vapor was extracted from SVB-518-201 for eight hours using a relatively constant extraction rate of 100 to 130 standard cubic feet per minute (scfm).
- On June 3, 1993, soil vapor was extracted from the well for five hours, with extraction rates continually increasing from 1.9 to 86.2 scfm.

Vapor samples were collected during both tests and analyzed for TCE. The results of the treatability tests are summarized in Berg et al. (1994; Tables B-1 and B-2). Due to equipment failure, the gas extraction rate for the June 2 test was derived using the relationship between flow rate and applied vacuum measured during the June 3 test.

During the two days of vapor extraction tests, approximately 1.2 gal (14.4 lbs) of TCE were removed from the subsurface and treated by GAC. The cumulative TCE mass removed was calculated using an approximate flow rate of 100 scfm and an average vapor concentration of 400 ppm (1.6 micrograms of TCE per liter of air at 25 °C). The total volume of vapor pumped during the extraction process was approximately 144,000 ft^3 (4,080 m^3). The influence of the SVE well was measured in piezometer SIP-518-101 at a distance of 50 ft (15.2 m). The horizontal radius of influence of the remediation system was therefore estimated to be at least this distance.

5. Vadose Zone Flow and Transport Modeling

5.1. Approach and Methodology

In addition to the analytical evaluation and the treatability test described above, a multiphase flow and transport model was used to:

- Evaluate the feasibility and long-term performance of the proposed Building 518 vapor extraction system, and
- Estimate the potential incremental contribution of TCE in the Building 518 Area vadose zone to ground water.

The NUFT code (Nitao, 1996) was selected for this task because NUFT is capable of simulating water/gas flow as well as VOC transport in both the vadose zone and ground water. The code simulates all physical transport processes described in the Building 518 conceptual model (Section 3).

To represent the hydrogeological conditions at the site in a detailed but expedient manner, the simulations considered flow and transport in two dimensions. To evaluate and calibrate selected model input parameters, initial simulations were performed using the simplifying assumption of uniform and homogeneous site conditions. Heterogeneous material properties based on geostatistical interpretations of site-specific data were incorporated into the conceptual model at later stages.

The model was calibrated using field data from the treatability test (Section 4.2). Subsurface property parameters and initial values were evaluated qualitatively regarding their uncertainty and their likely impact on the simulation results. The most uncertain and most sensitive parameters (i.e., intrinsic permeability and initial TCE mass) were allowed to vary as calibration parameters as discussed in Section 5.5.1.

5.2. Model Domain and Grid

To simulate radial flow toward a single SVE well, an axisymmetrical cylindrical modeling domain was chosen. The cylindrical domain consists of a radial computational grid comprised of 14 concentric cylinders (Fig. 6). SVE well SVB-518-201 is located at the axis of the domain. The maximum domain radius of 230 ft (70 m) exceeds the horizontal influence of the SVE well observed during the treatability test. The model domain is vertically subdivided into 33 horizontal layers from the ground surface to depth of 145 ft (45 m) bgs. The water table was simulated at 115 ft (35 m) bgs, and the bottom 30 ft (10 m) of the model domain was below the water table. Grid spacing ranged from 0.49 to 62.4 ft (0.015 to 19.0 m) horizontally, and 0.098 to 9.0 ft (0.03 to 2.74 m) vertically. To allow for a stable numerical solution and limit the effects of numerical dispersion, the maximum grid resolution is adjacent to the simulated extraction well, near the water table, and in areas with high initial VOC concentrations. Grid resolution is lower below the ground water table, and decreases with horizontal distance from the simulated extraction well (Fig. 6).

Because it is not possible to simulate regional ground water movement using an axisymmetric model grid, a rectangular grid was used in subsequent simulations to evaluate the impact of residual (post-SVE) VOCs on ground water. The rectangular grid can be visualized as a two-dimensional vertical plane through the cylindrical grid aligned parallel to the regional ground water flow direction as suggested by the depiction in Figure 5. The horizontal and vertical dimensions of cylindrical and rectangular grid cells are identical, with the exception of the two central columns that represent the SVE well in the cylindrical grid. These columns were removed from the rectangular grid because the SVE well was not simulated in the post-SVE period.

5.3. Boundary and Initial Conditions

Figure 7 shows the boundary conditions assigned to the model. At the ground surface, gas pressure was set equal to standard atmospheric pressure. Because humidity and the concentration of TCE vapor in the atmosphere can be assumed to be negligible compared to the subsurface, both were specified to be zero at the top of the model domain. A specified infiltration flux of 1.33 in./y (33.8 mm/y) was assigned to the top of the model domain, which represents a net infiltration of about ten percent of the annual average precipitation in the Livermore Valley.

Specified pressures were assigned to the lateral model boundaries in the vadose zone. The initial ground water table was defined by specifying hydraulic heads at the upgradient and downgradient model boundaries. The head elevations were chosen to simulate a ground water flow velocity of approximately 3.28 ft/y (1 m/y), which represents the estimated average ground water flow velocity at the site. Initial water saturation in the vadose zone was estimated by applying the boundary conditions described above and then simulating the system until steady state was achieved.

The extraction well was simulated as a column of cells at the center of the model domain. The well screen extended from 32.8 to 49.2 ft (10 to 15 m) bgs. To simulate SVE from the well, a specified pressure equal to the applied wellhead vacuum was assigned to the cells corresponding to the well screen.

5.4. Simulation of Homogenous Site Conditions

5.4.1. Input Parameters

To test the model setup and qualitatively evaluate sensitivities to various input parameters, homogeneous site conditions were initially simulated. Average uniform material parameters equivalent to a homogenous silty sand, which is the predominant sediment type in the Building 518 Area, were used for the entire model domain. If sufficient data were available, material properties were based on site-specific field data (Table 1).

Although soil parameters used to simulate homogeneous site conditions were uniform throughout the model domain, the initial distribution of TCE mass was spatially varied and was derived from sediment samples collected from borings in the Building 518 Area. Due to suspected variations in the analytical accuracy related to sample holding times, some of the data were discarded. TCE sediment concentrations used to derive the initial TCE mass were restricted to samples that were analyzed within three days of collection, because longer holding times may affect reported concentrations (Jenkins et al., 1993). The data used for model input consisted of a total of 112 data points from 11 of a total of 18 borings. EarthVision (Dynamic Graphic, Inc.), a three-dimensional interpolation program, was used to assign an initial TCE soil concentration to each cell in the model grid. The initial distribution of TCE concentrations is shown in Figure 8.

Table 1. Initial and calibrated model parameters for homogeneous silty sand site conditions.

Parameter	Unit	Value
Intrinsic permeability (k)	m^2	1.196×10^{-11}
Soil density (ρ_s)	kg/m^3	2.65
Porosity	–	0.28
Function used for capillary pressure (pc)	Pascals	linear 5.8×10^6 at pc = 0.0 5.37×10^5 at pc = 0.388
Function used for saturated hydraulic conductivity (K_s)	m/s	Van Genuchten m=0.192, S_r=0.242, S_a=0.96
Function used for tortuosity	–	Millington S_r=0
Soil/water partition coefficient (K_d) for TCE	L/kg	0.21

Notes:

m, S_a = Van Genuchten parameters.
S_r = Residual saturation.
L/kg = Liters per kilogram.
kg/m^3 = Kilograms per cubic meter.

5.4.2. Model Calibration

The model was calibrated to field measurements made during the treatability test. The objective was to match simulation results to:

1. The measured vapor flow rate (scfm);
2. The TCE concentrations in the effluent air stream (ppm on a volume-to-volume basis [$ppm_{v/v}$]); and
3. The total TCE mass removed during the June 2, 1993 eight-hour treatability test.

As a first step, measured vapor flow rates were used to calibrate gas flow through the vadose zone by using intrinsic permeability as the calibration parameter (Fig. 9a). A constant vacuum of 14.4 in. (366 mm) mercury (Hg) was applied at the wellhead, and the value of intrinsic permeability was adjusted iteratively until the computed flow rate matched the measured flow rate.

In the second step, contaminant transport in soil gas was calibrated using the measured TCE mass removal rates as calibration targets, and using initial soil TCE concentrations as the calibration parameter (Fig. 9b). A constant wellhead vacuum of 14.4 in. (366 mm) Hg the calibrated permeability, and corresponding vapor flow rate obtained in the first calibration step were held constant during transport calibration. TCE soil concentrations were adjusted up or down by a constant scaling factor until measured and computed extracted concentrations and mass removal rates were in reasonable agreement (Fig. 10). To calibrate the model, the simulated initial mass of TCE in the system had to be increased by a factor of five from 48.5 to 242.5 lbs (22 to 110 kg), indicating that the total VOC mass extrapolated from field data may have been initially underestimated.

5.4.3. Model Simulations

Simulations were conducted using a two-step process. First, gas flow and TCE transport were simulated. A cylindrical two-dimensional computational grid was used to simulate gas flow and TCE transport resulting from SVE at SVB-518-201. Then, a rectangular two-dimensional computational grid was subsequently used to simulate the migration of residual TCE through the vadose zone and into flowing ground water. The computed residual VOC soil concentrations were used as initial concentrations for the post-pumping simulations.

Mass removal was simulated for selected periods of SVE. The maximum simulated SVE period was 12 years. Post-remediation simulations estimated transport of residual TCE in the soil after the SVE system was shut down for 5,000 years.

Figure 11 shows the estimated increase in aqueous TCE concentrations at the water table throughout the first 500 years. Under the no-action scenario (i.e., no vapor extraction is conducted) a maximum increase of 280 ppb after 218 years is estimated. This is significantly higher than the 17 ppb TCE after 55 years predicted previously (Appendix G of Isherwood et al., 1990). The reasons for the change from earlier work are:

- Model calibration against data from the 1993 treatability test indicated that the total mass of TCE in soil may have initially been underestimated, perhaps by a factor of five.
- Unlike the 1990 model, this analysis includes the effects of rainfall infiltration, aqueous advection, and gaseous advection.
- The 1990 model used a TCE half-life of 50 years, whereas this analysis conservatively assumes no TCE degradation, as suggested by more recent analysis of site data by McNab and Narasimhan (1994).

The current simulations indicate that one year of continuous SVE reduces the subsequent incremental maximum TCE concentrations in ground water by over one order of magnitude (22 ppb vs 280 ppb) compared to the no-action case (Fig. 11). After continuous SVE for four years, simulations indicate that the subsequent maximum incremental TCE concentration in ground water is below the 5 ppb MCL.

5.5. Heterogeneous Site Conditions

5.5.1. Input Parameters and Qualitative Sensitivity Analysis

The objectives for simulating heterogeneous site conditions were to assess the effects of heterogeneous sediment properties on both the performance of the SVE system and the migration of TCE in the vadose zone. The processes that govern multiphase flow and transport through heterogeneous saturated and unsaturated soil depend on a large number of physical and chemical parameters. Field data were used to obtain site-specific parameter values where possible (Tables 2 and 3). For some of the parameters, such as the TCE source concentrations, data from boreholes in the Building 518 Area were used. For other parameters (intrinsic permeability, porosity, soil moisture retention curves), values were extrapolated from field and laboratory data from other parts of the Livermore Site. If no field data were available, estimates from research papers and textbooks were used to obtain parameter values.

