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DEVELOPMENT AND APPLICATION OF THE ECTRAN MODEL TO SUPPORT THE RI/FS AT THE FEMP SEPTEMBER 1993

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U.S. DEPARTMENT OF ENERGY
FERNALD
CINCINNATI, OHIO

HALLIBURTON NUS PROJECT NUMBER 4P94

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FERNALD ENVIRONMENTAL MANAGEMENT PROJECT
SEPTEMBER 1993

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TABLE OF CONTENTS

SECTION		PAGE
1.0	INTRODUCTION	1-1
2.0	OBJECTIVE AND CAPABILITIES OF THE SCREENING MODEL	2-1
2.1	MODEL STRUCTURE	2-1
2.2	SOURCE LOADING AND ATTENUATION PROCESSES	2-4
2.3	MODEL OUTPUT	2-4
2.4	MODEL PERFORMANCE	2-6
3.0	ECTran MODEL DEVELOPMENT	3-1
3.1	CONCEPTUAL MODEL	3-1
3.1.1	Stratigraphy	3-2
3.1.2	Hydrogeology	3-4
3.1.3	Contamination	3-4
3.2	ASSUMPTIONS	3-5
3.3	GOVERNING EQUATIONS	3-6
3.3.1	Model Layer 1	3-6
3.3.2	Model Layer 2	3-8
3.3.3	Underlying Saturated Zone	3-10
3.3.4	Downgradient Transport	3-11
3.4	SPREADSHEET IMPLEMENTATION	3-16
3.4.1	Coding	3-16
3.4.2	Input/Output Format	3-18
3.4.3	Example Output	3-18
3.5	MONTE CARLO SIMULATION	3-19
3.5.1	Implementation	3-26
3.5.2	Examples	3-26
4.0	DATA REQUIREMENT	4-1
4.1	CONTAMINANT AND GEOCHEMICAL INFORMATION	4-1
4.2	HYDROGEOLOGICAL INFORMATION	4-1
4.3	RISK ASSESSMENT SCENARIO INFORMATION	4-2
4.4	REMEDIAL ALTERNATIVE INFORMATION	4-2
5.0	COMPARISON AND VERIFICATION WITH SWIFT AND ODAST	5-1
5.1	MODEL RESOLUTION	5-1
5.2	MODEL RESULT	5-2
5.3	MODEL RUN TIME	5-7
6.0	APPLICATION	6-1
6.1	EXAMPLES OF PREVIOUS APPLICATIONS	6-1
6.2	PROPOSED APPLICATIONS AT FEMP	6-1
6.2.1	Working PRG Development	6-2
6.2.2	Scoping and Cross-Verification	6-3
6.2.3	Stochastical Modeling	6-3

477 5

TABLE OF CONTENTS (Continued)

SECTION		PAGE
7.0	REFERENCES	7-1

APPENDICES

A.1 MONTE CARLO SIMULATION REPORT, 20 YEARS PUMPING

A.2 MONTE CARLO SIMULATION REPORT, 30 YEARS PUMPING

B FORTRAN IMPLEMENTATION OF DOWNGRADIENT TRANSPORT

C.1 PREVIOUS APPLICATIONS

C.2 TYPICAL SENSITIVITY ANALYSES

TABLES

NUMBER		PAGE
3-1	ECTran Model Input and Output Table Format	3-17
3-2	ECTran Model Example, Baseline Conditions, Hypothetical FEMP, Fernald Ohio	3-20
3-3	ECTran Model Example, Source Removed and Age, Hypothetical FEMP, Fernald Ohio	3-22
3-4	ECTran Model Example, Source Removed, Age, and Pumping, Hypothetical FEMP, Fernald Ohio	3-24
5-1	Summary of Modeling Characteristics for Two OU2 Waste Units	5-3

