December 22, 1997

Chief, NY Remediation Branch
United States Environmental Protection Agency
290 Broadway, 20th Floor
New York, New York 10007

Attn: Mr. Lorenzo Thantu
        Remedial Project Manager

Re: Conceptual Groundwater Flow and Transport Models
        Continued RI/FS Activities
        Liberty Industrial Finishing Site
        Farmingdale, Nassau County, New York

Dear Mr. Thantu:

This letter transmits three (3) copies of the "Conceptual Groundwater Flow and Transport Models" deliverable. According to the requirements in the EPA letter of May 15, 1997, the enclosed document presents a conceptual groundwater flow model, a conceptual transport model, and conceptual hydrogeochemical models for the organic and inorganic constituents at the site. Responses to the general and specific comments contained in the May 15, 1997 EPA letter are presented in Appendix A.

Sincerely,
DAMES & MOORE

Matthias Ohr
Project Manager

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(PHL) cgw cover.doc

Enclosure

CONCEPTUAL GROUNDWATER FLOW AND TRANSPORT MODELS
LIBERTY INDUSTRIAL FINISHING SITE
FARMINGDALE, NEW YORK

December 22, 1997

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1.0 INTRODUCTION

Pursuant to Section 41(h) of the Administrative Order of Consent (Order) for Continued Remedial Investigation/Feasibility Study (CRI/FS) for Operable Unit II (Index No. II CERCLA-97-00203) at the Liberty Industrial Finishing Site, Dames & Moore transmitted a Fate and Transport Modeling Memorandum to the U.S. Environmental Protection Agency (EPA) on March 7, 1997. The numerical modeling study at the Liberty site was proposed to consist of the setup and calibration of a three-dimensional groundwater flow, contaminant transport, and geochemical model, which will be used to predict the fate and transport of the constituents of interest (COI) under existing natural conditions and various remedial alternatives.

The scope of the modeling study encompasses the following:

- Review of background information and identify data gaps;

- Formulation of a conceptual model of groundwater flow and COI transport at the site;

- Model setup and preparation of input data;

- Flow model calibration and sensitivity analysis for existing groundwater flow conditions;

- Model calibration for existing COI distribution and COI transport mechanisms at the site;

- Modeling using hydrogeochemical equilibrium model;

- Transport model calibration and sensitivity analysis for existing COI distribution and COI transport mechanisms at the site; and

- COI fate and transport modeling for various remedial alternatives.

A preliminary groundwater flow and COI transport conceptual model was previously presented in the Memorandum, dated March 7, 1997, and a groundwater flow model (MODFLOW) and contaminant transport model (MT3D), together with an equilibrium hydrogeochemical model (MINTEQA2), were proposed. Dames & Moore proposes to replace MT3D by a new transport model RT3D (Three-dimensional Multi-species Reactive Transport in Porous Media, developed by the U.S. Department of Energy, Clement et al., 1997).

The EPA provided comments on the Memorandum on May 15, 1997 and requested that Dames & Moore address the comments in this conceptual model deliverable. This report presents descriptions of the conceptual groundwater flow model (Section 3.1), COI transport (Section 3.2), and hydrogeochemical model (Section 3.3). Specific responses to the EPA comments are presented in Appendix A.

2.0   REVISED TRANSPORT MODEL

A recently released contaminant fate and transport model, RT3D, developed by the Pacific Northwest National Laboratory will be used in place of MT3D. RT3D is a new reactive transport simulator that has all the capabilities of MT3D, but can also be used for simulating reactive multispecies transport in three-dimensional saturated porous media. RT3D is a public domain FORTRAN-90 based software package. The current version of RT3D uses the basic input/output driver, advection, and dispersion routines from the version DOD_1.5 of the MT3D simulator. As with MT3D, RT3D requires that the USGS groundwater flow model MODFLOW be used to compute groundwater transport velocities.

RT3D is sufficiently flexible for simulating all of the relevant constituent reactions, microbial metabolisms, and microbial transport kinetics discussed below. As a research tool, RT3D has been used for modeling several laboratory and pilot-scale experiments; in addition, it is currently being used to model several sets of field-scale natural attenuation data.

3.0   CONCEPTUAL MODELS

This section presents detailed descriptions of the conceptual flow model (Section 3.1) and the conceptual organic and inorganic constituent transport and hydrogeochemical models (Sections 3.2 and 3.3).

3.1   Flow Model

A detailed three-dimensional conceptual groundwater flow model was developed for the study area. The hydrogeological setting, groundwater flow, basic model assumptions, and model domain, model grid, and boundary conditions are described below.

3.1.1   Hydrogeological Setting

The Liberty site is directly underlain by the Upper Glacial deposits of Pleistocene age. The Upper Glacial aquifer is composed of fine to coarse sands and gravel and is approximately 85 feet thick. The water table is currently approximately 17 to 19 feet below ground surface (bgs) at the site. The Magothy Formation is underlying the Upper Glacial aquifer. The predominant grain size of the Magothy Formation is fine sand with thin beds and lenses of silt and clay. The anticipated thickness of the Magothy Formation is 700 feet in the vicinity of the Liberty site. The Magothy Formation is underlain by the Raritan Clay, a confining unit comprised of impermeable clay.

3.1.2   Groundwater Flow

Groundwater of concern at the site occurs within two aquifers - the Upper Glacial and Magothy aquifers. A surface water body, Massapequa Creek, is located downgradient of the site. The Massapequa Creek originates approximately 1,000 feet south of the site, travels southwest

through several ponds along Massapequa Preserve to Massapequa Lake. The groundwater flow from the Upper Glacial aquifer continues downgradient within the aquifer with some portion discharging to Massapequa Creek. The Magothy aquifer discharges primarily to the south shore bays.

Groundwater elevation data generated during the remedial investigation (Roy F. Weston, January 1994) indicate that groundwater within the Upper Glacial aquifer moves predominantly in a south-southwesterly direction towards the Massapequa Creek. The average hydraulic gradient is reported to be 0.0022. The average effective porosity and horizontal hydraulic conductivity are reported to be 0.3 and 270 ft/day, respectively (Franke, et. al., 1972). The vertical and horizontal hydraulic conductivity ratio is reported to be 1:10 (Franke, et. al., 1972). The specific yield of the Upper Glacial aquifer is reported to be 0.2 (Warren et. al., 1968)

Groundwater in the Magothy aquifer is reported to migrate in a south-southeasterly direction (Roy F. Weston, January 1994). Hydraulic characteristics of the Magothy aquifer at and the downgradient of Liberty Site will be further investigated during continued RI/FS. Horizontal hydraulic conductivity and the anisotropic ratio of horizontal to vertical hydraulic conductivity are reported as 50 ft/day and approximately 1:36, respectively (Franke, et. al., 1972). The effective porosity of Magothy aquifer material is reported to be 0.25 (Warren et. al., 1968). The specific storage of Magothy aquifer is reported to be 6×10^{-7} ft^{-1} (Buxton, et. al., 1985)

3.1.3 Basic Model Assumptions

The following assumptions were made in the development of the conceptual groundwater flow model for the Liberty site:

- Steady-state flow conditions prevail in the aquifers;

- The Magothy aquifer is underlain by a confining layer, which dips in the general direction of groundwater flow;

- Groundwater recharge is uniform throughout the study area;

- The well fields are withdrawing water at constant pumping rates from the Magothy aquifer;

- The branches of Massapequa Creek in the study area are shallow and in hydraulic contact with the groundwater table.

3.1.4 Model Domain, Grid, and Boundary Conditions

The model grid may cover an area of approximately 29,000 feet by 23,000 feet (Figure 1). As shown in Figure 1, the southern boundary of the model domain may approximately follow the

limits of Merrick Road. The northern boundary of the model domain may extend to approximately 5,000 feet north of the Liberty site. The western boundary of the model domain may be defined to Hicksville Road in the northwest of the model domain and the Oyster Bay - Seaford Expressway in the southwest portion of the model domain. The eastern boundary of the model domain may extend to approximately 10,000 feet east of the Liberty site. The Massapequa Water District supply wells and South Farmingdale Water District supply wells that will be encompassed by the model domain are also shown in Figure 1.

Model Layers

The model may consist of a grid of ten layers. The first four layers may represent the Upper Glacial Aquifer, which has a saturated thickness of approximately 75 feet in the Liberty site area. The remaining six layers may represent the Magothy aquifer, which is approximately 700 feet thick, such that the depth of the model domain may extend to Raritan Clay. The domain is subdivided into ten model layers in order to allow an appropriate representation of vertical velocity variations and vertical variations in COI concentrations in the aquifers. Vertical velocity components are induced by the partially penetrating pumping wells and other three-dimensional hydrogeological features such as the various creeks and lakes.

The tops and bottoms of the model layers will be chosen such that they follow approximately the topographical surface and the water table. This may result in a relatively complex model geometry within each layer. The approximate layer thicknesses are presented in Table 1. Within each layer, all cells will be of equal thickness. Thus, the shape of each layer top and bottom will be identical, but the absolute elevation of the layers may differ by the layer thickness.

Three-Dimensional Model Grid

A grid of rectangular cells with side lengths varying from a minimum of 200 feet by 200 feet to an average of approximately 500 feet by 500 feet may used to discretize the domain in plan view. In areas where groundwater impacts or steep concentration gradients will be observed, the grid will be refined. Considering the model domain of 29,000 feet long and 23,000 feet wide, average rectangular cell dimensions of approximately 500 feet by 500 feet, and ten model layers, the model may consist of a total of 26,680 cells (i.e. 58 x 46 cells per layer).

Boundary Conditions

A groundwater divide, along which no-flow conditions are imposed, is present approximately 5 miles north of Liberty site. The major surface water feature is the Atlantic Ocean, located approximately 5 miles south of Liberty site. There are no significant hydraulic boundaries (specified head, no-flow, or specified flow) within 5 miles east or west of Liberty site.

It is sometimes not possible to choose the physical boundaries of the aquifer when designing a model for a hydrogeological site investigation. In these cases, hydraulic boundaries are selected

based on knowledge of the flow system. Typically, information is available on the general configuration of the regional flow system, but site information is sufficient to deduce long- term flow patterns. One approach consists of designing a nested set of grids so that the site grid, which has the finest nodal spacing, is embedded in a regional grid with coarser nodal spacing. The solution of the regional model is then used to define boundary conditions of the site model. Boundaries defined in this way are sometimes called artificial boundaries.