Table 2. Model parameters for TCE properties.

TCE properties	Source	Estimated degree of uncertainty	Used in calibration
Source concentration	Soil samples from Building 518 Area	High	Adjustable[a]
Spatial distribution	Geostatistical interpolation	Medium	Fixed
Soil/water partition coefficient	Lab measurements from samples throughout the Livermore Site	Medium	Fixed
Free diffusion coefficient	Literature	Low	Fixed
Molecular weight	Literature	Low	Fixed
Henry's constant	Literature	Low	Fixed

[a] Allowed to vary as calibration parameters.

To assess the effect of uncertainty in the model input parameters on simulations, a qualitative sensitivity analysis was performed. The quality and site-specificity of the available data were assessed, and professional judgment was used to estimate the relative degree of uncertainty of each parameter (Tables 2 and 3). The parameters with the highest degree of uncertainty, TCE source concentrations and intrinsic permeability, were chosen as calibration parameters. The initial values for these parameters were adjusted within a reasonable range until the field-measured calibration targets were met.

Table 3. Model parameters for water, air, and soil phases.

Parameter	Source	Estimated degree of uncertainty	Used in calibration
Water properties:			
Initial saturation	Calculated from rainfall data	Medium	Fixed
Free diffusion coefficient	Literature	Low	Fixed
Viscosity	Literature	Low	Fixed
Density	Literature	Low	Fixed
Air properties:			
Initial gas pressure	Atmospheric pressure	Low	Fixed
Viscosity	Literature	Low	Fixed
Density	Literature	Low	Fixed
Soil properties:			
Intrinsic permeability	Extrapolated from lab/field data	High	Adjustable[a]
Spatial soil distribution	Geostatistical interpolation	Medium	Fixed
Porosity	Measured throughout the Livermore Site	Low	Fixed
Soil moisture retention curves	Measured at Building 292 at the Livermore Site	Low	Fixed

[a] Allowed to vary as calibration parameters.

The sediments beneath Building 518 were classified as either high permeability or low permeability based on borehole lithologic data, estimates of sediment type from lithologic logs, and analysis and measurements of moisture content at various sample locations throughout the Livermore Site. These two permeability categories were expressed as indicators, with one (1) representing high permeability; and zero (0) representing low permeability. Lithologic data from Building 518 Area boreholes were used to assign permeability indicators to each cell of a closely-spaced, three-dimensional rectangular interpolation grid using a kriging interpolation algorithm (Fig. 12). The interpolation grid was then projected onto the more coarsely spaced two-dimensional NUFT model grid. A material type was assigned to each cell of the computational grid depending on the percentage of low- or high-permeability indicators within each computational cell (Table 4). A total of 11 material types were used, with Material Type 1 (M1) representing 100 percent low-permeability indicators, and Material Type 11 (M11) representing 100 percent high-permeability indicators. Incremental steps of ten percent were used for the material types between these two extremes.

The interpolated spatial distribution of intrinsic permeability along a two-dimensional east-west cross section through the model domain is shown in Figure 13. Table 4 lists the calibrated soil parameters for heterogeneous site conditions. Intrinsic permeability values ranged from 7.8×10^{-14} m^2 to 7.9×10^{-11} m^2.

Table 4. Calibrated soil parameters for heterogeneous site condition simulations.

Material type	Grain size	Intrinsic permeability (m^2)	Porosity	Partition coefficient K_d (L/kg)
	% fine /% coarse	Calibration parameter	Based on field measurements	
M1	100/0	7.8×10^{-14}	0.4	0.30
M2	90/10	1.6×10^{-13}	0.4	0.30
M3	80/20	3.1×10^{-13}	0.4	0.15
M4	70/30	6.2×10^{-13}	0.4	0.15
M5	60/40	2.5×10^{-12}	0.3	0.06
M6	50/50	2.5×10^{-12}	0.3	0.06
M7	40/60	4.9×10^{-12}	0.3	0.06
M8	30/70	1.0×10^{-12}	0.3	0.06
M9	20/80	1.9×10^{-11}	0.3	0.06
M10	10/90	4.0×10^{-11}	0.3	0.06
M11	0/100	7.9×10^{-11}	0.3	0.06

For each material type, a linear relationship between capillary pressure and water saturation was specified. Porosity was estimated to range from 0.3 to 0.4 (Table 4). The soil/water partition coefficient (K_d) of TCE was estimated to be 0.30 L/kg for M1 and M2, 0.15 L/kg for M3 and M4, and 0.06 L/kg for all other material types. This corresponds to higher TCE adsorption in soil of low-intrinsic permeability (e.g., clayey silt), and lower TCE adsorption in soil of high-intrinsic permeability (e.g., gravelly sand).

5.5.2. Model Calibration

The heterogeneous model was also calibrated to match results of the two-day treatability test. Calibration targets were the vapor flow rate, TCE concentration in the effluent air stream, and total mass of TCE removed from the soil. Calibration parameters were intrinsic permeability and the initial mass of TCE in the system. Calibration was achieved by an iteration procedure that involved increasing or decreasing the initial parameter values (within a reasonable range) until the model results matched the calibration targets. Only the magnitude of the calibration parameters were changed, while the spatial distribution was held constant.

The calibrated intrinsic permeability values ranged from 7.8×10^{-14} m^2 (M1) to 7.9×10^{-11} m^2 (M11) (Table 4). To match the TCE mass removed during the treatability test, the initial mass of TCE in soil was increased from the initial field-based estimate of 22 kg to 44 kg, 2.5 times less than the calibrated initial VOC mass used for the homogenous simulations.

5.5.3. Simulation Results

A no-action scenario and a series of SVE scenarios using existing extraction well SVB-518-201 were simulated. The no-action scenario used calibrated initial TCE concentrations and evaluated TCE migration through the unsaturated and saturated zones. The SVE simulations assessed the reduction in soil TCE concentrations resulting from operating the SVE well, and the subsequent migration of residual TCE through the subsurface after SVE ceased. Several durations of continuous SVE ranging from 0.5 to 12 years were evaluated.

Results of these simulations suggest that without SVE, TCE in soil in the Building 518 Area would reach ground water within the next 200 to 1,000 years (Fig. 14). TCE concentrations in ground water are estimated to reach a maximum of almost 300 ppb after 220 years (Fig. 15). Concentrations would decrease as the mass of TCE in the vadose zone is depleted and contaminants migrate downgradient in ground water, but it may take more than 500 years for TCE concentrations in ground water to fall below the 5 ppb MCL without SVE.

Simulations indicated that continuous SVE over a period of several years is likely to decrease TCE concentrations in soil and the underlying ground water. After five to six years of operation, TCE concentrations in soil above 20 to 30 ppb were estimated to be present in a small area close to the water table. Peak incremental TCE concentrations in ground water decreased from about 300 ppb for the no-action scenario to about 20 ppb after one year of SVE. After five to six years of continuous SVE, incremental TCE concentrations in ground water were estimated to be below the 5 ppb MCL (Fig. 15). Based on these calibrations and simulations, most of the TCE mass in the upper vadose zone interval would be removed after operating the system for one year (Fig. 16).

Simulation forecasts indicate that a SVE system using a single well screened in the upper VOC interval will effectively remove TCE mass. However, due to the heterogeneity of the subsurface sediments, soil near the water table will be remediated at a significantly lower rate. Figure 17 shows the simulated gas pressures and velocities induced by soil vapor extraction at SVB-518-201. The pressure gradient, which is commonly used to estimate the zone of influence of a SVE system, can be misleading in a heterogeneous environment. For systems in quasi equilibrium (e.g., affected by an extended period of SVE), pressure gradients are almost independent of the soil permeability distribution (Fig. 17). In contrast, the simulated distribution of vapor flow velocities clearly shows the expected channeling effect of the high-permeability soil layers, and the limited impact of the proposed SVE system on deeper intervals.

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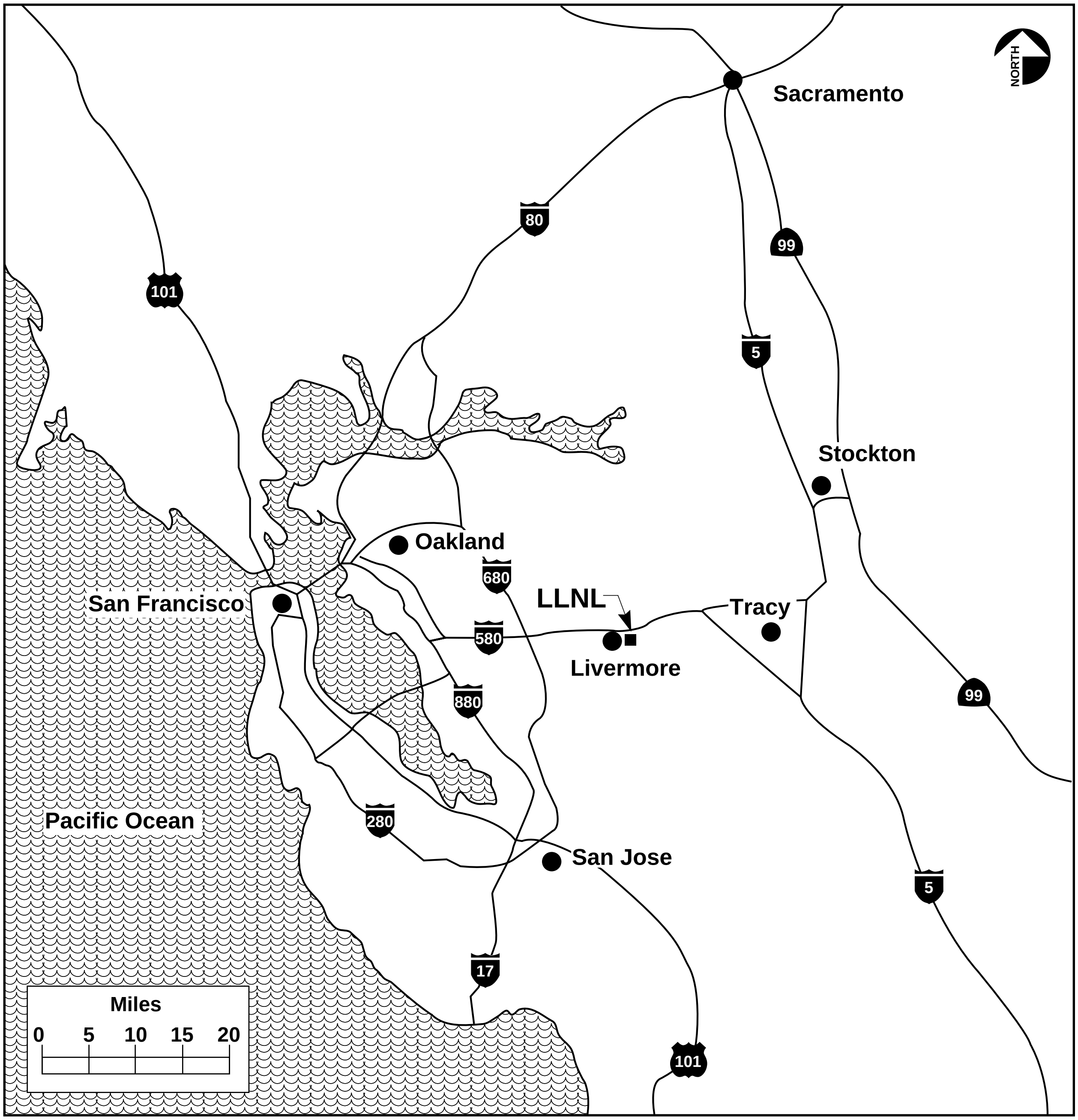
Figures



ERD-LSR-96-0034

Figure 1. Location of the LLNL Livermore Site.