FIGURES

NUMBER		PAGE
2-1	Buried Valley Aquifer Underlying the Fernald Site and Vicinity	2-2
2-2	Cross-Section of the New Haven Trough, Looking North	2-3
2-3	FEMP Operable Units	2-5
3-1	Representative Model Cross Section For FEMP Site	3-3
3-2	Representative Model Cross Section With Model Parameters	3-7
3-3	Conceptual Model of the Source Concentration	3-13
3-4	Conceptual Model of the Source Concentration with Hydraulic Barrier System	3-15
3-5	ECTran Model Example, Baseline Conditions, Hypothetical FEMP, Fernald Ohio	3-21
3-6	ECTran Model Example, Source Removed and Age, Hypothetical FEMP, Fernald Ohio	3-23
3-7	ECTran Model Example, Source Removed, Age, and Pumping, Hypothetical FEMP, Fernald Ohio	3-25
5-1	Comparison of ECTran and ODAST Models, Inactive Flyash Pile, Source Area	5-5
5-2	Comparison of ECTran and ODAST Models, Solid Waste Landfill, Source Area	5-5
5-3	Comparison of ECTran and SWIFT Models, Inactive Flyash Pile, Source Area	5-6
5-4	Comparison of ECTran and SWIFT Models, Inactive Flyash Pile, Source Area	5-6

1.0 INTRODUCTION

An efficient and robust groundwater contaminant fate and transport model implemented on Excel 4.0 and Crystal Ball 3.0 (ECTran) has been developed and is proposed to support the Remedial Investigation/Feasibility Study (RI/FS) processes at the Fernald Environmental Management Project (FEMP). This screening-level model can be utilized to supplement existing more complex fate and transport models during parameter estimation, risk assessment, cleanup goal development, Alternate Concentration Limit (ACL) determination, and stochastical sensitivity analysis. The ECTran (which stands for Excel-Crystal Ball Transport) model is based on straightforward mass-balances and advection/dispersion analytical equations, but can be used to simulate a variety of complex conditions. To date, Halliburton NUS has employed similar models to determine soil cleanup goals, ACLs, cleanup time estimations, and to support baseline risk assessments for both CERCLA and RCRA applications in U.S. EPA Regions III, VI, and X. This report presents the required capabilities, development processes, and proposed applications of the screening-level spreadsheet-based groundwater contaminant fate and transport model (i.e., ECTran) at the FEMP.