The hydraulic boundary conditions for the Liberty site may be based on the Nassau County Department of Public Works (NCDPW) Regional Groundwater Flow Model. However, necessary modifications of this model may be made to characterize the localized hydrogeologic conditions of the study area. The NCDPW Regional Groundwater Flow Model is a calibrated representation of multiple aquifer system underlying Nassau, Queens, and Western Suffolk Counties. The boundaries of the regional model were Long Island Sound and the Atlantic Ocean. The nodal spacing of the regional model is approximately 5,000 feet. However, a smaller local grid will be developed within the regional grid.

Representation of Surface Water Bodies

The interactions between the aquifers and the Massapequa Creek, ponds, and Massapequa Lake within the Massapequa Preserve will be in incorporated in the model. Additional surface water bodies in the model may include Seaford Creak within the Tackapausha Preserve, Jones Creek, Carman Creek, Amityville Creek, and Woods Creek. The surface water bodies will be represented as features that either supply water or act as drains, depending on the local flow conditions in the aquifer.

The water levels in the surface water bodies will be set in accordance with ground surface data obtained from the corresponding USGS topographic maps (Amityville, N.Y.). A limited amount of data on water levels within the model domain may be collected during remedial investigation studies. Where available, these data will be used to confirm or adjust the water levels specified in the model.

Recharge

The two natural sources that provide most of the recharge are precipitation and subsurface inflow. Annual precipitation in the study area averages about 45 inches, fifty percent of which is lost mainly by surface and near-surface evapotranspiration and by direct runoff. Direct runoff is reported to be approximately 5 to 15 percent of the total precipitation of the drainage basin (Perlmutter et. al., 1979). The remainder of the precipitation, which averages 22 inches annually, seeps down to the water table. Recharge from precipitation will be set 22 inches/year throughout the study area. Additional recharge, including cesspool, waterline leakage, and recharge basin effects will be taken directly from the regional model.

Discharge

Groundwater is discharged from the aquifers by subsurface outflow, withdrawal by pumping wells, seepage into Massapequa Creek, and evapotranspiration. Two public water supply well fields, operated by the Massapequa and South Farmingdale Water Districts, are located approximately 8,000 feet south/southeast of the site. These well fields withdraw groundwater from the Magothy aquifer. The pumping wells within the model domain will be incorporated in the model. The discharge into Massapequa Creek may be taken directly from the regional model.

3.1.5   Groundwater Flow Modeling

A detailed three-dimensional groundwater flow model will be constructed for the study area. The modeling of the groundwater flow system will be conducted with the USGS MODFLOW model. The model will be calibrated against observed head data in order to allow the subsequent prediction of COI migration under various remedial alternatives.

3.1.6   USGS MODFLOW Model Description

USGS MODFLOW (MacDonald and Harbaugh, 1988) is currently the most widely used groundwater flow model. It simulates groundwater flow in three dimensions by using a block-centered finite-difference approach. The subsurface can be described as a sequence of layers, each of which may contain cells of spatially varying properties. The model can handle unconfined, confined, leaky, or a combination of such conditions in any one of its model layers. Flow associated with wells, areal recharge, evapotranspiration, drains, and streams can be simulated.

3.1.7   Flow Model Calibration

The flow model will be calibrated against static groundwater conditions, as observed during the continued RI/FS. Monitoring wells will be installed at various vertical intervals in Upper Glacial and Magothy Aquifers well clusters, according to the revised monitoring well installation proposal, dated December 22, 1997. Measured water levels in each model layer will be checked against the simulated water levels during the calibration process.

The quality of a model calibration is expressed by plotting the observed versus calculated hydraulic head values. For a perfect calibration, the resulting data points fall onto a correlation line; for practical hydrogeological model applications, however, the observed versus calculated data points will scatter about this line. The model calibration will be further checked by computing the residual mean error. In addition, the residual mean will be normalized against the observed range of values (i.e. difference between maximum and minimum observed head value), in order to determine the quality of the model in the context of the site. The calibration statistics will be presented in the final report.

3.1.8 Sensitivity Analysis

Subsurface conditions can never be accurately defined, and any analysis based on assumptions (input parameters) regarding these conditions will result in some uncertainty. The major uncertainties involved with the prediction of the advective migration of COI at the site will be identified during model development. Thus, thorough sensitivity analyses of the flow model's input parameters will include magnitude and distribution of horizontal and vertical hydraulic conductivity, storativity, and recharge and may be conducted as part of the calibration process.

3.1.9 Input Parameters

Aquifer properties were collected from published sources and are presented in Table 2. Uniform aquifer properties will be assumed for each aquifer for the initial simulation. If necessary, these properties may be adjusted for each model layer during the calibration process.

The hydraulic properties of the Upper Glacial and Magothy aquifers on Long Island have been extensively studied, which allows a reliable estimation of aquifer properties in the study area. Horizontal hydraulic conductivity, K_H, in the Upper Glacial Aquifer were verified during the RI (Roy F. Weston, January 1994) by performing slug tests in selected on-site and off-site monitoring wells. The reported K_H ranged from 122 to 629 ft/day, which correspond well with established regional and local K_H of 270 ft/day (Franke, et. al., 1972). Dames & Moore will perform slug tests in selected on-site and off-site monitoring wells to verify local K_H with reported regional K_H of the Magothy aquifer.

It should be noted that slug tests determine the characteristics of a small volume of aquifer material surrounding the well. This aquifer material may have been disturbed during well installation. However, slug tests do provide fairly accurate estimates of local K_H. The vertical hydraulic conductivity, specific yield, and specific storage cannot be determined from slug tests.

The tabulated values (Table 2) of aquifer properties may be used as input parameters for initial simulation. Model calibration will be performed through a trial and error procedure in which aquifer properties are adjusted until a reasonable match between simulated water elevations and measured water elevations are obtained. The calibrated aquifer properties will be used for subsequent simulations.

3.2   Transport Model

3.2.1   Distribution of Constituents of Interest

The results of on-site and off-site groundwater screening were submitted to the EPA in the November 7, 1997 monitoring well installation proposal. The November 7, 1997 proposal contained plan view maps showing the concentrations of specific COI within the Upper Glacial and Magothy Aquifers, and cross section maps showing the vertical concentration distribution of specific COI. Note that, in general, the groundwater quality information needed to complete the conceptual models of inorganic and organic constituent source location(s), mass, and distribution will be based upon groundwater sampling of the proposed and existing monitoring wells.

3.2.2   Fate and Transport Processes

The processes governing the fate of the primary organic COI (PCE and TCE) are summarized in Table 3, and discussed below.

3.2.2.1 Physical Processes

Contaminants are transported in groundwater by advection, i.e., the movement of a solute at the speed of the average linear velocity of groundwater as given by:

$$v = \frac{K \, x \, i}{n_e} \qquad \text{(Eqn. 1)}$$

where, $K =$ hydraulic conductivity in the direction of groundwater flow
$i =$ hydraulic gradient in the direction of groundwater flow
$n_e =$ effective porosity

Another major physical process that affects contaminant movement in groundwater is dispersion. Dispersion refers to spreading of contaminants caused by the fact that not all of the contaminant actually moves at the same speed as the average linear velocity. Contaminant movement is strongly influenced by the presence of local heterogeneities that cause deviations from the average linear velocity. Typically, these deviations are assumed to be represented by a relation similar to Fick's law of diffusion. The dispersion term, D, is usually calculated from

$$D = \alpha \, x \, v + D^* \qquad \text{(Eqn. 2)}$$

where, α = Dispersivity
D^* = Coefficient of molecular diffusion

3.2.2.2 Chemical Processes

Sorption

Sorption and desorption describe the chemical solid-aqueous solution exchange potential and are often estimated by an equilibrium partition coefficient, K_d, and assumed to be linear. Under these assumptions, mass transfer is symmetrical with respect to the forward and backward direction. Estimates of K_d are typically used to determine a retardation factor for the COI, which is used in solute transport models and expressed as:

$$R = 1 + \frac{\rho K_d}{\omega} \qquad\qquad \text{(Eqn.3)}$$

where, R = retardation factor
ρ = soil bulk density
ω = soil moisture content.

K_d can be approximated by the following expression:

$$K_d = f_{oc} K_{oc} \approx f_{oc} 0.63 K_{ow} \qquad\qquad \text{(Eqn.4)}$$

$f_{oc} \equiv$ fraction organic carbon

$K_{oc} \equiv$ chemical organic carbon to water partition coefficient

$K_{ow} \equiv$ chemical octanol to water partition coefficient

Typical K_{ow} values for of the primary organic COI and their daughter-products (1,1-DCE, 1,2-DCE, and VC) are summarized in Table 4.

At many sites, however, a significant "tailing effect" in constituent concentrations has been observed during remediation. One potential explanation of this phenomena is the apparent slow desorption of constituents from soil matrices. Under these assumptions, sorption is non-linear (the forward rate of sorption differs from desorption) and can be approximated with a Freundlich-type expression. The rate of retardation due to sorption non-linearity is then inversely related to the constituent concentration (i.e., sorption increases as concentration decreases) and can be expressed as:

$$R = 1 + \frac{\rho K_d N}{\omega} C^{N-1} \qquad\qquad \text{(Eqn.5)}$$

where, R = retardation factor
ρ = soil bulk density

ω = soil moisture content

N is the Freundlich constant (N<1).

Precipitation / Dissolution

Precipitation and dissolution describe chemical aqueous solution-organic exchange potential and are characterized by the solubility of a compound. The solubility of the primary organic COI and their daughter-products are summarized in Table 4.

Volatilization

Volatilization describes how compounds behave at a gas-liquid surface such as the partitioning between air-water and air-organic systems. In dilute systems, the volatilization potential can be estimated from Henry's law constant and vapor pressure of a particular compound. In concentrated systems or when non-aqueous phase liquids (NAPL) exist, volatilization potential can be estimated using Raoult's law and the activity coefficient, mole fraction, and vapor pressure of a particular compound. Values of Henry's law constant, and vapor pressure for of the primary organic COI and their daughter-products are summarized in Table 4.

Diffusion

Molecular diffusion is the process that brings reactants into contact with each other and enables the physicochemical processes described above to occur. In addition, molecular diffusion transports chemicals across boundaries, for example, into a living cell, onto a particle surface, or across the air-water interface.

Combined, these physicochemical processes govern chemical equilibria and distribution between the four phases: aqueous, solid (including colloids), gas, and organic (NAPL). The thermodynamics and kinetics of these physicochemical processes will ultimately decide a compound's fate in a subsurface environment. For example, if a compound is sorbed to organic matter in the subsurface then it may not be readily available for microbial degradation or volatilization. The kinetics and thermodynamics of desorption, dissolution, and diffusion will then determine how quickly, if at all, a compound becomes available for these actions. Subsurface environmental conditions that affect physicochemical processes include pressure, temperature, pH, redox condition, and aqueous solution composition (organic solute and solvent, and inorganic salt concentrations).