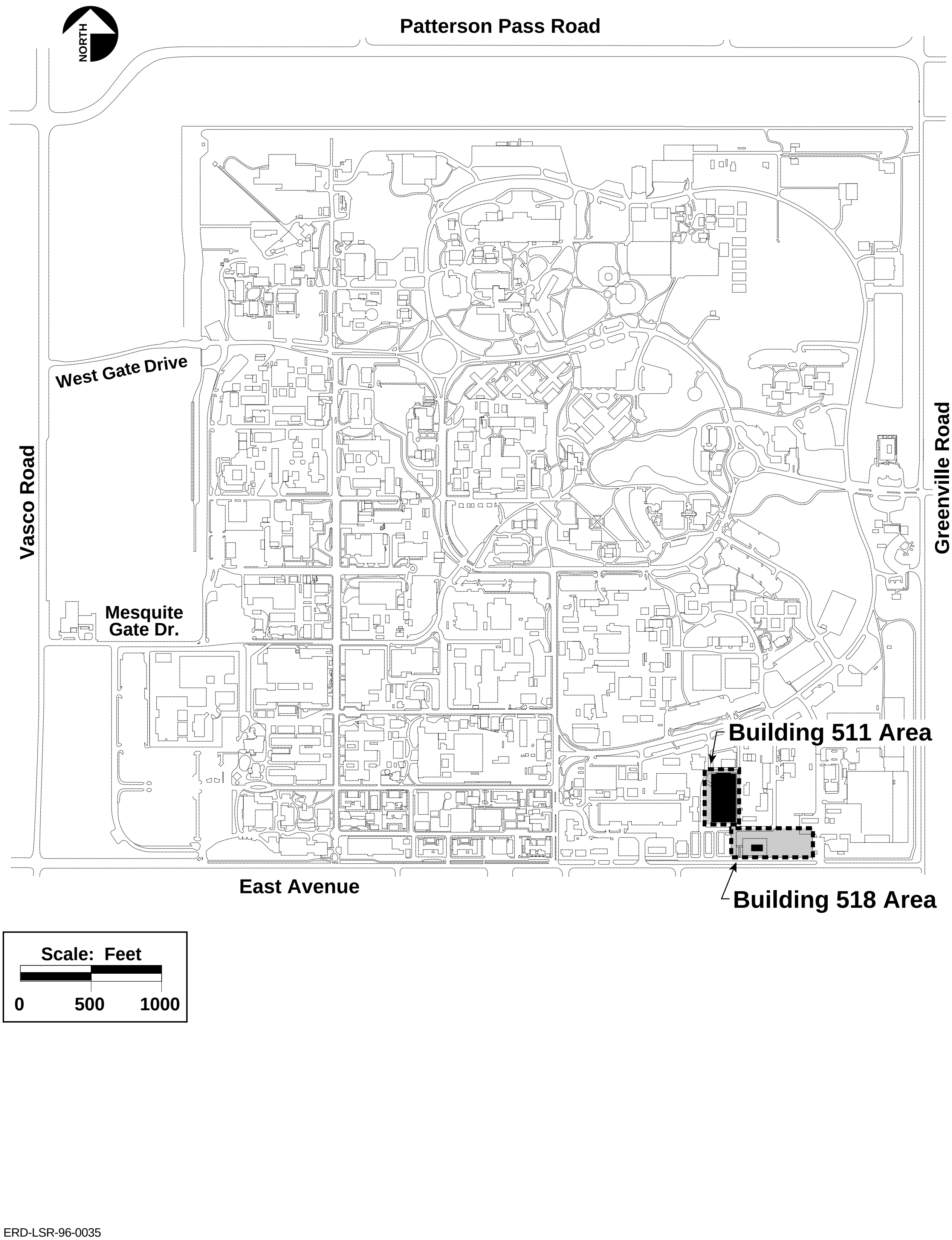


Figure 2. Location of the Building 518 Area.

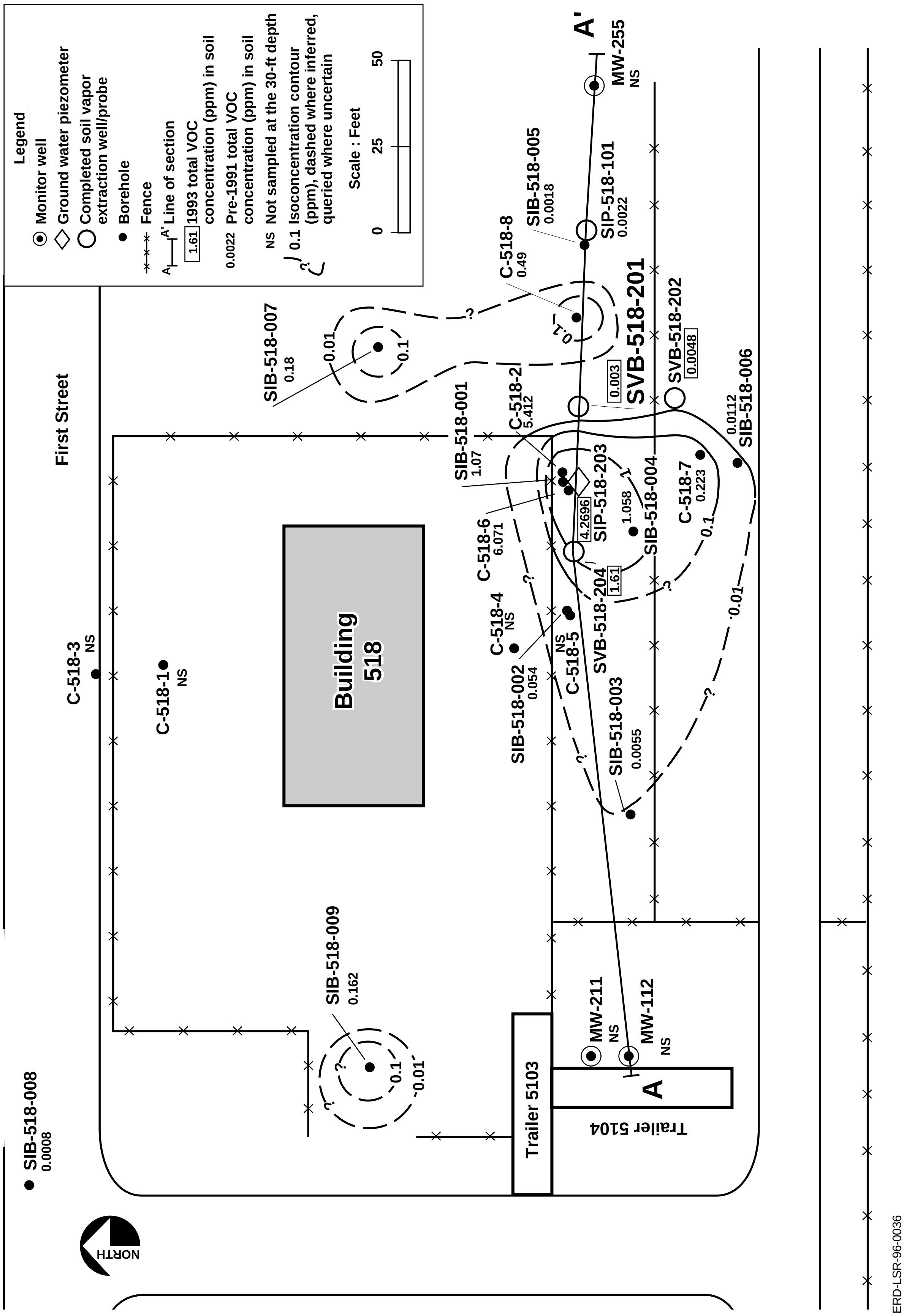
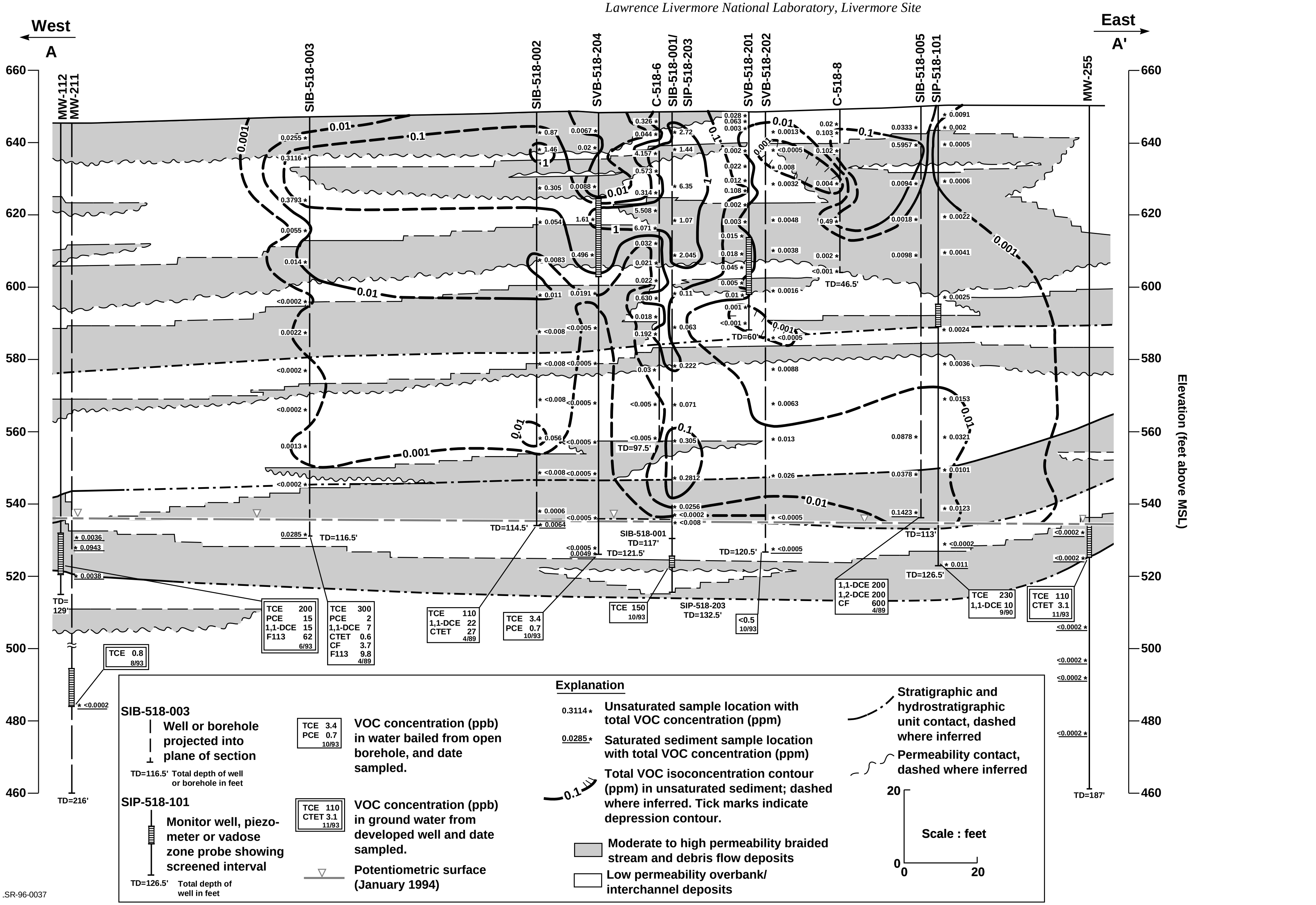


Figure 3. Borehole, monitor well, piezometer, and soil vapor extraction well/probe locations in the Building 518 Area. Total VOC soil isoconcentration contours are for approximately 30-ft depth.



ure 4. Hydrogeochemical cross section A-A' in the Building 518 Area.