2.0 OBJECTIVE AND CAPABILITIES OF THE SCREENING MODEL

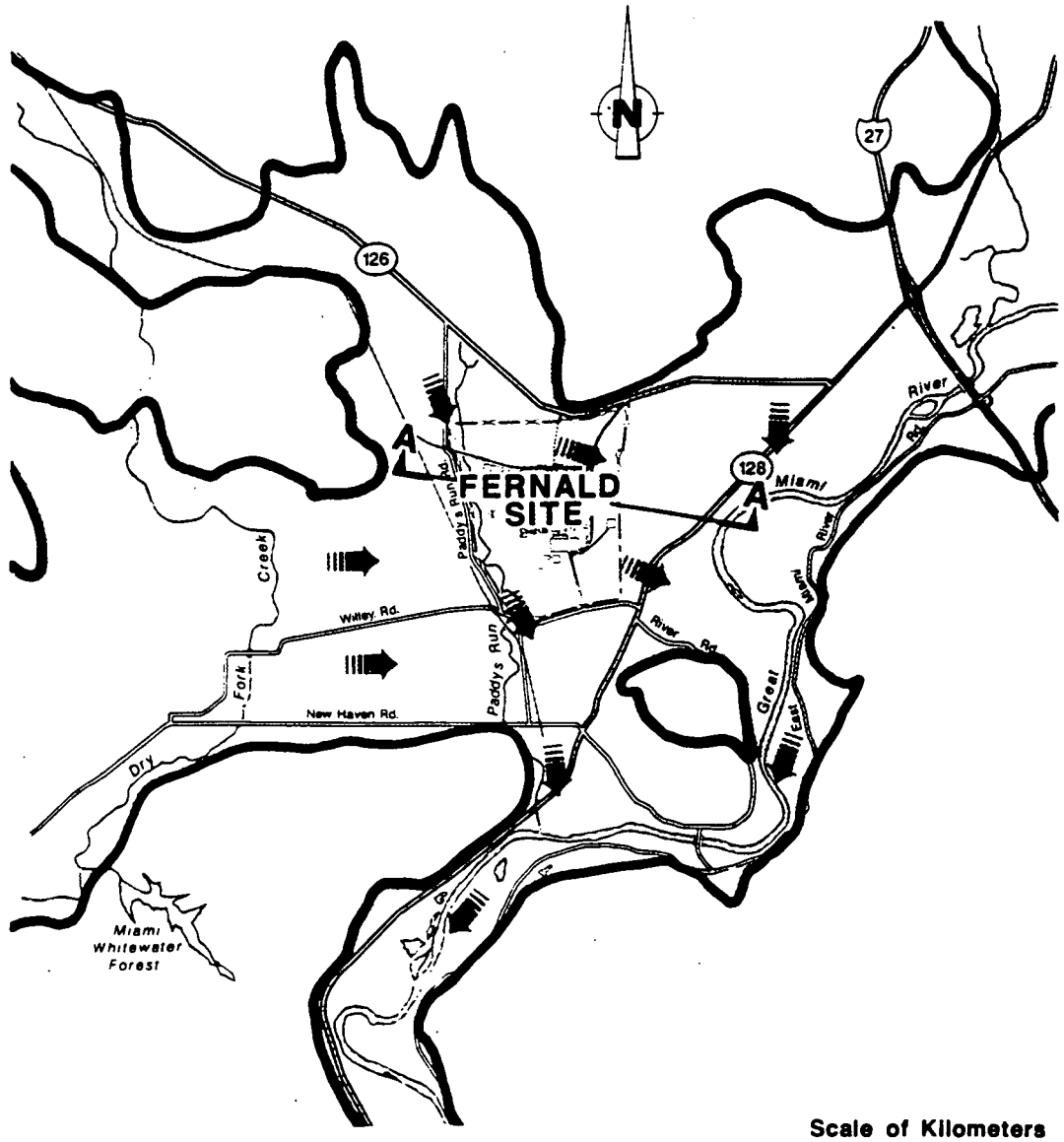
Groundwater fate and transport models, developed using ODAST and SWIFT codes, have been applied in various Removal Actions and RI reports at the FEMP. Based on the experiences of these modeling tasks, a screening-level contaminant fate and transport model was determined necessary to supplement the existing modeling tools. Due to their complexities, the current models are not efficient during model parameter estimation, model calibration, remedial alternative screening, long-term simulation, and stochastical sensitivity analysis. Because of this limitation, the usefulness of computer models in supporting RI/FS processes has not been fully utilized at the FEMP. The primary objective of the proposed screening model is to efficiently support the current models in tasks where larger numbers of long-term modeling runs are required. The screening model can be used to scope the necessary scenarios or final ranges of parameter values that the primary groundwater models need to simulate and verify. In order to achieve this objective, this auxiliary model should be robust and flexible. Desired capabilities of this model are summarized in the following subsections.

2.1 MODEL STRUCTURE

Figures 2-1 and 2-2 show the general hydrogeological conditions (setting) in the vicinity of FEMP. In order to support the existing models which simulate these conditions, the conceptual structure of the proposed screening model needs to:

- Include both the glacial overburden and sand and gravel aquifer underlying the FEMP.
- Use any specified groundwater flow conditions directly.
- Use a mixing-depth concept in the saturated zone instead of the fixed thickness of the entire saturated zone.
- Employ analytical solutions, so that no model grid is required.
- Be separately and flexibly applied in any localized source areas.

Figure 2-1 Buried Valley Aquifer Underlying the Fernald Site and Vicinity



Scale of Kilometers

0 1 2

1 Kilometer = 0.62 Mile

LEGEND

- Buried Valley Aquifer
- General Direction of Groundwater Flow
- Plant Perimeter
- A A Location of Cross-Section Shown in Figure 2-2