3.2.2.3 Biological Processes

Potential Biodegradation Pathways

Biodegradation potential is dependent upon two factors: (1) the compound must be biodegradable, and (2) microorganisms capable of degrading the compound must be present and

evenly distributed in the impacted area. If these factors are not satisfied, then appreciable *in situ* biodegradation will not occur. Intrinsic (naturally occurring) biodegradation of chlorinated solvents, such as PCE and TCE, typically occurs under anaerobic conditions. One of the predominant mechanisms for transformation of chlorinated solvents is reductive dehalogenation. A brief review of anaerobic reductive dehalogenation and the specific anaerobic degradation pathway of PCE and TCE by this mechanism is presented below.

Anaerobic Reductive Dehalogenation

Anaerobic reductive dehalogenation results in the replacement of a halogen by hydrogenolysis or dihalo-elimination. The process proceeds sequentially until all halogens have been removed. The reductive process is usually supported through co-metabolism. Under this scenario, the halogenated organic compound acts as an alternative electron acceptor for either sulfate reducing or methanogenic bacteria. The reductive dehalogenation is carried out by electrons from the oxidation of the primary substrate (electron donor). The success of the process relies on a proper balance between appropriate electron acceptors and electron donors.

PCE and TCE Degradation Pathway

The microbially mediated degradation pathway of PCE and TCE is illustrated in Figure 2. As shown in Figure 2, PCE degrades sequentially to TCE, then to *cis*-DCE, and then to VC, and finally to ethane or ethene via reductive dehalogenation.

Biodegradation Kinetics

The kinetics of biodegradation must allow for the remediation to be completed in a reasonable time frame. The rate of *in situ* biodegradation is a complex function of intrinsic biokinetic parameters, mobile and immobile microorganism concentration, electron acceptor and contaminant physicochemical properties, and soil moisture content.

Currently there is no systematic methodology to quantitatively determine biodegradation kinetics *in situ*. Most often, an overall rate of *in situ* biodegradation is quantified by measuring the rate of consumption (disappearance) or production of indicator compounds. This method will be used to determine site-specific biodegradation rates for PCE, TCE, *cis*-DCE, and VC based on site-specific groundwater concentration data, and then compared to published values.

Another technique that may used to derive the site-specific biodegradation rates is an exponential regression analysis of contaminant concentration versus time data, measured at individual wells. Alternatively, a method developed by Bushcheck and Alcantar (1995) could be used to separate the contributions of advection, dispersion, sorption, and biological decay to the total observed decay rate. This technique uses constituent concentrations observed at multiple wells along a transect coincident with the predominant groundwater flow in an analytical solution to one-dimensional contaminant transport with first-order decay.

In either case, the site-specific biodegradation rate for each COI will then be used in the contaminant fate and transport model RT3D.

Microbial Inhibition Potential

Several factors may inhibit *in situ* biodegradation; these include: (1) low constituent bioavailability; (2) microbial metabolic requirements; and (3) the presence of toxins and grazing protozoa.

Contaminant Bioavailability

In the subsurface, biodegradation generally occurs in the pore and (soil) bound water phase, primarily by microorganisms that exist in biofilms immobilized on soil particle surfaces and suspended in pore water. In order for biodegradation to occur, the target constituent must therefore be in an aqueous phase, within the microenvironment of the acting microorganisms (Alexander, 1994). Inhibition of *in situ* biodegradation will occur when constituents are bound to soil matter through sorption processes, or are contained in an organic phase, or otherwise resist dissolution into an aqueous phase and are not bioavailable.

Microbial Metabolic Requirements

Microorganism metabolic requirements (or factors) can be divided into two groups: chemical and physical (Gaudy and Gaudy 1988). Of the chemical requirements, a carbon and energy source (electron donor), an electron acceptor, and proper nutrients are among the most important. Important physical factors are pH, temperature, and salinity. Physical factors in general act as selective agents by determining the types of organisms that can grow, and by influencing the growth rates of those organisms that can grow under the prevailing conditions. Inhibition of *in situ* biodegradation will occur when microorganism metabolic requirements are not met, and result in less than optimal microorganism growth conditions. The role of electron acceptors and electron donors in this process are discussed below.

Electron Acceptors

The availability of electron acceptors in anaerobic systems affects reductive dehalogenation by competing with the halogenated compounds for reducing potential. The influence of electron acceptors is explained by thermodynamic principles. Recalling that microorganisms will couple redox half reactions that yield the greatest free energy provides the basis for understanding these principles. In the absence of molecular oxygen, the electron acceptor successive levels are $Mn(IV)$, NO_3, $Fe(III)$, organic compounds, SO_4, and CO_2. In the case of reductive dehalogenation, "organic compounds" are analogous to chlorinated solvents. The specific influence of electron acceptors, however, can not be generalized. Different microbial systems and

different soil-water chemical conditions undoubtedly cause shifts in the thermodynamic equilibrium, and therefore, multiple electron-accepting processes are ongoing simultaneously.

Electron Donors

In general, almost any substrate that can be degraded anaerobically to either acetate or hydrogen will serve as an electron donor. Hydrogen and acetate are used by sulfate reducing microbes and/or methanogenic bacteria that use the chlorinated solvents as electron acceptors. If substrate is limited, ethanol or benzoate may be added as a supplemental substrate to further stimulate biological activity. Ethanol is rapidly degraded anaerobically resulting in the rapid production of hydrogen. Benzoate is more slowly degraded anaerobically resulting in a slower production of hydrogen.

Toxicity and Protozoa Grazing

The presence of toxins such as certain heavy metals and metabolic intermediates (e.g., daughter products and "suicidal enzymes") can also inhibit *in situ* biodegradation. In addition, protozoa grazing on indigenous bacteria can inhibit *in situ* biodegradation. This effect, however, is averaged out as the population of indigenous protozoa and bacteria rise and fall in response to each other.

3.3   Hydrogeochemical Model

3.3.1   Distribution of Constituents of Interest

The results of on-site and off-site groundwater screening were submitted to the EPA in the November 7, 1997 monitoring well installation proposal. The November 7, 1997 proposal contained plan view maps showing the concentrations of specific COI within the Upper Glacial and Magothy Aquifers, and cross section maps showing the vertical concentration distribution of specific COI. Note that, in general, the groundwater quality information needed to complete the conceptual models of inorganic and organic constituent source location(s), mass, and distribution will be based upon groundwater sampling of the proposed and existing monitoring wells.

3.3.2   Physicochemical Processes

Multiple physical and chemical processes affect the interaction of groundwater and soil and determine the fate of inorganic COI in the subsurface. These processes are listed in Table 5, along with example chemical reactions, and are discussed further below in the context of chromium and cadmium fate and transport in the subsurface. In contrast to chromium, cadmium [Cd(II)] is a simple metal that is not redox sensitive although other components of minerals containing Cd(II) may be affected by the redox potential of the subsurface.

3.3.2.1 Speciation

The dominant chromium species in groundwater are shown in Figure 3 along with the stability field for the chromium solid $Cr(OH)_3$. In the range of natural groundwater pH and under reducing to slightly oxidizing redox potential, cationic and neutral species of Cr(III) ($CrOH^{2+}$, $Cr[OH]_2^+$, and $Cr[OH]_3^0$) dominate with the solid $Cr(OH)_3$ and are stable over a large portion of the pH/Eh region. Under more oxidizing conditions, the Cr(VI) anionic species $Cr_2O_7^{2-}$ (dichromate), $HCrO_4^-$ (bichromate) and CrO_4^{2-} (chromate) are dominant (Nikolaidis et al., 1994; Rai et al., 1984). The groundwater pH at the Liberty site appears to be depth dependent, with higher pH values in the upper aquifer (6.0 to 6.8), and the lower pH values in the Magothy Aquifer (4.7 to 5.5).

The dominant cadmium species in groundwater are shown in Figure 4 along with the stability field for the cadmium solid CdS. In the range of natural groundwater pH and redox conditions, the cationic species of Cd(II) predominates. Under more reducing conditions, the neutral species CdS is stable, and at groundwater pH in excess of 9, the hydrolyzed cationic, neutral and anionic species of $CdOH^+$, $Cd(OH)_2^0$ and $Cd(OH)_3^-$ become dominant.

3.3.2.2 Complexation

In addition to hydroxyl and other inorganic species, Cr(III) may form complexes with organic acids (e.g., humic and fulvic acids) and water-soluble organic matter, thereby enhancing the mobility of chromium (James and Bartlett, 1983).

Cd(II) may undergo stepwise formation of complexes involving ligand species, such as chloride, hydroxides, and water soluble organic matter. In subsurface environments with pH values less than about 9, the formation of the complex $CdOH^+$ is unlikely, and cadmium-chlorine complexes will dominate.

3.3.2.3 Sorption

Cr(III) and Cd(II) exhibit typical cationic sorption behavior (Deutsch, 1997). Adsorption increases with pH as the adsorbent surface sites become more negatively charged and attractive to cations. Specific adsorption of Cr(III) onto iron and manganese oxides likely occurs under oxidizing conditions (Korte et al., 1976). Solid organic matter may also be an important sorbent, although complexation with dissolved organic ligands may reduce adsorption. Because of the low solubility of the reactive Cr(III) solid $Cr(OH)_3$, the effect of the Cr(III) sorption on chromium mobility is generally not considered an important factor (Deutsch, 1997).

The dominant Cr(VI) species, chromate, exhibits typical anionic sorption behavior. Adsorption decreases with increasing pH as the sorbent surfaces become more negatively charged. Adsorption also decreases when competing dissolved anions are present (Deutsch, 1997). Adsorption onto iron oxides and hydroxides has been shown to be suppressed by 50 to 80 percent

in the presence of typical groundwater concentrations of dissolved HCO_3^- and SO_4^2 (Zachara *et al.*, 1987). Orthophosphate (PO_4^{3-}) also competes for adsorption sites with chromate (Barlett and Kimble, 1976). Adsorption of chromate is not affected by the presence of cations.

The adsorption edge (i.e., the pH at which 50 percent of the total species of interest is sorbed) for Cd(II) sorption onto iron oxyhydroxides and aluminous oxides (i.e., clays) is located at pH values of about 5.5 to 6.5, and complete sorption will occur at a pH value of about 8. Adsorption of Cd(II) is suppressed by the presence of the sorption inhibitors (i.e., compounds that are competitively sorbed and, therefore, limit the sorption capacity for Cd) chloride and sulfate.