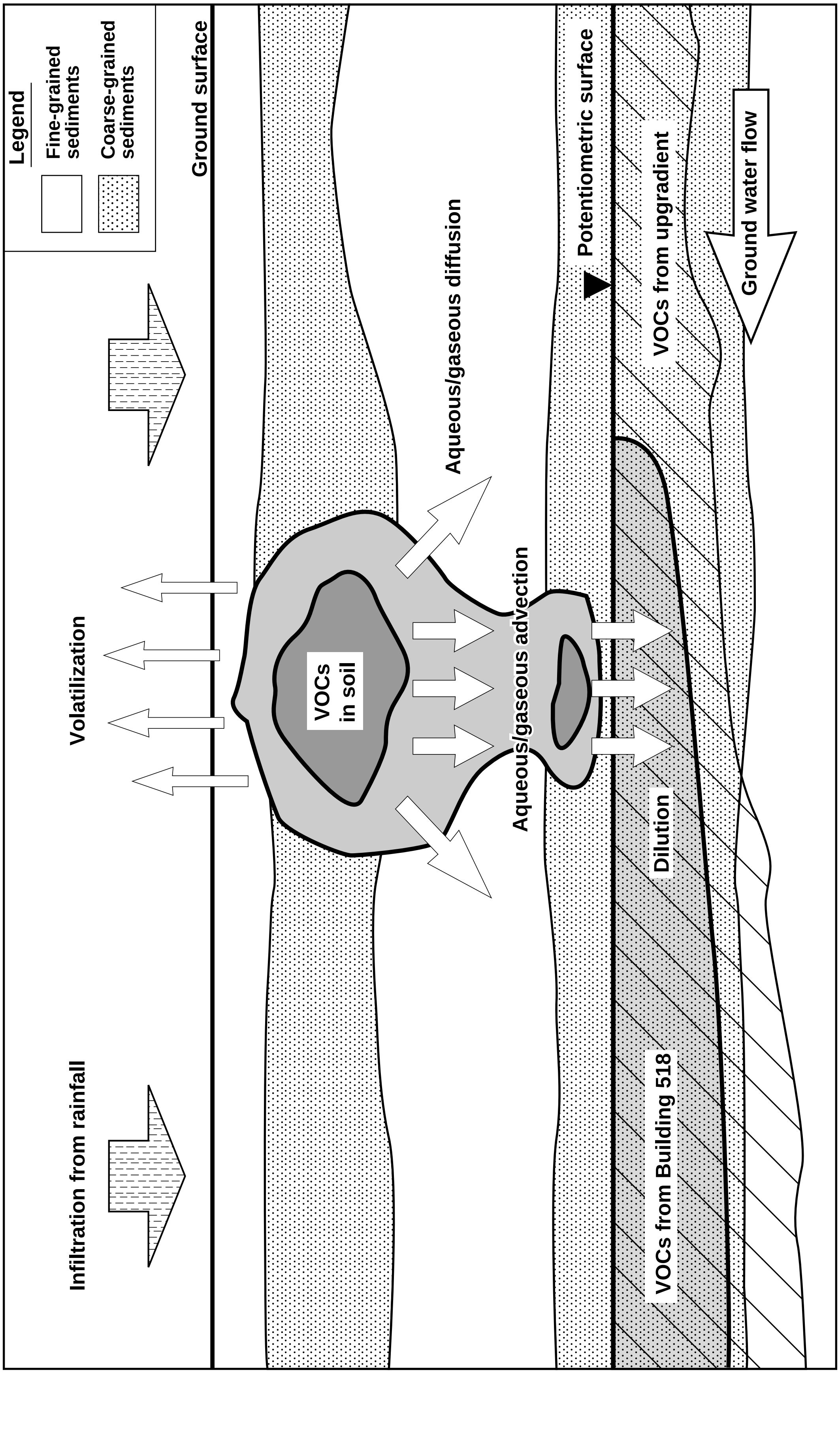


Figure 5. Conceptual model of the Building 518 Area subsurface.

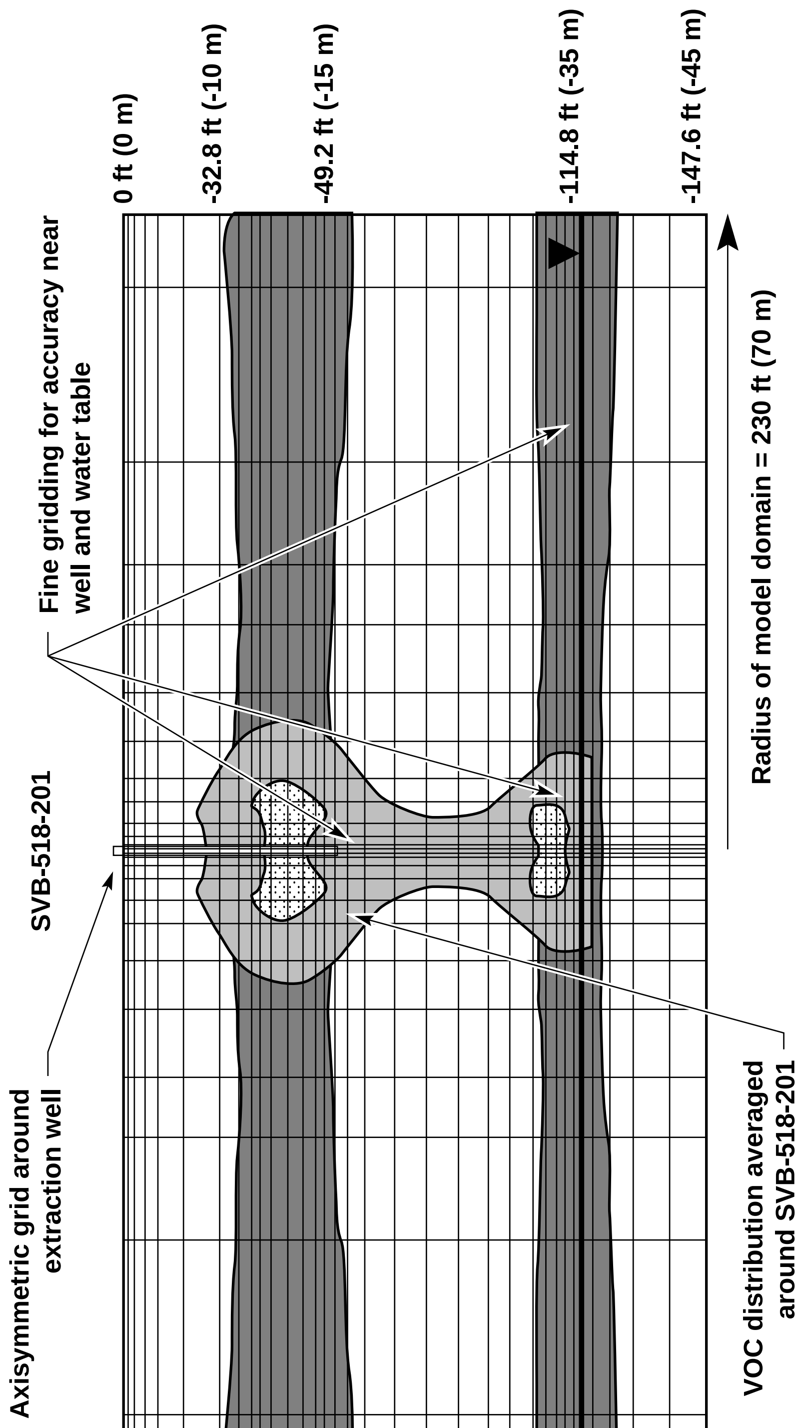


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Figure 6. Computational grid for the Building 518 transport model.