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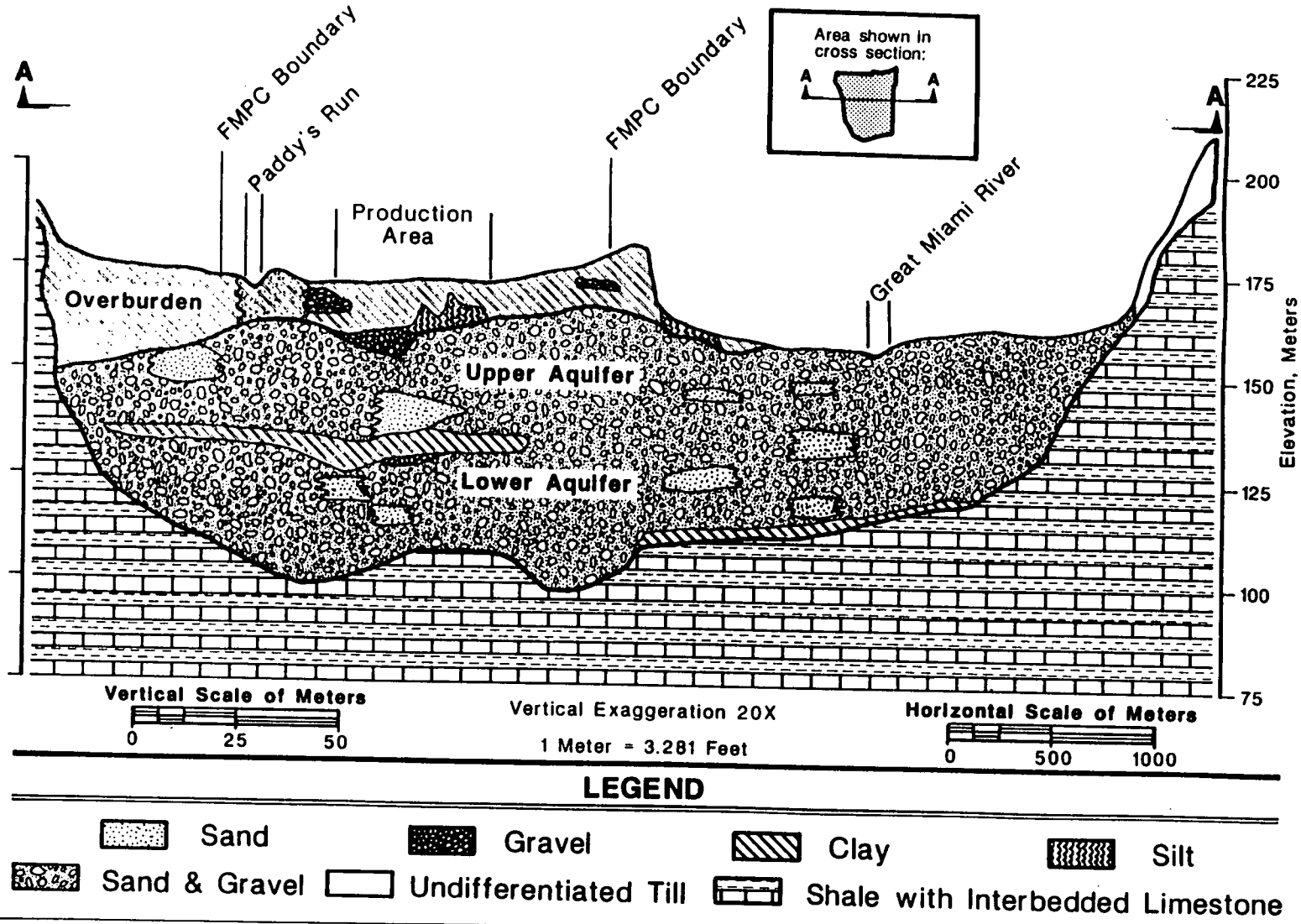
Figure 2-2: *Cross-Section of the New Haven Trough, Looking North*



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2.2 SOURCE LOADING AND ATTENUATION PROCESSES

Figure 2-3 shows the Operable Unit (OU) designations in the FEMP. Each of the five OUs presents different contaminant source loading characteristics and hydrogeological conditions that affect the attenuation of contaminants. Therefore, a realistic screening model for the FEMP should be able to:

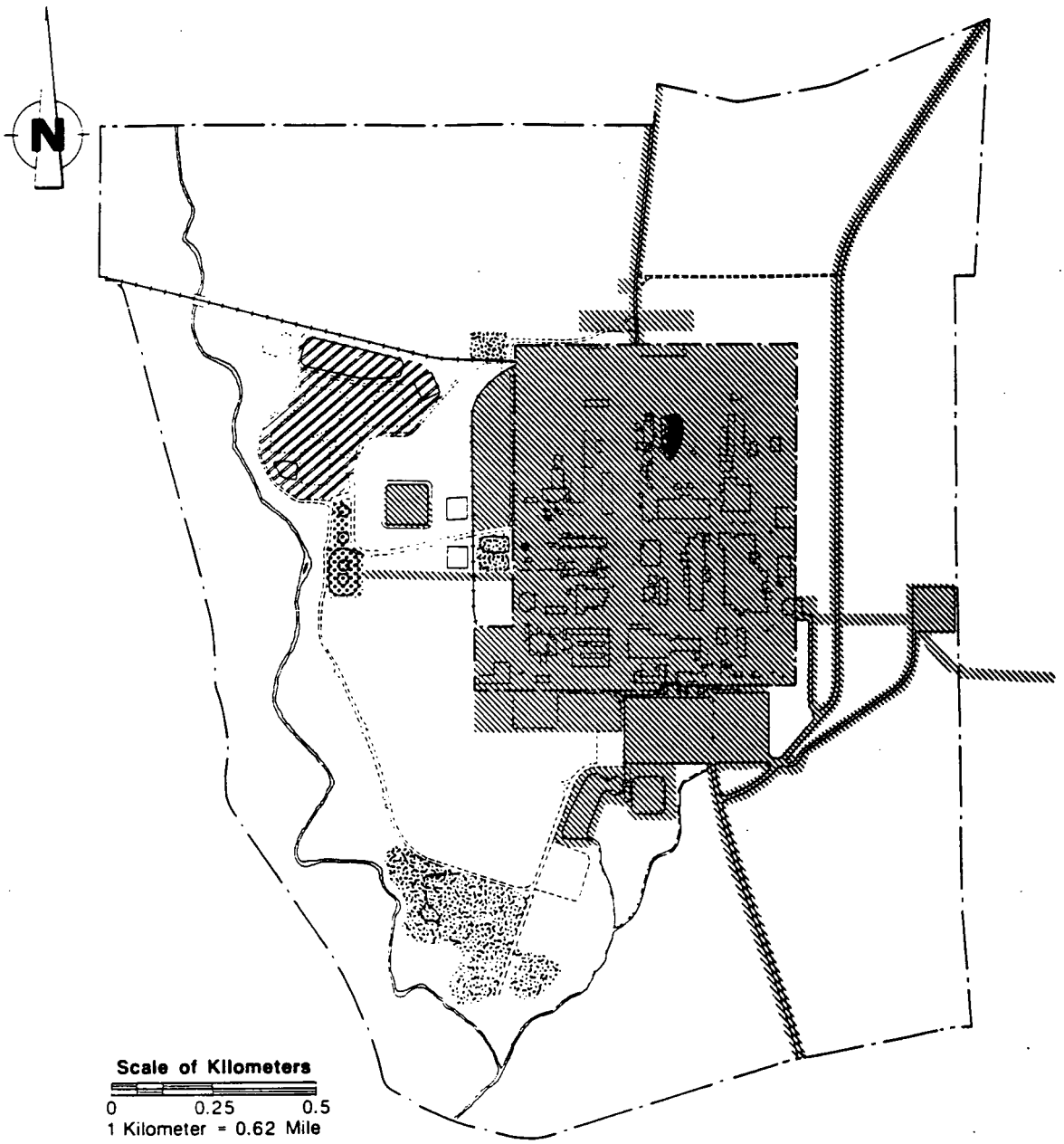
- Simulate all major physical and chemical processes that affect the contaminant fate and transport.
- Accept zone- and layer-specific initial contaminant concentrations, chemical decay rates and distribution coefficients.
- Include the source loading from the waste units.
- Include additional source loading in the glacial overburden.
- Consider contaminated or clean upgradient groundwater recharge.
- Consider impacts of pumping and/or containment in the source area on the exposure point concentrations.
- Consider age of the source to estimate the current downgradient concentrations.

2.3 MODEL OUTPUT

The modeling results need to be easily accessible and clearly understandable. Therefore, the screening model should be designed to:

- Present layer- and zone-specific contaminant concentrations vs. time.
- Present concentrations along the projected centerline of the contaminant plume at a downgradient location such as the FEMP property line.
- Present the output statistically and graphically without the need of post-processing.