3.3.2.4 Dissolution / Precipitation

Mineral solubility is another geochemical process that affects the fate of inorganic constituents in the subsurface environment. The challenge in modeling mineral equilibrium is in selecting reactive minerals that might form in the subsurface. The solubility of a mineral can vary over many orders of magnitude and is dependent on such factors as the pH, Eh, ionic strength, and dissolved concentrations of ligands for each particular system. Because of the variability of mineral solubility, the concentration of chromium in groundwater, as limited by the solid concentrations, will be site-specific. The reactive minerals that are typically present in most subsurface environments are listed in Table 6, along with specific chromium and cadmium minerals.

3.3.2.5 Oxidation / Reduction

Oxidation-reduction processes play a major role in affecting the mobility of chromium because it is relatively mobile as Cr(VI) and immobile as Cr(III). It has been shown that where abundant reactive organic matter is present, Cr(VI) can be reduced to Cr(III) (Barlett and Kimble, 1976). Under somewhat acidic conditions, it has been found that Cr(VI) reduction by Fe(II) may occur. In that case, the reduction of chromium may be followed by the precipitation of the low-solubility solid $(Fe,Cr)(OH)_3$ (amorphous), depending on the prevailing pH (Eary and Rai, 1991). The natural sources of ferrous iron in the environment that may reduce chromate include residual amounts of reduced iron in minerals such as hematite and biotite. Other naturally occurring reductants such as dissolved sulfides have also been shown to be capable of reducing Cr(VI) (Schroeder and Lee, 1975).

The rate of reduction of Cr(VI) to Cr(III) increases with decreasing pH (Henderson, 1994). At pH values near 5, the half-life of Cr(VI) is ca. one month, whereas at a pH of 7 the half-life may be several years (Deutsch, 1997). In the case where ferrous iron is the reductant, the pH effect may be due to the greater solubility of iron minerals under low-pH conditions and the resulting higher dissolved concentration of Fe^{2+}. In general, the redox condition of most subsurface environments favors the reduction of Cr(VI) to Cr(III); however, it has been shown that oxidized manganese in the form of $MnOOH$ and MnO_2 can oxidize Cr(III) to Cr(VI) (Barlett and James, 1979). This oxidation is fairly slow under slightly acid to basic conditions and is probably limited

by the solubility of $Cr(OH)_3$ (Eary and Rai, 1987). Cr(III) does not appear to be significantly oxidized by the presence of dissolved oxygen in natural water (Eary and Rai, 1987).

3.3.3 Mathematical Modeling Approach

The coupling of a complete geochemical modeling code such as MINTEQA2 (Allison *et al.* 1991) with a finite difference or finite element transport code (MODFLOW/RT3D) has not been considered a feasible approach to mass transport modeling with extensive geochemical reactions because of the computationally intensive requirements of modeling the geochemistry at each node of the grid. An approach that has lent itself to solving complex chemical interactions is the 'mixing cells in series' concept. In this approach, a packet of water influenced by physical and chemical processes is followed along a flow path. Physical processes affect the rate of flow and transfer of mass by dispersion and diffusion with adjacent packets. Geochemical processes allow for mass transfer between the solution and solid phases and a gas phase. The physical and geochemical transport processes are calculated separately and then combined to couple the processes (Deutsch, 1997). This approach will be adopted using MODFlOW and RT3D to simulate the physical processes, and MINTEQA2 to simulate the geochemical processes.

Initially, the unique composition (speciation) of inorganic COI in each area (or areas with significantly different geochemistry) will be determined by running MINTEQA2 separately for each area. Temporal and spatial changes in chemical composition from dissolution / precipitation and sorption / desorption processes will be simulated by using the non-equilibrium Mass-transfer-limited Sorption (or dissolution) Model option available in RT3D.

The groundwater and soil parameters that may be evaluated for the organic and inorganic COI fate and transport modeling are listed in Table 7 and Table 8, respectively. It may not be necessary to evaluate all of the parameters that are listed (e.g., an easily measurable parameter such as chloride may be used a proxy for other halogen sorption inhibitors, using accepted abundance ratios). The groundwater parameters (unless otherwise specified in the CRI/FS work plan) will be evaluated from selected Upper Glacial and Magothy aquifer wells. The soil parameters will be evaluated from selected on-site and off-site stratigraphic characterization borings.

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TABLE 1
MODEL LAYER GEOMETRY

Layer No.	Thickness (feet)	Aquifer
1	not specified	Upper Glacial
2	25	Upper Glacial
3	25	Upper Glacial
4	25	Upper Glacial
5	50	Magothy
6	50	Magothy
7	100	Magothy
8	100	Magothy
9	200	Magothy
10	200	Magothy

Note: Layer 1 will contain the water table;
the water table position will be calculated
iteratively by the model and therefore
the thickness for layer 1 is not specified.

TABLE 2
FLOW MODEL INPUT PARAMETERS FOR INITIAL SIMULATION

Input Parameters	Start-up Value	Source
Longitudinal Horizontal Hydraulic Conductivity, K_x ft/day	Upper Glacial = 270 Magothy Formation = 50	Franke, et. al., 1972
Horizontal Hydraulic Conductivity, K_y, ft/day	Upper Glacial = 270 Magothy Formation = 50	Franke, et. al., 1972
Vertical Hydraulic Conductivity, K_z, ft/day	Upper Glacial = 27 Magothy Formation = 1.4	Franke, et. al., 1972
Specific Yield, S_y	Upper Glacial = 0.24	Warren et. al., 1968
Specific Storage, S_s, , ft^{-1}	Magothy Formation = 6×10^{-7}	Buxton, et. al., 1985
Porosity, n	Upper Glacial = 0.30 Magothy Formation = 0.25	Franke, et. al., 1972 Warren et. al., 1968
General Head Boundary, H, ft		Solution of Regional Model
Recharge, inches/year	Upper Glacial = 22	Warren et. al., 1968
Evapotranspiration, inches/year	Upper Glacial ~ 0	Wexler, et. al., 1988
Seepage Rates		Regional Model
Well Fields		Well location, screen interval, and pumping rate of all pumping wells within the model domain will be determined and included in the model

TABLE 3
PROCESSES GOVERNING THE FATE OF ORGANIC CONSTITUENTS

Physical	*Chemical*	*Biological*
Advection	Sorption	Potential Biodegradation Pathways
Dispersion	Precipitation / Dissolution	Biodegradation Kinetics

	Volatilization	Microbial Inhibition Potential
		    - Contaminant Bioavailability
		    - Metabolic Requirements
		    - Toxins

	Diffusion	

TABLE 4
PHYSICAL / CHEMICAL PROPERTIES OF ORGANIC CONSTITUENTS

Compound	Specific [a] Gravity	K_{ow} [b]	Solubility [b] (20°c) (mg/L)	Vapor Pressure [c] (mm Hg)	Henry's Constant [c] (atm-m^3/mol)
PCE	1.63	398	150	17.8	0.0259
TCE	1.47	240	1,100	57.9	0.0091
1,1-DCE	1.25	69.2	400 - 2,500	600	0.034
1,2-DCE	1.27	3.02 - 5.01	600 - 6,300	208 - 324	0.00656 - 0.00758
VC	0.91	2.4	1.1 - 60	2660	0.0819

Sources:

a   Deutsch, W.J. 1997. *Groundwater Geochemistry: Fundamentals and Applications to Contamination.* Lewis Publishers. New York, NY.

b   USEPA. 1990. Basics of Pump-and-Treat Ground-Water Remediation Technology. EPA-600-8-90/0003. March.

c   Schwarzenbach, R.P., P.M. Gschwend, D.M. Imboden. 1993. Environmental Organic Chemistry. John Wiley & Sons, Inc. New York, NY.

TABLE 5
PROCESSES GOVERNING THE FATE OF INORGANIC CONSTITUENTS

Process	*Example Chemical Reaction*
Ion Speciation	$Cr(OH)_2^+ + H^+ \leftrightarrow Cr(OH)^{2+} + H_2O$ $Cd(OH)^+ + H^+ \leftrightarrow Cd^{2+} + H_2O$
Ion Complexation	$Cr(OH)_2^+ + Cl^- + 2H^+ \leftrightarrow CrCl^{2+} + 2H_2O$ $Cd(OH)^+ + Cl^- + H^+ \leftrightarrow CdCl^+ + H_2O$
Mineral Dissolution/Precipitation	$Cr(OH)_2^+ + H_2O \leftrightarrow Cr(OH)_3\,(a) + H^+$ $Cd(OH)^+ + H_2O \leftrightarrow Cd(OH)_2\,(a) + H^+$
Oxidation/Reduction	$Cr(OH)_2^+ + O_2 \leftrightarrow CrO_4^{2-} + 2H^+$
Adsorption/Desorption	$CrO_4^{2-} + Fe(OH)^{2+} \leftrightarrow FeOH \cdot CrO_4$ $Cd^{2+} + Fe(OH)^{2+} \leftrightarrow FeOH \cdot Cd$

TABLE 6
TYPICAL REACTIVE MINERALS IN THE SUBSURFACE ENVIRONMENT

Carbonates	*Oxides / Hydroxides*
Calcite [$CaCO_3$]	Ferrihydrite [$Fe(OH)_3$]
Dolomite [$CaMg(CO_3)_2$]	Goethite [$FeOOH$]
Siderite [$FeCO_3$]	Gibbsite [$Al(OH)_3$]
Rhodochrosite [$MnCO_3$]	Pyrolusite [MnO_2]
Magnesian Calcite [$(Ca,Mg)CO_3$]	
Sulfates	*Sulfides*
Gypsum [$CaSO_4 \bullet 2H_2O$]	Pyrite [FeS_2]
Alunite [$KAl_3(SO_4)_2(OH)_6$]	Mackinawite [Fe/S]
Jarosite [$KFe_3(SO_4)_2(OH)_6$]	Orpiment
Jurbanite [$AlSO_4(OH)_6$]	
Silica	*Silicates*
Chalcedony	Clays
Amorphous Silica [SiO_2 am]	Zeolites

Chromium Specific Minerals

Oxidizing Conditions	*Reducing Conditions*
Chromite Cr_2O_3	$Cr(OH)_3$ amorphous
Chromatite ($CaCrO_4$)	$(Fe,Cr)(OH)_3$
Hashemite ($BaCrO_4$)	$FeCr_2O_4$
Crocoite ($PbCrO_4$)	Cr_2O_3
Iranite ($PbCrO_4 \bullet H_2O$)	

Cadmium Specific Minerals

Oxidizing Conditions	*Reducing Conditions*
Otavite ($CdCO_3$)	Greenockite (CdS)
$Cd_3(PO_4)_2$	$Cd(OH)_2$ amorphous

Source: Adapted from Deutsch (1997)

TABLE 7
GROUNDWATER PARAMETERS FOR GEOCHEMICAL MODELING

Data	Use
Major Ions Ca^{2+}, Mg^{2+}, Na^+, K^+, HCO_3^-, CO_3^{2-}, Cl^-, NO_3^-	Calculation of solution complexes; calculation of ionic strength and solute activity; saturation indices for minerals with these components
pH	Ion speciation / complexation and mineral solubility
Eh and Redox Potential	Ion speciation / complexation and mineral solubility of redox-sensitive elements
Dissolved Gases O_2, CO_2	Qualitative measure of redox potential Stability of groundwater pH
Minor / Trace Elements Fe, Mn, Al	Clay and oxyhydroxide mineral equilibria
Trace Metals Ba, Cr, Pb, Cu, Zn Hg, Cd	Mineral equilibria, competitive adsorption
Trace Semi-Metals As, Se	Mineral equilibria, competitive adsorption
Trace Non-Metals F, Br, P	Complexation, mineral equilibria, competitive adsorption
Organic Compounds VOCs Humic / Fulvic acids	Complexation, oxygen consumption, sorption and redox reactions

Source: Adapted from Deutsch, 1997.