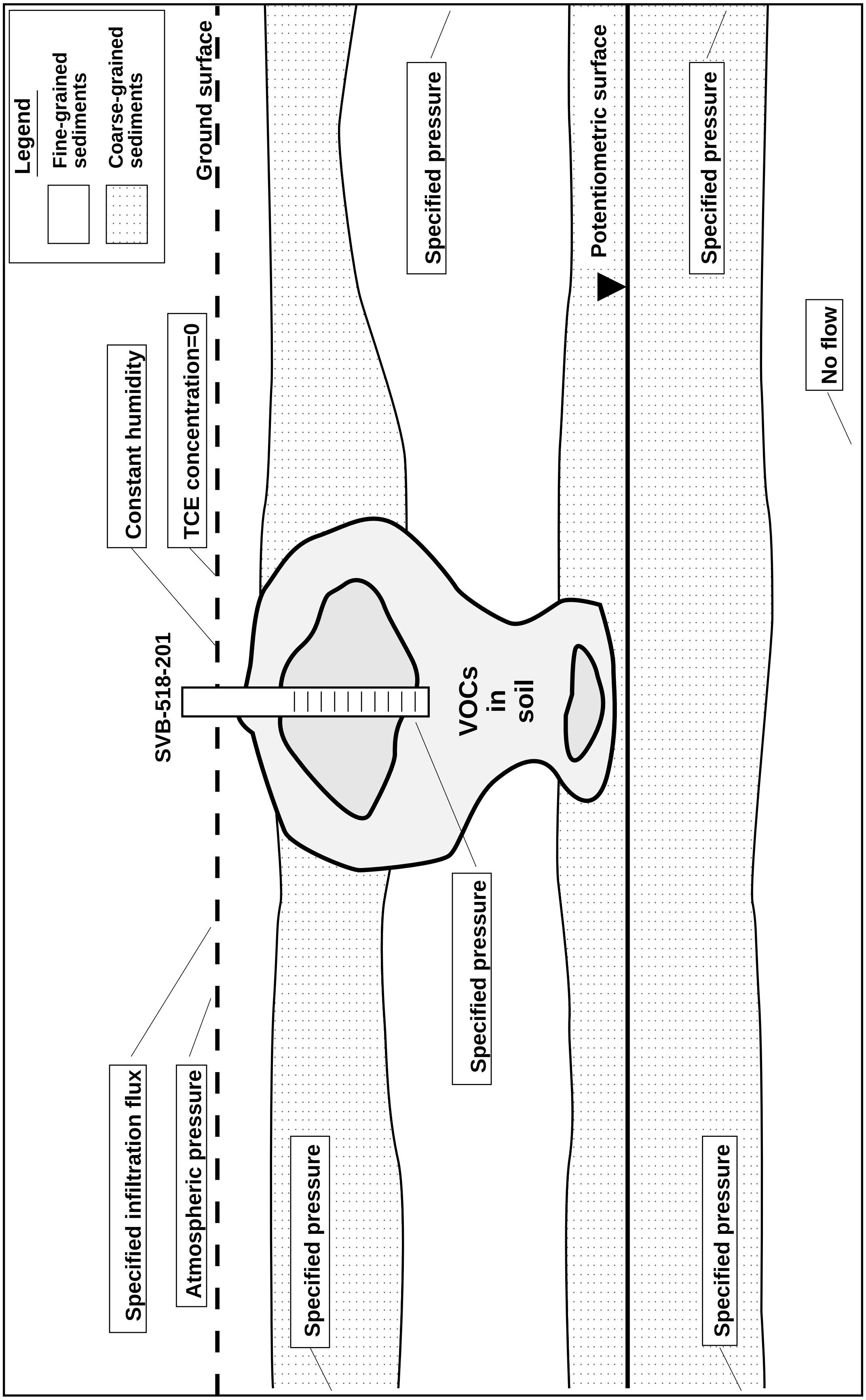

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Figure 7. Building 518 model boundary conditions.

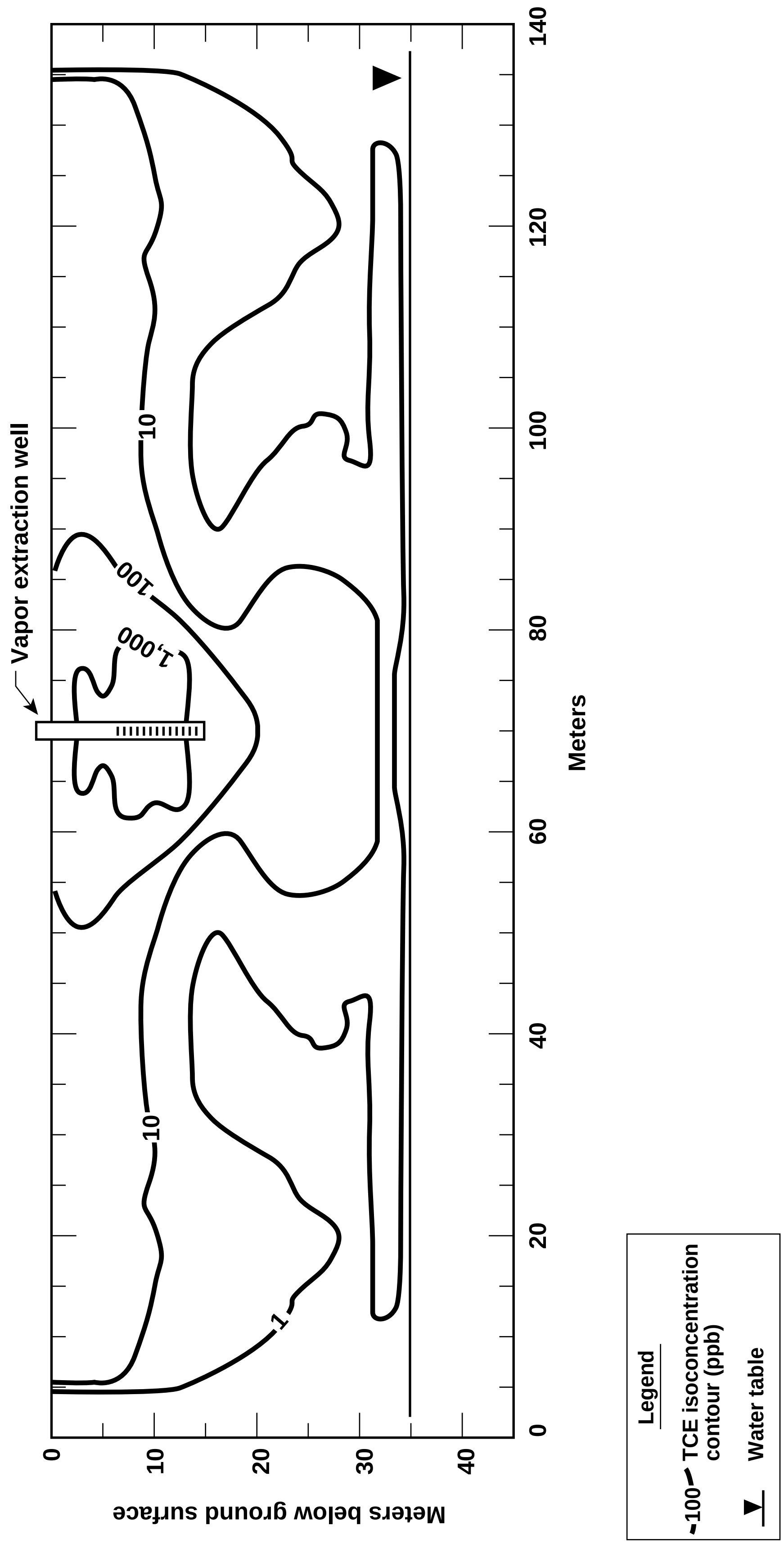

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Figure 8. Spatial distribution of initial TCE soil concentrations.

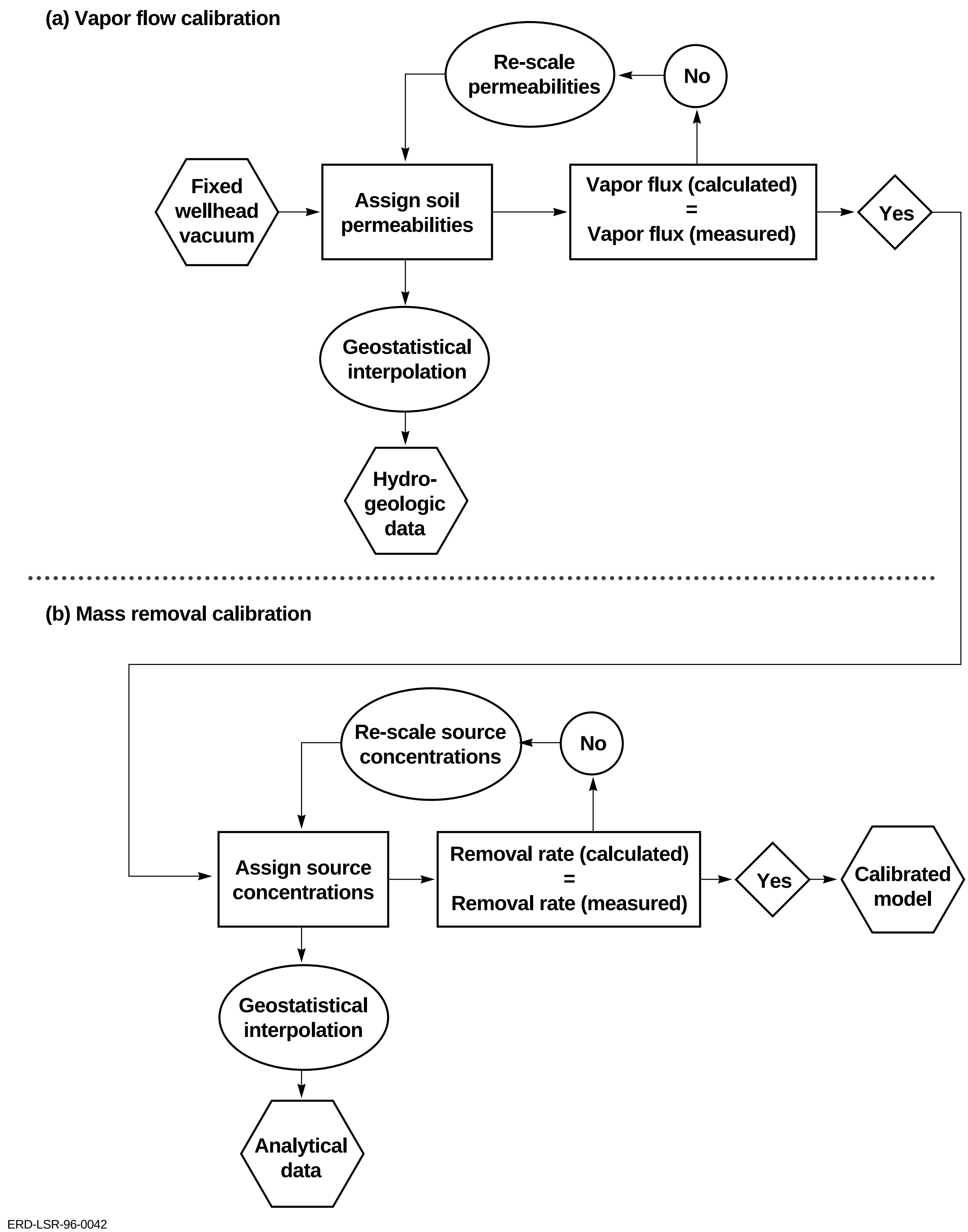

Figure 9. Model calibration process for: (a) vapor flow and (b) mass removal.