Figure 2-3 : FEMP Operable Units



LEGEND

- Operable Unit 1
- Operable Unit 2
- Operable Unit 3
- Operable Unit 4

Operable Unit 5 (Not Shown)

2.4 MODEL PERFORMANCE

The most desired characteristic of the screening model is the capability to support fast, flexible, but realistic applications. Under these performance criteria, the screening model should:

- Apply and calibrate to field conditions easily.
- Support stochastical analysis.
- Have a very short run time that is not sensitive to contaminants being simulated.

3.0 ECTran MODEL DEVELOPMENT

Based on the required capabilities, a spreadsheet-based approach was selected to develop the screening fate and transport model. This section describes the development process of the ECTran model. Discussions on the development of the conceptual model, assumptions, governing equations, spreadsheet implementation (i.e., Excel 4.0), and Monte Carlo simulation capability (i.e., Crystal Ball) are all included within this section.

To develop a mathematical/computer model, the natural physical and chemical systems in question must first be characterized or conceptualized. This delineation of the natural systems on site with necessary assumptions and simplifications is usually called a conceptual model. Governing equations based on the conceptual model and assumptions are then derived. Next, suitable computer tools are utilized to implement the governing equations. The developed computer model with proper input data must then be applied to simulate a measured event and to verify the validity of the model development process. If the appropriate conceptual model, assumptions, and governing equations have been used for model development, the model will simulate the natural system properly.

Once the basic functions (i.e., deterministic simulations of the natural physical and chemical processes) of the model have been implemented and verified, auxiliary capabilities can be developed and incorporated to improve the overall usefulness of the model. Typical auxiliary functions can include: statistical calculations, Monte Carlo simulation, graphical presentation, and on-line user's guide.

3.1 CONCEPTUAL MODEL

Since the screening model will be independently applied in many localized source areas at the FEMP, the model should have sufficient flexibility and be easily customized to a specific source area during model applications. Therefore, a general conceptual model of fate and transport of a contaminant in the groundwater system underlying the FEMP should be determined. Information gathered during previous site and contaminant characterization tasks was utilized for this purpose. The general conceptual model for scoping the screening model development identified and incorporated the following information:

- General configuration of the water-bearing zones of interest.
- Possible hydrologic behavior of, and interconnections between, all major geologic formations.
- Ranges of velocities and directions of groundwater flow.
- Extent and configuration of potential contaminant sources.
- Chemical properties of major contaminants of concern.
- Geochemical properties of aquifer materials that affect contaminant transport.
- General contaminant migration pathways.
- Locations of potential exposure points to be considered in the risk assessment.

Detailed information on geology, hydrogeology, and contaminants has been collected at the FEMP during RI/FS and Removal Action activities. This information was used to develop a general conceptual model which could be applied over most of the site. Figure 3-1 depicts the general conceptual model determined for developing the proposed screening model. The following sections describe the rationale for the conceptual model.

3.1.1 Stratigraphy

In general, the geologic conditions at the FEMP site can be categorized into four general units. The uppermost unit consists of the waste unit and unsaturated weathered till. The next-lower unit consists of generally unweathered glacial overburden interbedded with glaciofluvial sand and gravel stringers. Some of the stringers are saturated and have been labeled as perched groundwater. The next-lower unit consists of unsaturated sand and gravel outwash deposits existing above the Great Miami Aquifer (GMA). The lowest geologic unit of interest is the GMA. This aquifer is a well-sorted sand and gravel water table system consisting of glacial outwash deposits located within a 2- to 3-mile-wide subterranean valley known as the New Haven Trough. This aquifer is divided by a 10- to 20-foot-thick clay aquitard at an approximate depth of 120 feet. The aquifer overlies limestone/shale bedrock at an approximate depth of 200 feet.