VOCs and major and trace metals contained in TAL inorganics will be collected from existing and new monitoring wells, according to the SAP. Field measurements, using flow-through-cells will include pH, redox potential and dissolved oxygen. Analyses for major anions, dissolved carbon dioxide, and humic and fulvic acids will be performed from selected groundwater samples throughout the impacted area. Chlorine data may be used as proxies for fluorine and bromine, using accepted abundance ratios.
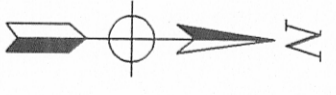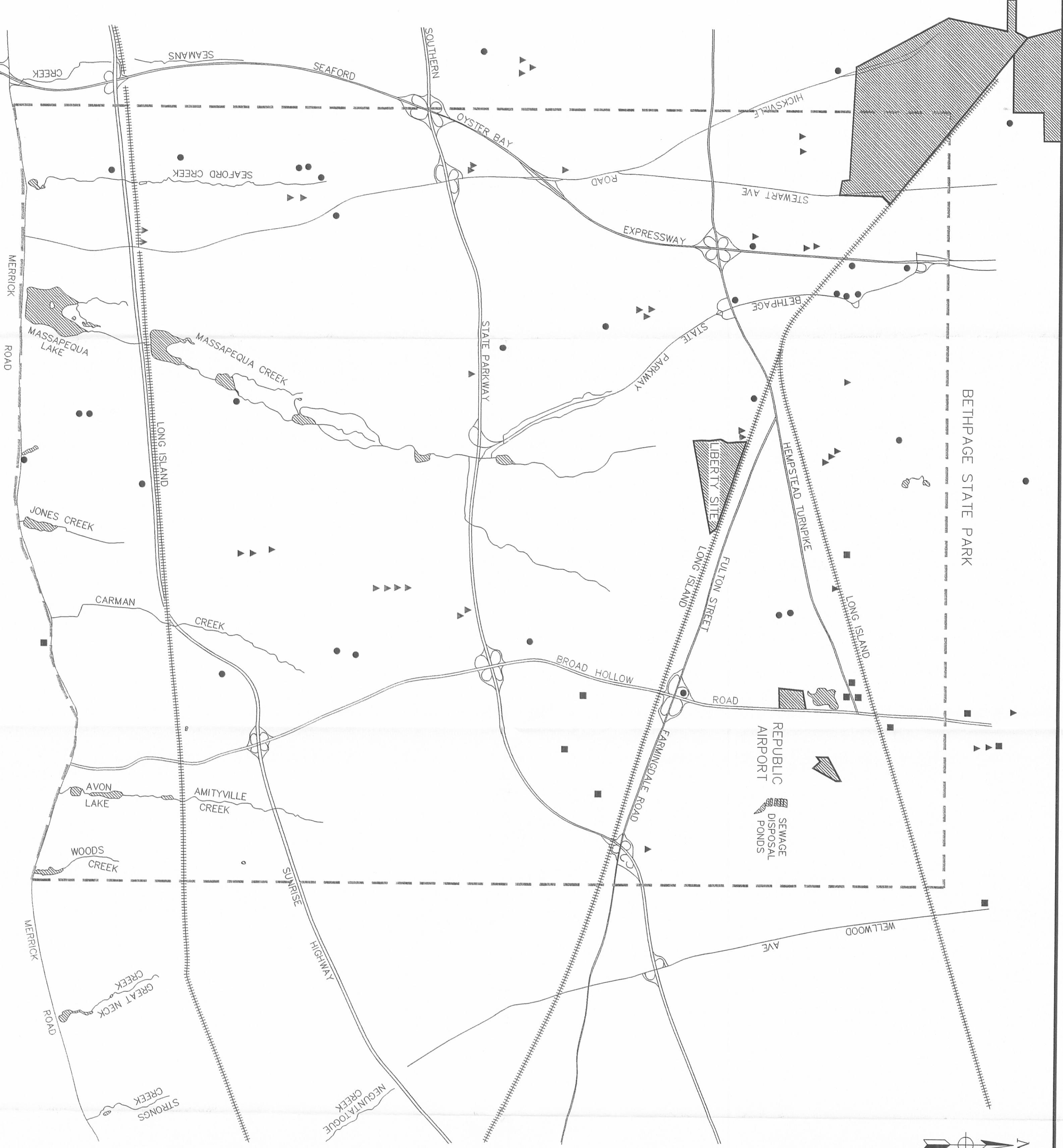
TABLE 8
SOLID PHASE PARAMETERS FOR GEOCHEMICAL MODELING

Constituent of Solid Phase	Potential Impact on System
Calcite	Mineral solubility control on solution concentration, partial measure of neutralization capacity
Gypsum	Mineral solubility control on solution concentration
Dolomite	Source of constituents to solution, partial measure of neutralization capacity
Clay mineral identification, quantification & cation exchange capacity	Exchange sites for major cations, mineral solubility control on solution concentration
Ferric and Manganese oxyhydroxides	Mineral solubility control on solution concentration, adsorption substrates for minor/trace elements
Pyrite	Mineral solubility control on solution concentration, source of acidity under oxidizing condition
Silicate Minerals	Sources of many dissolved constituents
Organic Carbon	Adsorbent medium for organic and inorganic compounds, reducing agent, source of dissolved carbon

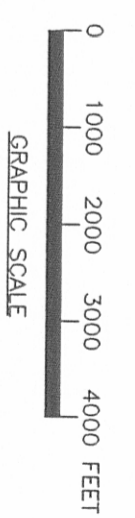Source: Adapted from Deutsch, 1997

At least two stratigraphic characterization borings will be completed during the well installation program, according to the revised monitoring well installation proposal, dated December 22, 1997. Selected soil samples collected from these borings will be analyzed for grain size, mineral abundance by x-ray diffraction (major silicates, calcite, gypsum, dolomite, oxides and hydroxides, pyrite), cation exchange capacity, and fractional organic carbon.

NOTE:
ALL FEATURES ADAPTED FROM AMITYVILLE, NEW YORK, 7.5' QUADRANGLE.

SEAMANS CREEK

SEAFORD

SOUTHERN

OYSTER BAY

SEAFORD CREEK

HICKSVILLE

STEWART AVE

ROAD

EXPRESSWAY

BETHPAGE

MERRICK ROAD

MASSAPEQUA LAKE

MASSAPEQUA CREEK

LONG ISLAND

STATE PARKWAY

BETHPAGE STATE PARKWAY

BETHPAGE STATE PARK

JONES CREEK

LIBERTY SITE

HEMPSTEAD TURNPIKE

FULTON STREET

LONG ISLAND

LONG ISLAND

CARMAN CREEK

BROAD HOLLOW

ROAD

REPUBLIC AIRPORT

SEWAGE DISPOSAL PONDS

FARMINGDALE ROAD

AVON LAKE

AMITYVILLE CREEK

WOODS CREEK

SUNRISE HIGHWAY

MERRICK ROAD

GREAT NECK CREEK

STRONGS CREEK

NEGUNTATOGUE CREEK

WELLWOOD AVE

N

GRAPHIC SCALE
0   1000   2000   3000   4000   FEET

EXPLANTION:

———— HEAVY-DUTY ROADS
———— MEDIUM DUTY ROADS
———— WATER BODIES
+++++ RAILROADS
● MONITORING WELL
▶ WATER SUPPLY WELL
◤ SUPERFUND SITE
▶ MASSAPEQUA WATER DISTRICT SUPPLY WELL
▶ SOUTH FARMINGDALE WATER DISTRICT SUPPLY WELL
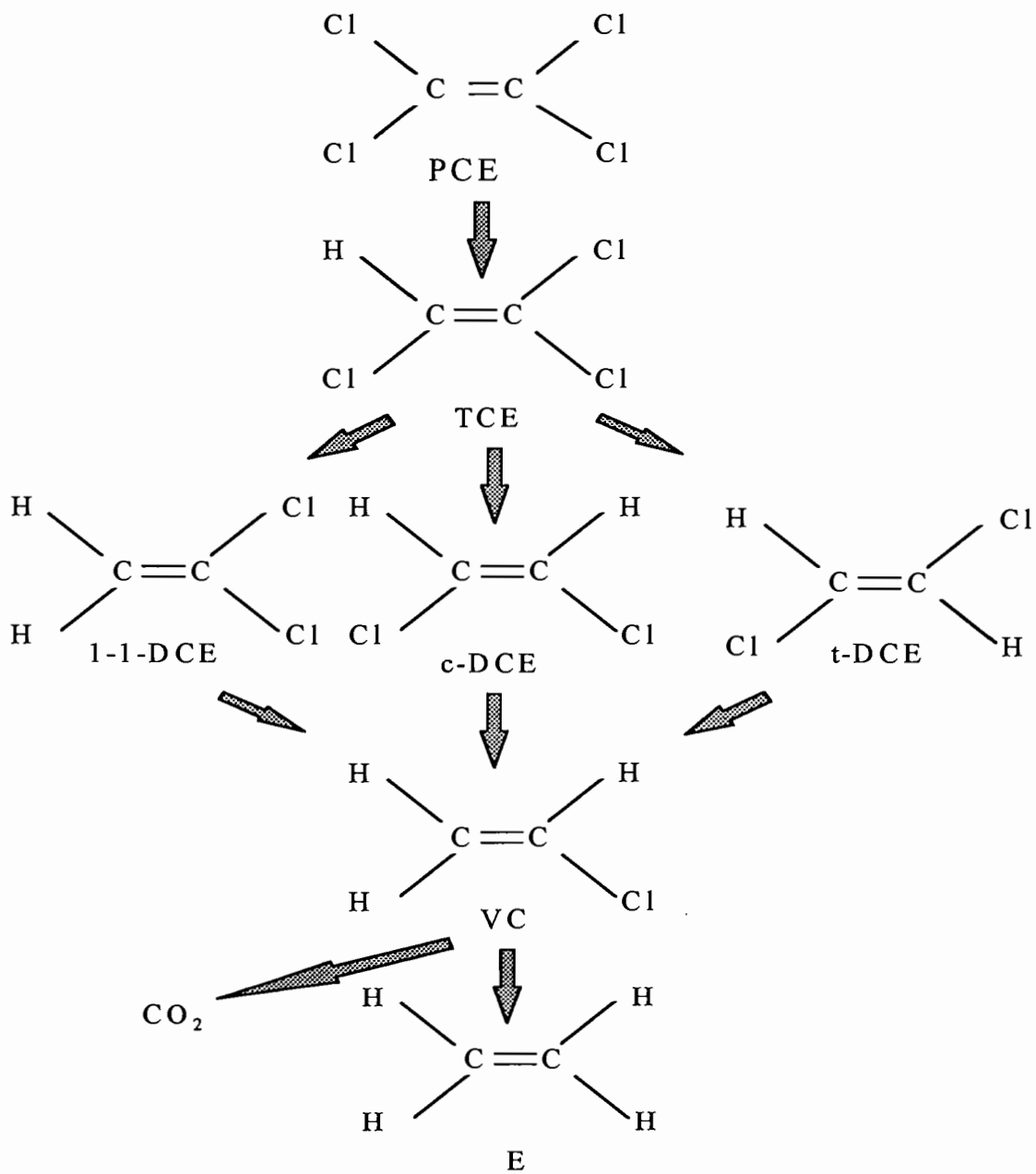■ PROPOSED MODEL DOMAIN