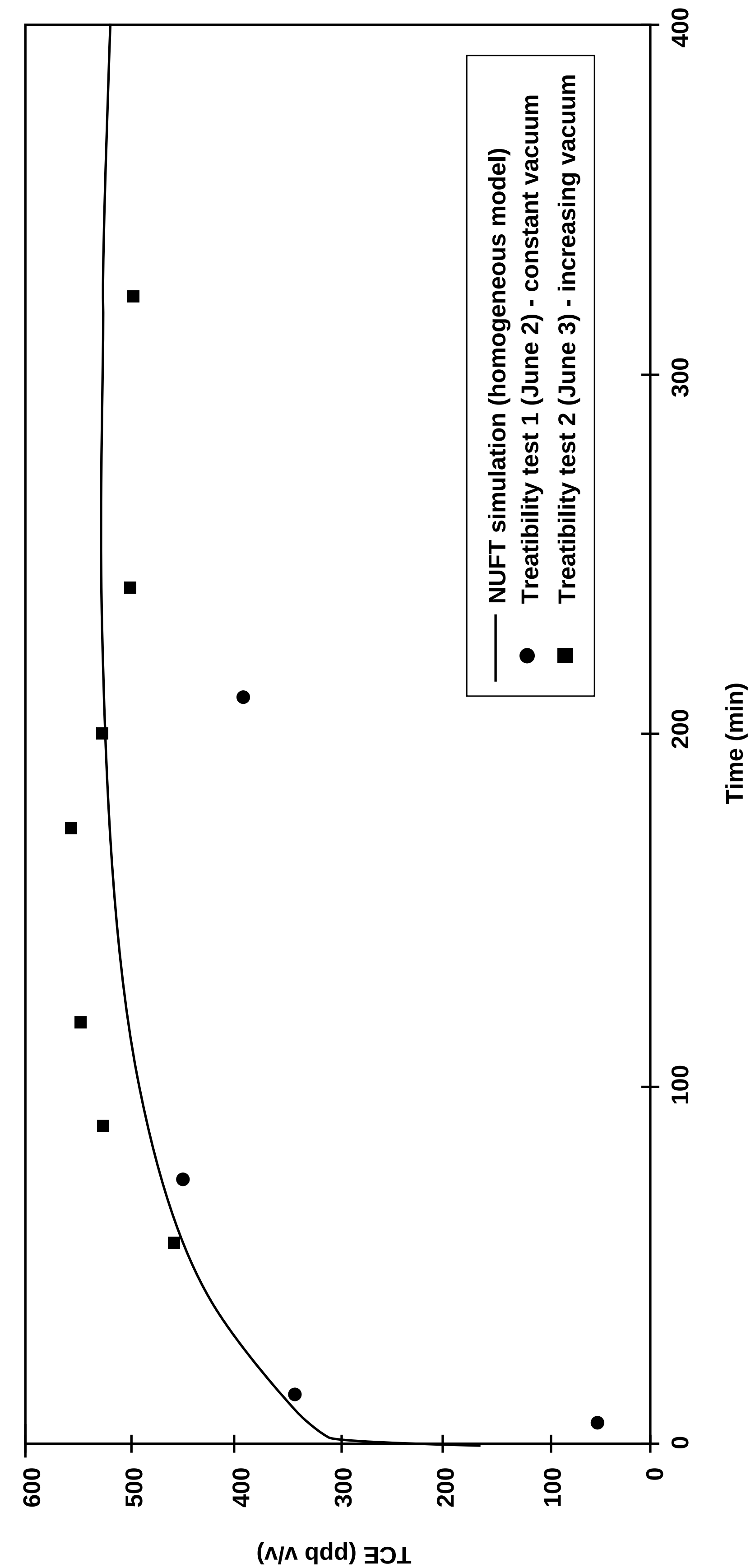

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Figure 10. Vapor flow calibration for homogeneous site conditions.

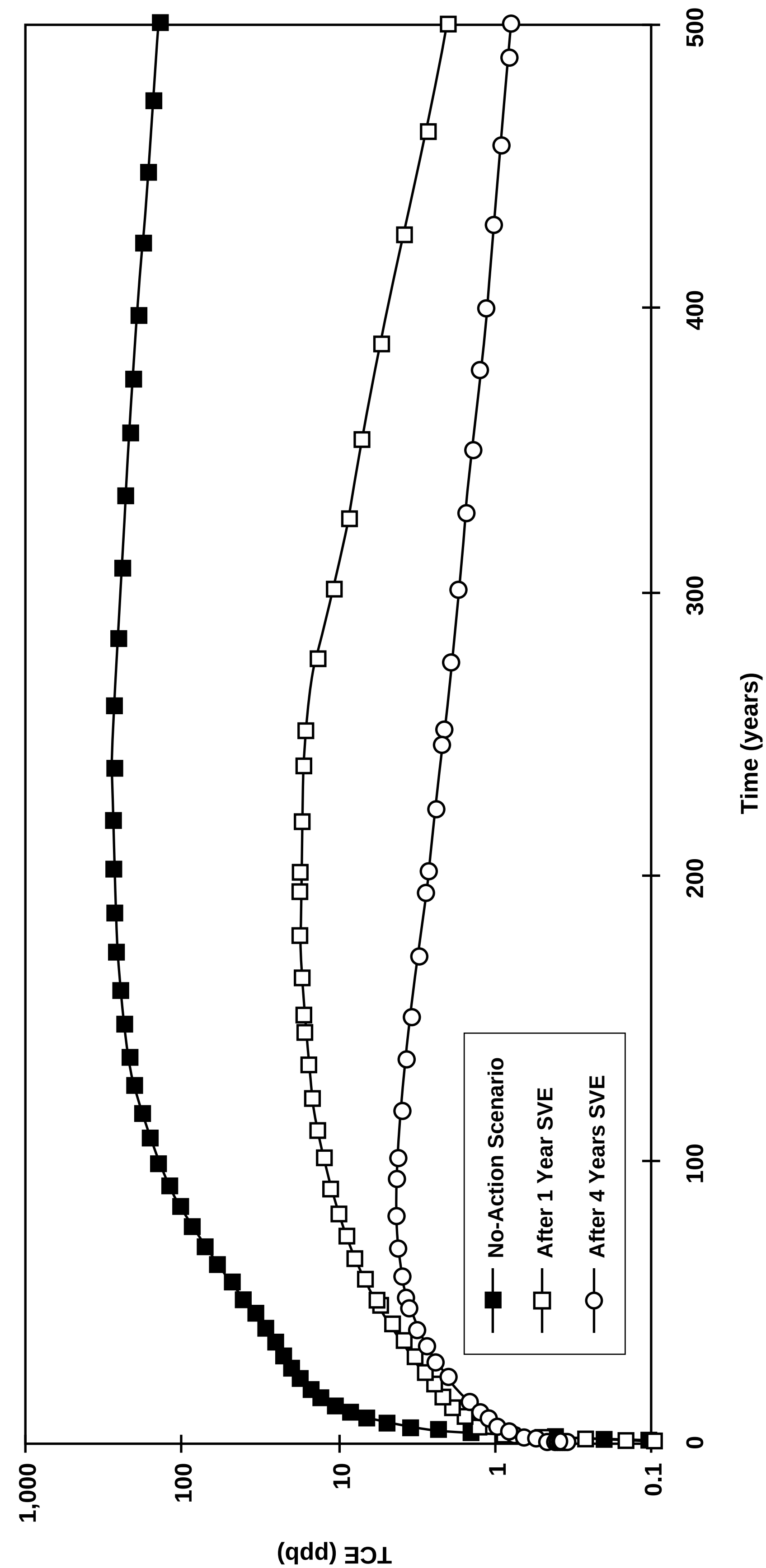

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Figure 11. Estimated TCE concentrations in ground water, homogeneous conditions.

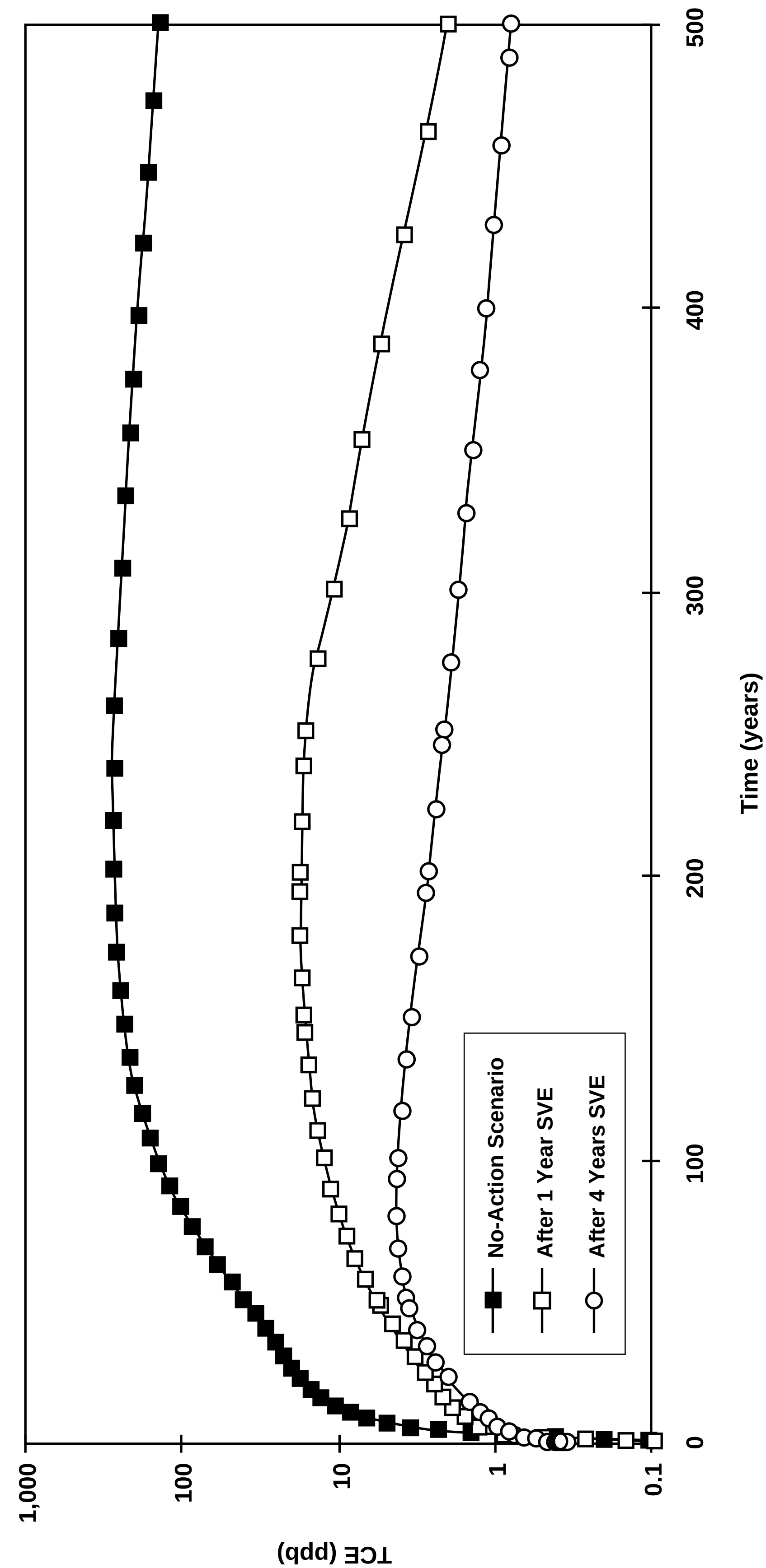

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Figure 11. Estimated TCE concentrations in ground water, homogeneous conditions.