This information was used to determine that the screening model should have three potential layers (i.e., Layer 1, Layer 2, and Saturated Zone (GMA)). Layer 1 was used to represent the glacial overburden, Layer 2 was used to represent the unsaturated sand and gravel, and the bottom model layer represented the upper portion of the GMA. The conceptual model did not directly represent the waste unit and weathered till, but indirectly modeled it by using the leachate loadings from the waste unit as inflows to Layer 1. The reason for not considering the lower portion of the GMA is that the maximum contaminant

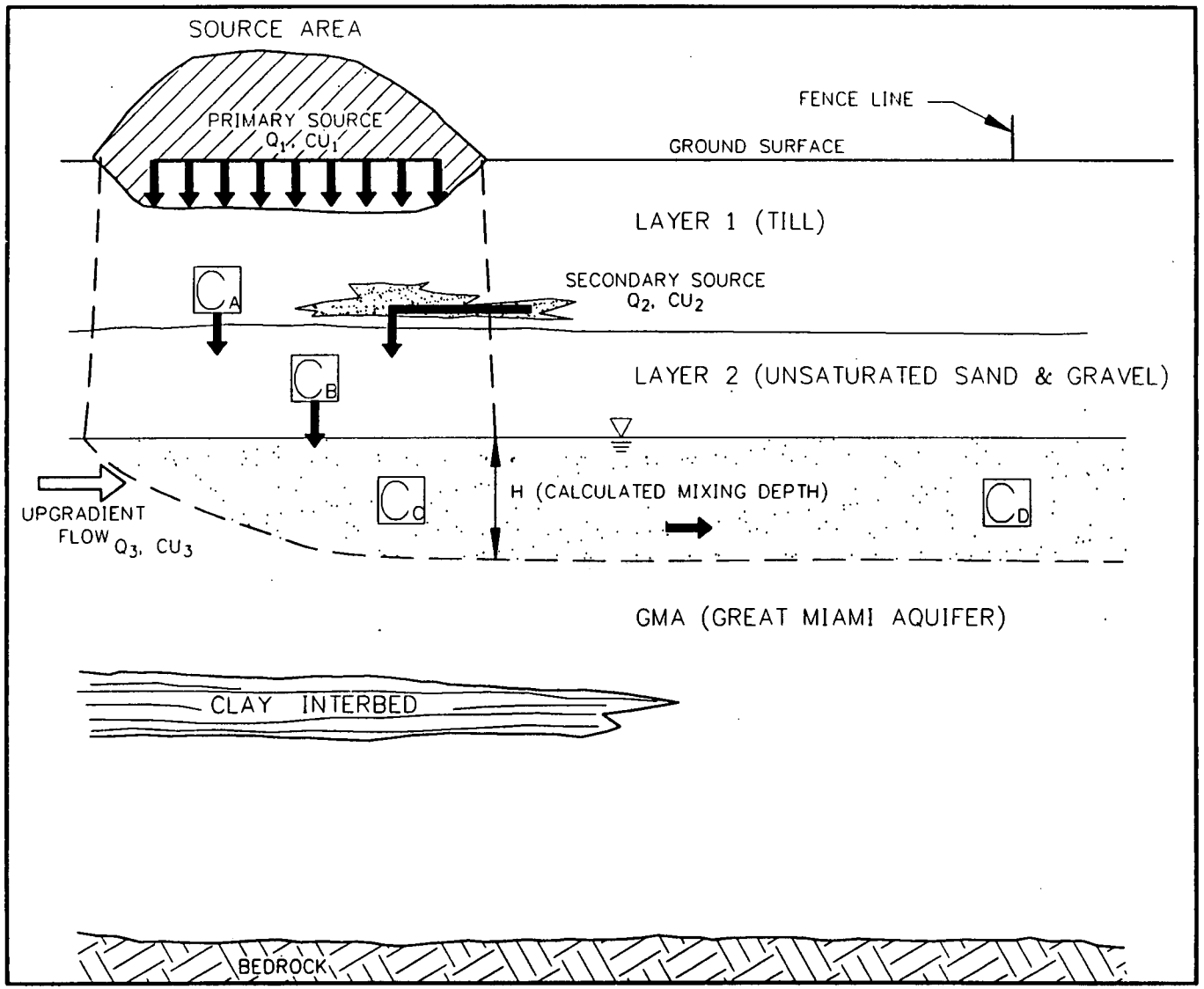


FIGURE 3-1
REPRESENTATIVE MODEL CROSS SECTION
FOR FEMP SITE

concentration will most likely occur in the upper portion of GMA. This approach seems reasonable for the ECTran model since the purpose of a screening model is to estimate the peak contaminant concentration.