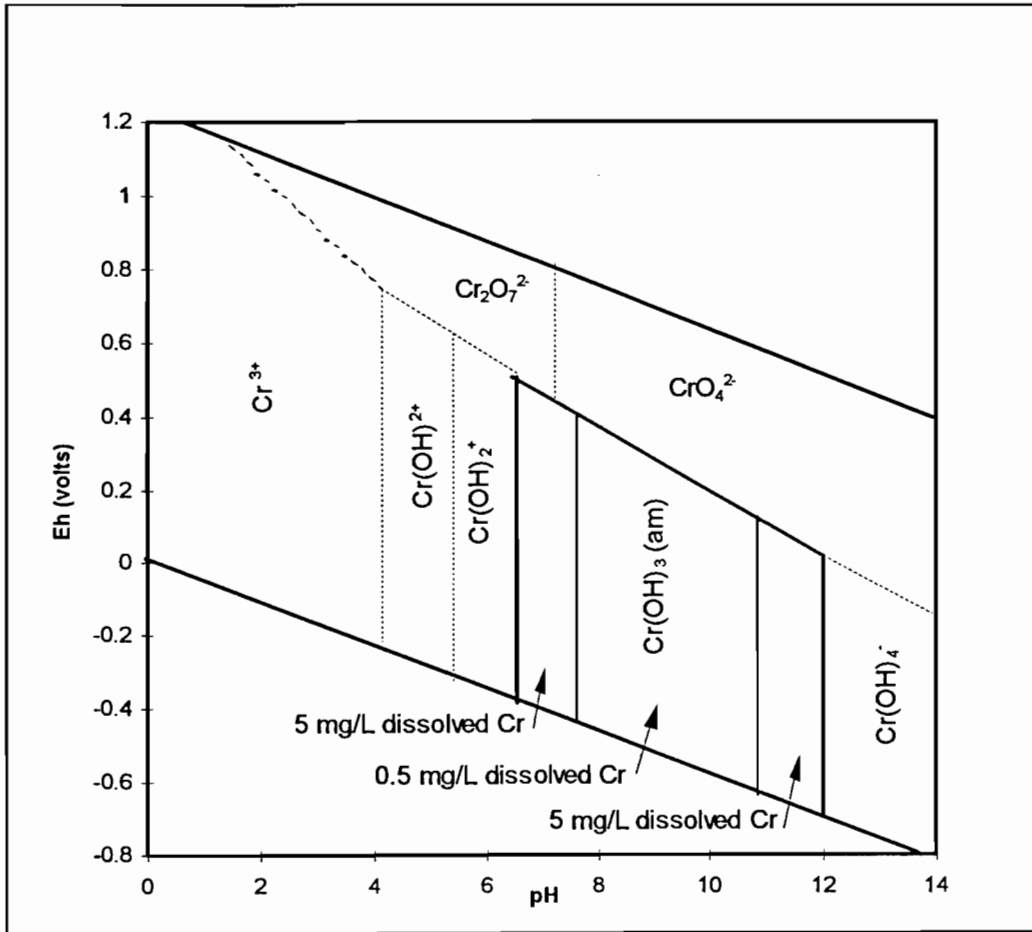**FIGURE 2   ANAEROBIC DEGRADATION PATHWAY OF PCE, TCE, DCE, and VC**

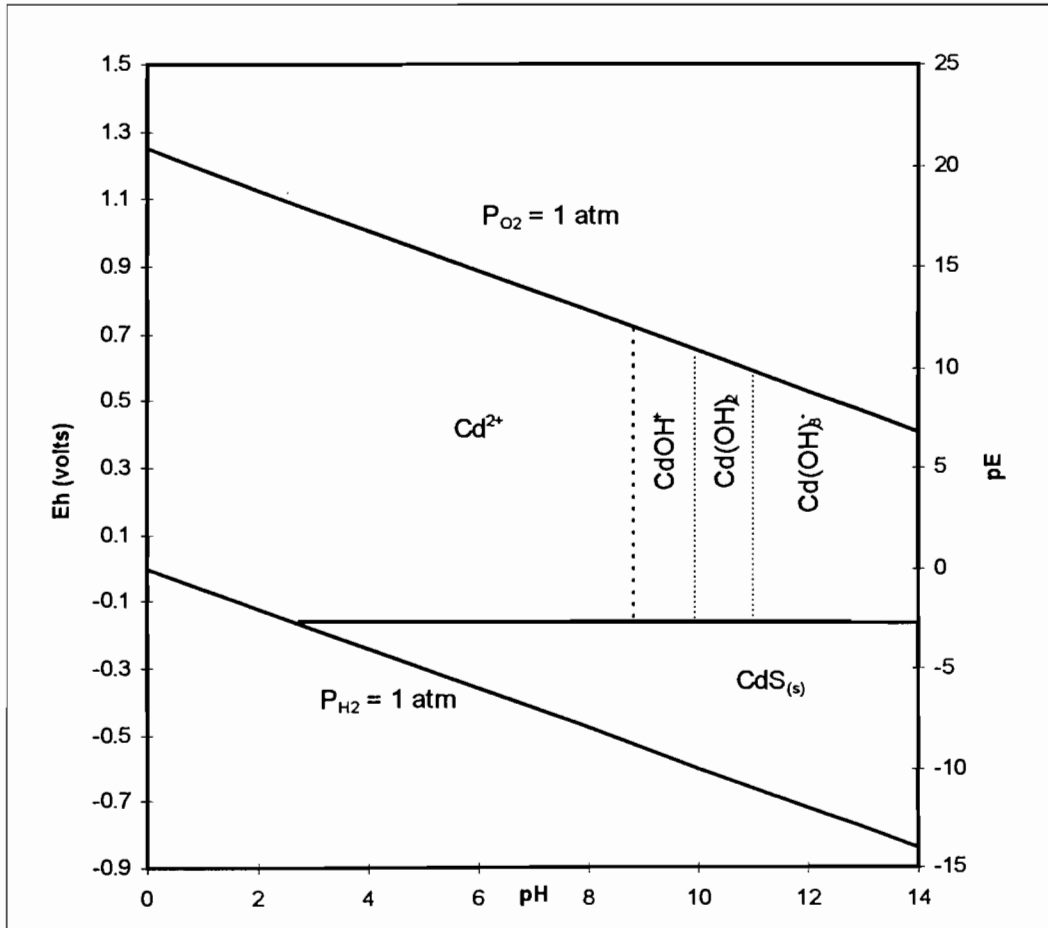**FIGURE 3   CHROMIUM SPECIATION AND MINERAL EQUILIBRIUM**

FIGURE 4   CADMIUM SPECIATION AND MINERAL EQUILIBRIUM

APPENDIX A
RESPONSE TO EPA COMMENTS

GENERAL COMMENTS

Comment 1:

The overall modeling approach presented in Dames & Moore's (D&M's) March 7, 1997 Fate and Transport Modeling Memorandum is generally well presented and thorough. The groundwater flow and trichloroethene (TCE) transport modeling are fairly straight forward efforts, and, other than some minor clarifications that are needed, are proposed well in the Memorandum. The hexavalent chromium modeling, however, is a more complex effort and requires a more involved analysis. The modeling programs MT3D and MINTEQA2 are useful and industry accepted tools for addressing the hexavalent chromium transport and geochemical issues. However, additional discussions need to be provided indicating how MINTEQA2 will be used to characterize the complex hexavalent chromium geochemistry, and how these results will be implemented in the MT3D model to adequately simulate the retardation of hexavalent chromium across the large Liberty contaminant plume and under variations in geochemical and hydraulic conditions. As stated in the cover letter, these additional specifics on how MINTEQA2 will be performed, as well as the following comments, unless otherwise stated, can be fully addressed in the conceptual flow model deliverable, to be submitted by D&M with its July 1997 Monthly Progress Report.

Response:

Section 3.3.3 of this deliverable provides detailed specifications on how MINTEQA2 will be performed.

Comment 2:

As explained in EPA's April 15, 1997, letter that transmitted the Agency's and the New York State Department of Environmental Conservation's (NYSDEC's) comments on Dames & Moore's February 20, 1997, Proposed Sample Location Maps, the recent regional groundwater flow and transport modeling conducted by the Nassau County Department of Public Works (NCDPW) for the South Farmingdale Water District (SFWD) and the Massapequa Water District (MWD) indicated that six of SFWD and MWD drinking water supply wells are directly downgradient of the Liberty site and, therefore, that there exists the potential impact of the MWD and SFWD supply wells by the Liberty groundwater contaminant plume. Due to the concerns raised by the NCDPW's modeling effort, boundary conditions for D&M's site-specific fate and transport model should be constructed south of the two SFWD drinking water supply wells (Wells N-05147 and N-06149) and the four MWD drinking water supply wells (Wells N-04602, N-05703, N-08214, and N-09173).

Response:

As shown in Figure 1, which indicated the proposed model domain, the boundary conditions for the site-specific fate and transport model will be constructed approximately 5,000 feet south of MWD drinking water supply wells.