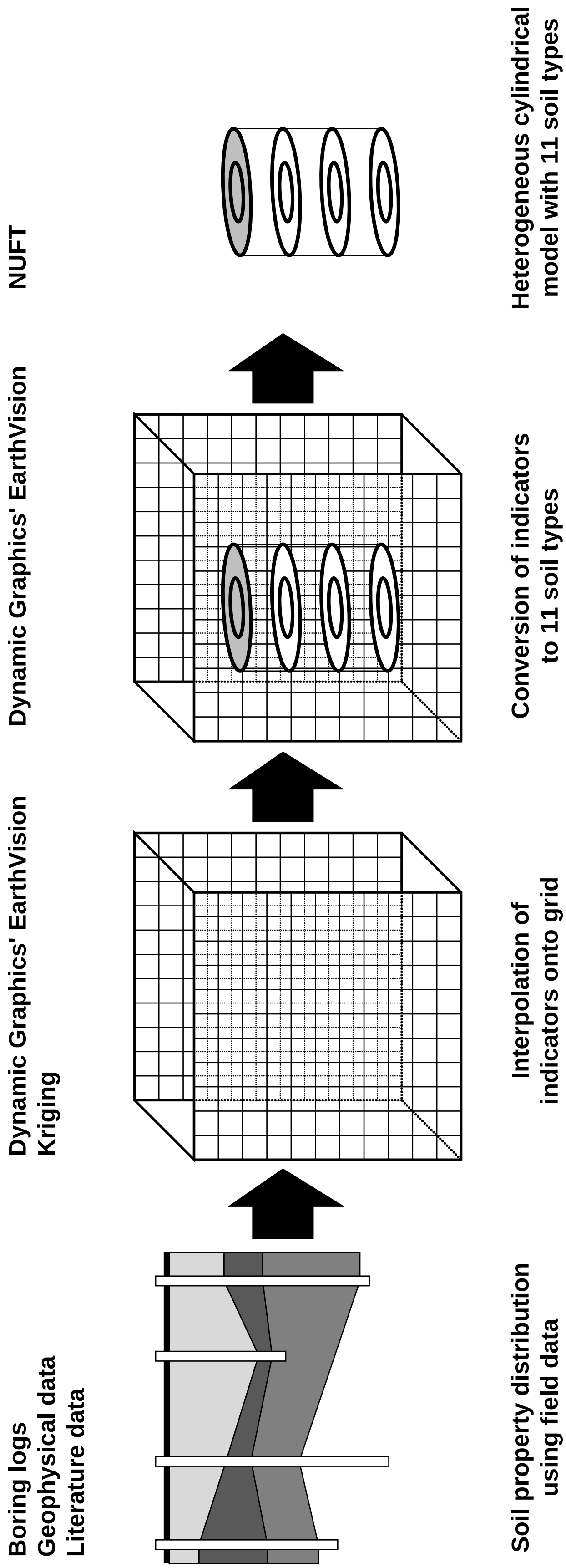

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Figure 12. Geostatistical interpolation of model parameters.

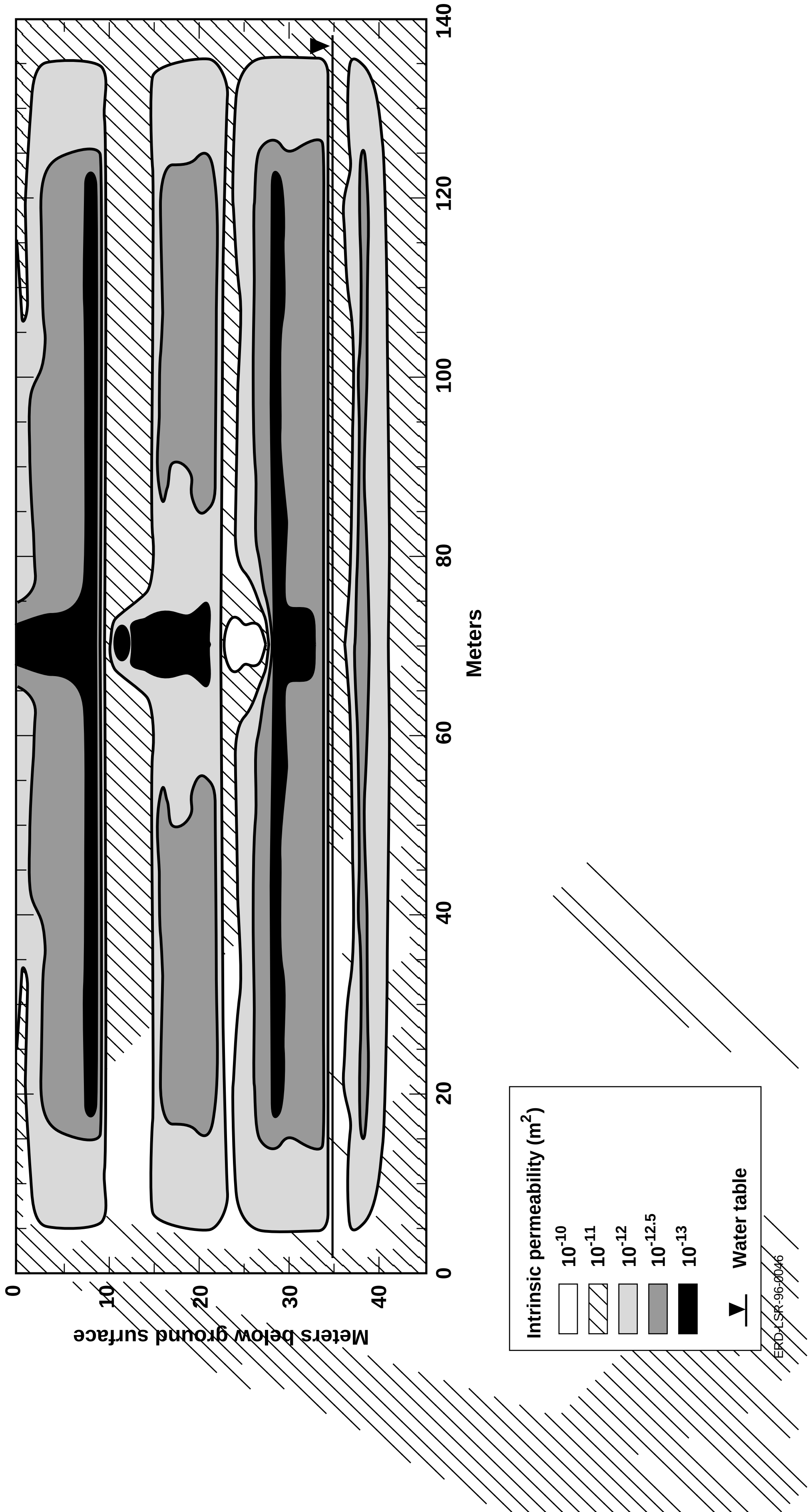

Figure 13. Spatial distribution of intrinsic permeability used for heterogeneous site conditions.

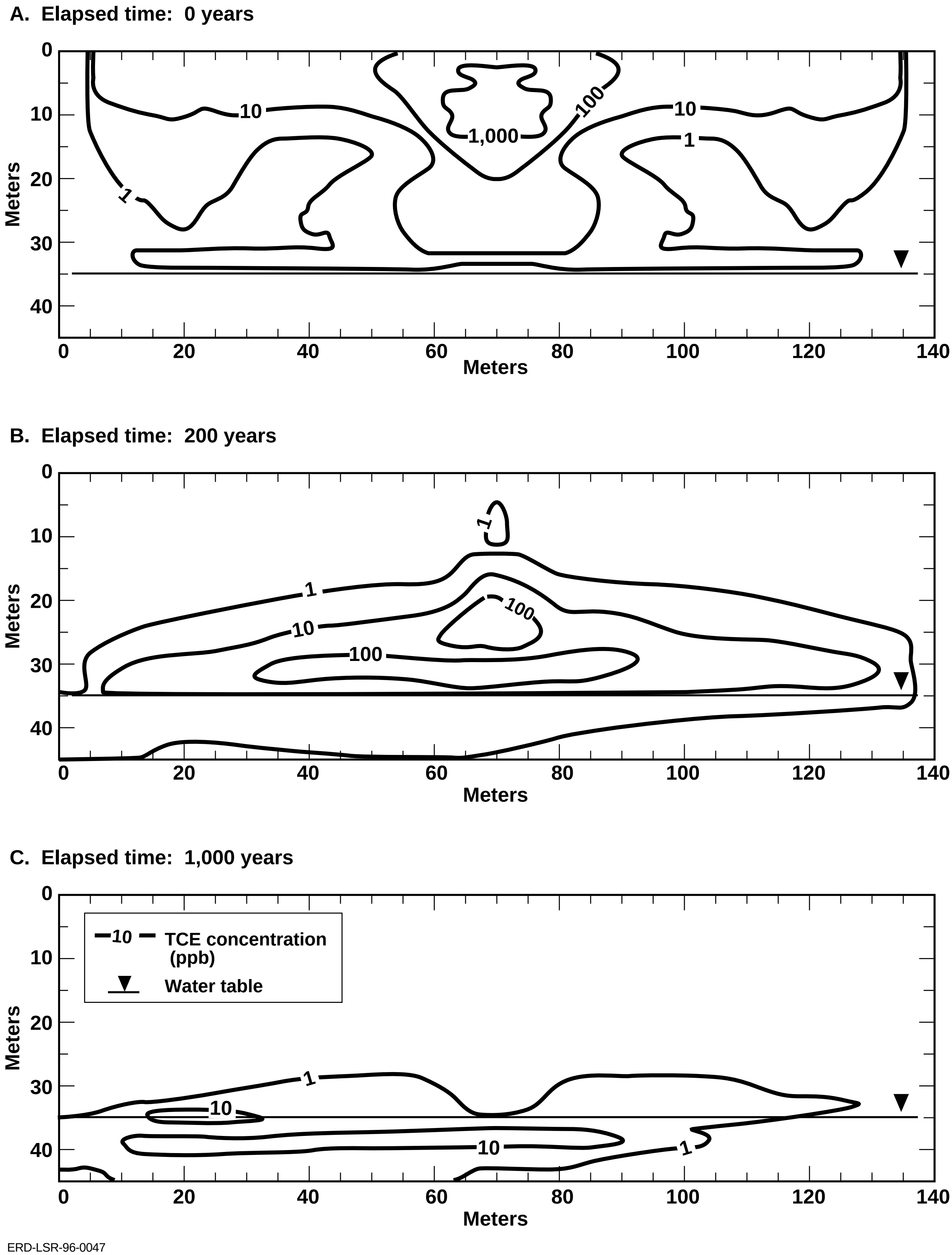

Figure 14. Estimated TCE migration in soil and ground water with time for the no-action scenario, heterogeneous conditions.