Comment 3:

To ensure EPA's adequate review of D&M's fate and transport modeling effort, please submit, in accordance with software licenses, copies of the model manuals and codes, input files, and output files at least two weeks in advance of the submittal of the modeling results, which, according to the Administrative Order on Consent (Index No. II CERCLA-97-0203), are to be provided in the Operable Unit II (OU II) Remedial Investigation (RI) and Feasibility Study (FS) reports.

Response:

Copies of the model manuals and codes, input files, and output files will be submitted two weeks in advance of the submittal of the modeling results.

SPECIFIC COMMENTS

Comment 1

Section 1.0, Third Paragraph, Objectives: Please clarify what the difference is between the second and third objectives.

Response:

The third paragraph does not specify objectives; it specifies the individual phases of the modeling effort. The second phase, predictive mass transport modeling, is intended to predict the transport of constituents of interest (COI) under natural conditions. The third phase, remedial alternatives evaluation, may include, but not be limited to, several pumping scenarios in order to capture impacted groundwater. Other remedial alternatives may be evaluated.

Comment 2:

Section 2.0, Second Bullet, Conceptual Model: A preliminary groundwater flow and contaminant transport conceptual model is presented in this memorandum. A similar geochemical conceptual should also be presented, based upon the data generated during the OU II RI. More detailed flow, transport, and geochemical conceptual models should be provided in the July 1997 progress report.

Response:

Detailed flow, transport, and geochemical conceptual models have been prepared and are described in this submittal. Note that groundwater quality data will be based on groundwater sampling of existing and new OU II monitoring wells, according to the SAP.

Comment 3:

Section 2.0, Sixth Bullet, RI Report: EPA recommends that all efforts relating to the development, calibration, and performance of sensitivity analyses on the flow, transport and geochemical models be presented in the RI report.

Response:

All efforts relating to the development, calibration, and performance of sensitivity analyses on the flow, transport and geochemical models will be presented in the RI report.

Comment 4:

Section 4.0, Data Requirements: In order to adequately model the Magothy aquifer, the conceptual hydrogeologic model must discuss how the vertical gradient within the thick Magothy unit will be determined. This information will be needed to establish the model layering and what the lower boundary conditions will be and to what depth in the Magothy the numerical models will extend.

Response:

Monitoring wells will be installed in the form of well clusters at various vertical intervals in the Magothy Aquifer. Vertical hydraulic gradients can be determined from the static water level measurements within the well clusters. Measured water levels in each model layer will be checked with the simulated water levels during the calibration process. The model layers, boundary conditions, and vertical extent of the numerical models in the Magothy aquifer are described in Section 3.1.4 of this deliverable.

Comment 5:

Section 4.0, Sixth Bullet, Groundwater Quality Parameters: Please list what additional groundwater quality parameters (and soil analyses if anticipated) that will be collected are, and how they will be used to support the modeling efforts. Specifically, please indicate how the additional data will be used to develop appropriate distribution coefficients (Kd) for TCE and hexavalent chromium in the MT3D transport model, and whether the data will be used to vary the Kd spatially in the model.

Response:

Site groundwater and soil parameters that may be used for organic and inorganic constituent fate and transport modeling are listed in Table 7 and Table 8. Also listed in Table 7 and Table 8 are the intended uses of each of these parameters (it may not be necessary to evaluate all of the parameters that are listed; e.g., an easily measurable parameter such as chloride may be used a proxy for other halogen sorption inhibitors, using accepted abundance ratios). Soil fractional organic carbon data will be collected to better estimate the distribution coefficients (K_d) for trichloroethene (TCE) and chromium [Cr(VI) and Cr(III)] species. The groundwater concentrations of the trace metals, semi-metals, and non-metals listed in Table 7 will also be measured in selected samples to assess the potential for competitive adsorption between these compounds and chromium. In addition, the groundwater concentration of VOCs and, in selected samples, humic and fulvic acids will be used to assess the potential for chromium complexation, sorption and redox reactions which affect chromium mobility. These parameters will be measured at selected locations (both horizontally and vertically) to assess spatial variability. If necessary, spatially variable distribution coefficients will be used in model simulations.

Comment 6:

Section 5.0, Groundwater Flow Modeling: Please discuss in general the anticipated vertical and horizontal extent of the flow and transport modeling. What will the boundaries be for the model and are they natural hydrologic boundaries? What depth will the model be extended to, and approximately how many layers will it be? What surface water bodies will be included in the model? Because the available groundwater sampling data is more than three years old, the plume may have migrated further down gradient than it is currently mapped. Therefore, the numerical models need to extend beyond the currently mapped extent of the plume, especially if a natural attenuation option will be simulated.

In addition, as stated above, due to the concerns raised by the NCDPW's recent modeling effort that there exists the potential impact of the six MWD and SFWD supply wells by the Liberty groundwater contaminant plume, the model will need to extend far enough to include these supply wells and any other nearby municipal well fields, and incorporate their associated drawdown cones into the model baseline and predictive simulations.

Response:

Model Domain: The model grid may cover an area of approximately 29,000 feet by 23,000 feet (Figure 1). The southern boundary of the model domain may approximately follow the limits of the Merrick Road. The northern boundary of the model domain may extend to approximately 5,000 feet north of the Liberty site. The western boundary of the model domain may be defined to Hicksville Road in the northwest of the model domain and Oyster Bay Expressway in the southwest portion of the model domain. The eastern boundary of the model domain may extend to approximately 10,000 feet east of the Liberty site. The Massapequa Water District supply

wells and South Farmingdale Water District supply wells that will be encompassed by the model domain are also shown in Figure 1.

Model Layers: The model may consist of a grid of ten layers. The first four layers may represent the Upper Glacial Aquifer, which has a saturated thickness of approximately 75 feet in the Liberty site area. The remaining six layers may represent the Magothy aquifer, which is approximately 700 feet thick. The domain may be subdivided into ten model layers in order to allow an appropriate representation of vertical velocity variations and vertical variations in COI concentrations in aquifers. Vertical velocity components are induced by the partially penetrating pumping wells and other three-dimensional hydrogeological features such as the various creeks, and lakes. The tops and bottoms of the model layers will be chosen such that they follow approximately the topographical surface and the water table. This may result in a relatively complex model geometry within each layer. The approximate layer thicknesses are presented in Table 1. Within each layer, all cells will be of equal thickness. Thus, the shape of each layer top and bottom will be identical, but the absolute elevation of the layers may differ by the layer thickness.

Boundary Conditions: A groundwater divide, along which no-flow conditions are imposed, is present approximately 5 miles north of Liberty site. The major surface water feature is the Atlantic Ocean, located approximately 5 miles south of Liberty site. There is no significant hydraulic boundaries (specified head, no-flow, or specified flow) within 5 miles east or west of Liberty site. It is sometimes not possible to choose the physical boundaries of the aquifer when designing a model for a hydrogeological site investigation. In these cases, hydraulic boundaries are selected based on knowledge of the flow system. Typically, information is available on the general configuration of the regional flow system, but site information may be sufficient to deduce long-term flow patterns. One approach consists of designing a nested set of grids so that the site grid, which has the finest nodal spacing, is embedded in a regional grid with coarser nodal spacing. The solution of the regional model is then used to define boundary conditions of the site model. Boundaries defined in this way are sometimes called artificial boundaries.

The hydraulic boundary conditions for the Liberty site may be based on the Nassau County Department of Public Works (NCDPW) Regional Groundwater Flow Model. However, necessary modifications of this model may be made to characterize the localized hydrogeologic conditions of the study area. The NCDPW Regional Groundwater Flow Model is a calibrated representation of multiple aquifer system underlying Nassau, Queens, and Western Suffolk Counties. The boundaries of the regional model were Long Island Sound and Atlantic Ocean. The nodal spacing of the regional model is approximately 5,000 feet. However, a smaller local grid will be developed within the regional grid.

Representation of Surface Water Bodies: The interactions between the aquifers and the Massapequa Creek, ponds, and Massapequa Lake within the Massapequa Preserve will be in incorporated in the model. Additional surface water bodies in the model may include Seaford Creak within the Tackapausha Preserve, Jones Creek, Carman Creek, Amityville Creek, and

Woods Creek. The surface water bodies will be represented as features that either supply water or act as drains, depending on the local flow conditions in the aquifer. The water levels in the surface water bodies will be set in accordance with ground surface data obtained from the corresponding USGS topographic maps (Amityville, N.Y.). A limited amount of data on water levels within the model domain may be collected during remedial investigation studies. Where available, these data will be used to confirm or adjust the water levels specified in the model.

Comment 7:

Section 5.2, Sensitivity Analysis: In order to adequately evaluate the models' uncertainty, sensitivity analysis runs should be conducted under the calibrated (non-pumping) conditions, and also under the hydraulic stresses that are simulated in the FS Report, such as pumping, etc.

Response:

Sensitivity analysis runs will be conducted under the calibrated (non-pumping) conditions. Additional sensitivity analysis runs under the hydraulic stresses that may be simulated in the FS Report (such as pumping, etc.) may be performed, if deemed necessary.

Comment 8:

Section 6.1, First Paragraph, Biodegradation: TCE naturally biodegrades to other daughter products such as dichloroethene, vinyl chloride, and eventually ethene. However, under natural conditions, this is typically a relatively slow process and, therefore, it is difficult to predict the biodegradation rate. Is it anticipated that any biodegradation will be assumed for TCE, and if so, how will the biodegradation rate be estimated?

Response:

A term for TCE biodegradation will be included in the constituent fate and transport modeling. The TCE biodegradation rate will be derived from site-specific groundwater TCE concentration data, and compared to published values. One technique that may be used to derive the site-specific biodegradation rates is an exponential regression analysis of constituent concentration versus time data, measure at individual wells. Alternatively, a method developed by Bushcheck and Alcantar (1995) could be used to separate the contributions of advection, dispersion, sorption, and biological decay to the total observed decay rate. This technique uses constituent concentrations observed at multiple wells along a transact coincident with the predominant groundwater flow direction (downgradient from the contaminant source) in an analytical solution to one-dimensional transport with first-order decay.

In either case, the site-specific biodegradation rates will then be used in the model RT3D (Clement, 1997) to simulate contaminant transport. RT3D has extended reaction capabilities that will allow for simulation of reductive anaerobic (first-order sequential) biodegradation of

tetrachloroethene (PCE), TCE, *cis*-1,2-dichloroethylene (*cis*-DCE), and vinyl chloride (VC). If this approach is adopted, site-specific biodegradation rates for *cis*-DCE and VC will also be derived and compared to published values.

Comment 9:

Section 6.1, MT3D Transport Model Simulations: One of the challenges of the Liberty transport modeling effort is that the plume is so large (more than 1.5 miles long). The numerical models will need to be at least two layers (possibly more), with relatively small model nodes located around pumping centers and large concentration gradients. This will require a relatively large number of active model nodes during the transport model scenarios. Please explain how this memory and simulation time problem will be addressed, without compromising the model predictions.

Response:

Computers equipped with Pentium II processors that operate at speeds of 233 to 300 MHz, and 64 to 96 megabytes of RAM will be used for the transport modeling. Computer memory and model simulation time requirements, therefore, are not anticipated to be problem.

Comment 10:

Section 6.2, MINTEQA2 Modeling: In natural systems, chromium exists in either the trivalent (+3) or hexavalent (+6) oxidation (valence) state. Both pH and oxidation potential (Eh) affect the chromium species present in groundwater. The hexavalent form is extremely soluble and moves readily in groundwater, whereas the trivalent form may exist in soluble form or precipitate as a chromium hydroxide under neutral or high pH conditions. Both forms are also affected by sorption onto the aquifer soils under certain conditions. Data collected during the original RI indicate that chromium exists in groundwater at the site in the soluble hexavalent form, and in both the soluble and insoluble trivalent form (January 1994 RI Report).

D&M proposes to model transport of two contaminants, TCE and hexavalent chromium. MINTEQA2 is an equilibrium model that will indicate if a water quality sample is undersaturated, supersaturated, or in equilibrium with respect to the minerals which make up the aquifer matrix. It will also indicate the speciation, hence mobility, of the various inorganic complexes present. MINTEQA2 is proposed to be used to simulate equilibrium concentrations of hexavalent chromium (presumably for groundwater samples that will not be analyzed for hexavalent chromium, but only total chromium). It is assumed but not specifically stated that the reasoning is that the retardation and dissolution factors in the MT3D model would then be adjusted, depending on the proportions of species of chromium (i.e., hexavalent and trivalent forms retard differently and have different solubilities in groundwater systems). The accuracy of the speciation results from MINTEQA2 are affected by many variables, including organic compounds such as TCE, which cannot be accounted for in the model.

Given the current site conditions and the hydrogeochemical modeling as proposed by D&M, EPA provides, below, the specific comments that need to be addressed for further clarification:

Comment 10a

A geochemical conceptual model is usually presented to support the selection and procedures for use of a geochemical model. A clear understanding of the site's groundwater/contaminant chemistry is essential for selecting a suitable model. A geochemical conceptual model should be presented to support the proposal. This should include how colloidal transport of chromium will be addressed.

Response

A geochemical conceptual model is presented in Section 3.2 and 3.3 of this deliverable to aid in selecting a suitable mathematical model. The issue of colloidal transport of chromium will require further investigation. One potential method of addressing this issue might be to simulate colloidal transport as a mobile solid phase that may contain sorbed chromium species (e.g., chromium-iron oxyhydroxides) or colloidal-sized minerals containing chromium.

Comment 10b

MINTEQA2 should generally not be used in place of actual data to estimate hexavalent chromium values because too many variables are known to affect chromium speciation. These variables translate to additional data needs which were not originally proposed in the February 1995 Sampling and Analysis Plan (SAP), prepared by Roy F. Weston, Inc. Variables that determine speciation include dissolved oxygen, sulfur, organic matter, mineralogy of the aquifer soils, manganese oxide coatings on the aquifer soils, and iron (dissolved and oxide coatings on aquifer soils). In addition, the concentrations of dissolved Cr^{+3} species are affected by precipitation, sorption, and complexation processes, which are functions of pH, Eh, and concentrations of the anions sulfate, nitrate, chloride, and fluoride, and various ligands (Vertical Distribution and Partitioning of Chromium in a Glaciofluvial Aquifer, Nikolaidis *et al, Ground Water Monitoring and Remediation,* Summer 1994, p. 150-159).

As with any model, the accuracy of the modeling results is directly dependent on the accuracy and completeness of the input data. The proposal should, in general, evaluate the relative advantages and disadvantages of measuring hexavalent chromium directly versus indirectly with MINTEQA2. Specifically, a discussion should be provided whether any of these additional data will be collected; how they will be collected; and, if not, how the accuracy of the model results will be impacted.

Response:

To address these additional data needs, groundwater and soil samples will be collected at selected locations (both horizontally and vertically) throughout the impacted area. The samples will be analyzed for the parameters listed and qualified in Table 7 and 8 of this submittal. The metal constituents (including hexavalent chromium) in the groundwater samples will be analyzed as total and dissolved samples, according to the SAP. This will be accomplished through the collection of field filtered (0.45 µm in-line filter) groundwater samples.

Comment 10c

MINTEQA2 requires the use of dissolved (filtered) samples; otherwise model results may appear supersaturated with respect to mineralogy, if the total (unfiltered) metals are greater than dissolved metals. Therefore, samples to be used for MINTEQA2 should be filtered in the field, unless it can be demonstrated that unfiltered metals are not significantly different from filtered metals. Sampling for dissolved metals may go beyond the scope of sampling included in the site February 1995 SAP.

Response:

See response to #10b.

Comment 10d

Oxidation potential (Eh) is difficult to measure in the field. The proposal should describe how this will be measured.

Response:

Oxidation/reduction (redox) potential will be recorded while purging groundwater from monitoring wells at a low flow rate (less than 0.4 L/min or the minimum capabilities of the pump) in accordance with the USEPA Region I Draft SOP - "Low Flow (minimum stress) Purging and Sampling Procedure for the Collection of Groundwater Samples from Monitoring Wells". A flow-through-cell will be used while measuring all groundwater field parameters, including redox potential.

Comment 10e

The potential exists at the Liberty site for the aquifer soils to represent a future continuing source of metals to groundwater from desorption. Temporal or spatial variations of changes (such as pumping, pH and Eh) may result in significant changes or differences in speciation, and consequently, changes in sorption of chromium onto the aquifer soils. The MT3D transport model can simulate desorption as long as Kd remains constant. However, Kd can change or vary

spatially as the chromium speciation changes. The proposal does not discuss how speciation temporal changes or spatial variations and potential desorption of metals will be evaluated, and what role, if any, MINTEQA2 will play.

Response:

As previously stated, groundwater and soil samples will be collected at selected locations (both horizontally and vertically) and analyzed for the constituents listed and qualified in Tables 7 and 8. These parameters will then be evaluated for spatial variations. If spatial variations are identified, multiple organic or inorganic source areas can be simulated in RT3D. The unique composition (speciation) of inorganic COI in each area can be determined by running MINTEQA2 (Allison *et al.*, 1991) separately for each area. Temporal changes in source composition from dissolution / precipitation and sorption / desorption processes will be simulated by using the non-equilibrium Mass-transfer-limited Sorption (or dissolution) Model option available in RT3D. In addition, RT3D allows for user-defined reactions to be used. With this capability, the user can defined any kinetic or equilibrium geochemical reaction.

Comment 11:

Section 6.2, third paragraph, Dissolution: The last sentence indicates that the results of the MINTEQA2 modeling will be used as input into the MT3D model by adjusting factors such as retardation and dissolution. However, the text in the second paragraph of section 6.0 indicates that MT3D cannot simulate dissolution. Please clarify.

Response:

A recently released contaminant fate and transport model, RT3D (Clement, 1997), will be used in place of MT3D. RT3D is a new reactive transport simulator that can be used for simulating reactive multispecies transport in three-dimensional saturated porous media. RT3D is a FORTRAN-90 based software package. The current version of RT3D uses the basic input/output driver, advection, and dispersion routines from the version DOD_1.5 of the MT3D simulator. As with MT3D, RT3D requires that the USGS groundwater flow model MODFLOW be used to compute groundwater transport velocities. RT3D is capable of simulating dissolution processes.

Comment 12:

Section 6.3, Contaminant Transport Model Calibration: The first paragraph indicates that during calibration of the transport model, as many as eight input parameters will be varied in order to match the current plume. Please briefly indicate what data will be used to calibrate the transport model, and how the calibration will be done. What information is known about the source concentrations and source life? It would be beneficial to establish a potential range that is considered to be reasonable for all of the transport modeling input parameters, prior to adjusting them to achieve calibration.

Response:

Transport Model Calibration: The transport model will be calibrated by varying input parameters over the approximate range of values specified in Table A1, until predicted constituent plume concentrations closely match the observed concentrations. Comments concerning the source concentrations and source life are addressed below with Comment #13.

Table A1 - Transport Model Input Parameters

Control Parameters	*Range*	*Notes*
time step, dt	$C_o < 1$	Courant number (C_o) will be maintained at less than one, $C_o \equiv v \, (dt \, / \, dx)$
maximum grid size, dx	$P_e < 2$	Peclet number will be maintained at less than two, $P_e \equiv dx \, / \, \alpha_L$

Aquifer Properties	*Range*	*Notes*
soil porosity, n	0.20 - 0.40	
soil bulk density, ρ_b	1.5 - 2.0 g/cm^3	
soil moisture content, ω	5 - 25 %	
soil fraction organic carbon, f_{oc}	0.01 - 0.5 %	
longitudinal dispersivity, α_L	50 - 150	ratio of α_L to α_T between 5:1 and 2:1
transverse dispersivity, α_T	10 - 50	ratio of α_L to α_T between 5:1 and 2:1

Chemical Properties	*Notes*
retardation factor, R	will be calculated for individual constituents in accordance with Eqn. (1) and Eqn. (2) of the Organic Contaminant Conceptual Model
biodegradation rate, k	will be calculated for individual constituents as specified in Response to EPA Comment #8

Constituent Distribution: The results of groundwater screening were submitted to the EPA in the November 7, 1997 monitoring well installation proposal. The November 7, 1997 proposal contained plan view maps showing the concentrations of specific constituents within the Upper Glacial and Magothy Aquifers, and cross section maps showing the vertical concentration distribution of specific constituents. Note that, in general, groundwater quality information to complete the conceptual models of inorganic and organic constituent source location(s), mass,

and distribution will be based upon groundwater sampling of the proposed and existing monitoring wells.

Comment 13:

Section 7.0, Transport Model Predictive Simulation: During the transport model predictive simulations, will the assumption be made that all source material is removed (or isolated), or will simulations be made to model an ongoing source? If it is anticipated that an ongoing source will be modeled, how will the mass input be simulated?

Response:

Initial transport modeling will assume an ongoing source of contamination exists, which will be simulated by multiple vertical input wells injecting constituents at a concentration equal to the constituents solubility in water at a fixed flow rate. Subsequent modeling may be performed to simulate various remedial alternatives (e.g., source removal actions).