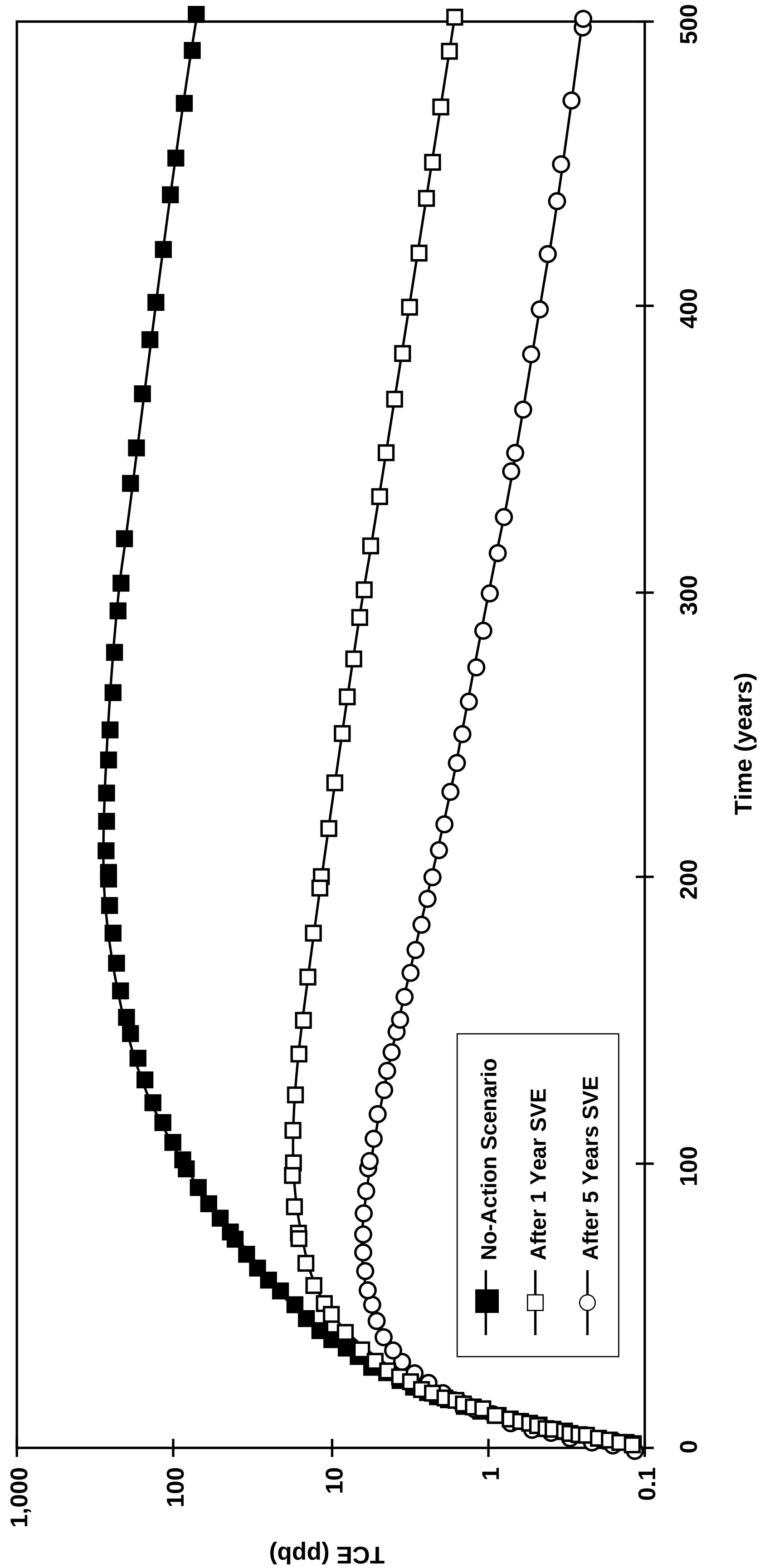

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Figure 15. Estimated TCE concentrations in ground water, heterogeneous conditions.

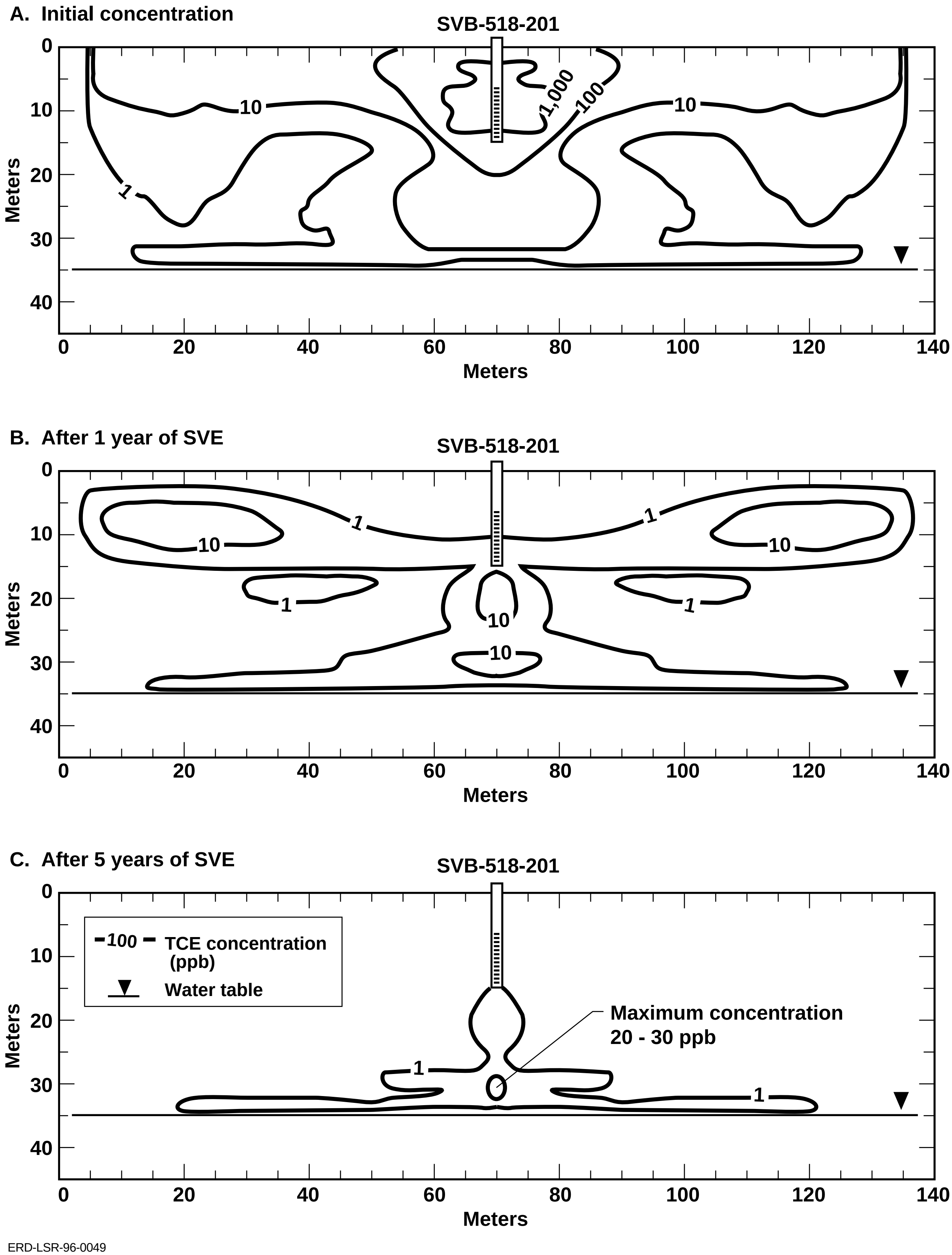

Figure 16. Estimated TCE soil concentrations for SVE simulation, heterogeneous conditions.

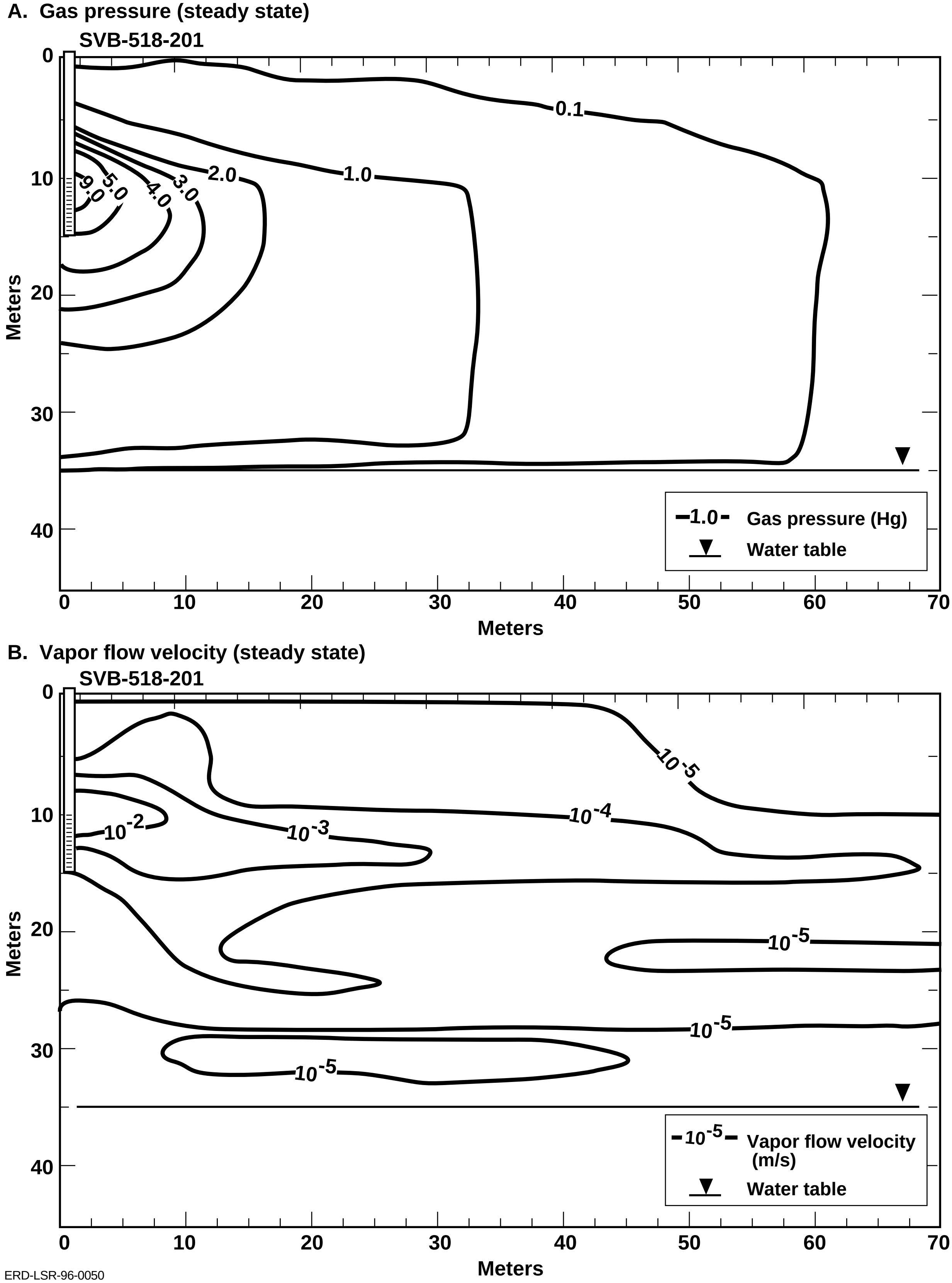

Figure 17. Estimated pressure gradients and vapor flow velocities, heterogeneous conditions.

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