3.1.2 Hydrogeology

The hydrogeology of the FEMP and the surrounding area is a textbook example of a glaciofluvial buried valley aquifer (Walton, 1970; Fetter, 1989; Freeze and Cherry, 1979). The primary aquifer in the region is the GMA, a well-sorted sand and gravel water table system consisting of glacial outwash deposits. As shown in Figure 2-1, groundwater in the aquifer enters the FEMP area via buried channels on the west, north, and east. Under natural conditions, the primary flow would be across the site to the south. However, large pumping wells east of the FEMP in the Big Bend area of the Great Miami River have created a pronounced cone of depression causing groundwater flow at the FEMP to have easterly, southeasterly, and southerly components.

Within the glacial overburden, there are numerous water-bearing zones (i.e., perched groundwater) that have limited interconnection. The majority of these zones are of glaciofluvial origin and consist of small beds of highly-sorted sands and gravels. These beds are probably the result of small meltwater streams that occurred along the ice margin and within the glacier itself. This information was used to determine that the screening model should allow potential subsurface perched water flow into and/or out of the model domain in the glacial overburden.

3.1.3 Contamination

The primary contaminant at the FEMP site is uranium. Other secondary contaminants at the site include radioactive contaminants such as radium and thorium and inorganic/organic contaminants such as lead, bis(2-ethylhexyl)phthalate and trichloroethene. The conceptual model was developed to be general enough to allow for modeling of each type of contaminant (i.e., radionuclide or inorganic/organic) and to take into consideration the contaminant geochemistry and transport at the site. The depositional characteristics and the hydrostratigraphic units present at the FEMP impart general contaminant transport characteristics on solutes migrating from the individual waste areas to receptor locations. These characteristics include:

- **Solute Migration Potential.** Solutes have a high migration potential through the upper weathered tills due to the fractured nature of the sediment. Solute migration can also occur through the unweathered till, however, at a much slower rate. Once the solute reaches the

glacial outwash, the solute migration potential is high, based on the hydraulic conductivity of the matrix.

- **Hydraulic Interconnection.** The intercommunication between perched water-bearing zones is limited in the glacial environment. Communication between the upper water-bearing zones within the glacial overburden and the GMA is likely over an extended period of time. Communication between the upper and lower zones within the GMA will be controlled by transverse (vertical) dispersion and will therefore be extremely limited.

- **Adsorption/Attenuation Characteristics.** Sediments found within the glacial overburden generally have sufficient organic carbon content (e.g., 0.5 percent to 1 percent) to cause retardation of organic constituents. The clay mineralogy would result in cation retardation for inorganic constituents. Given the till matrix, it is also unlikely that adsorption/attenuation breakthrough would occur. Adsorption/attenuation will occur at lower rates in the regional aquifer due to the lower organic carbon and clay content in the outwash.

This information was used to conclude that the screening model should allow zone- or layer-specific adsorption, attenuation, and decay parameters to be specified.

3.2 ASSUMPTIONS

In order to develop a spreadsheet-based analytical fate and transport model, the following simplified but conservative assumptions were incorporated into the proposed ECTran model:

- External source loadings and upgradient conditions are constant.

- Dispersion is negligible in the overburden.

- Vertical dispersion is negligible in the Great Miami Aquifer.

- Downgradient aquifer can be approximated as homogeneous with uniform groundwater flow.

- Layer-averaged input conditions and model predictions are sufficient in the overburden for screening purposes.

- Zone-averaged contaminant concentrations in the mixing zone underlying the source area and concentrations at the fence line are sufficient in the GMA for screening purpose.

3.3 GOVERNING EQUATIONS

The differential equations which govern groundwater flow and transport of contaminants were used to develop analytical solutions in ECTran. The developed model relies on key information inside the waste units and uses simple and robust, but conservative, fate and transport equations to describe the relatively complex modeling domain and contaminant migration pathways encountered at the FEMP. Important parameters included in the ECTran model to describe each layer and zone in the conceptual model is shown in Figure 3-2. The following subsections discuss the development and rationale of the governing equations in each model layer or zone using these parameters (shown in Figure 3-2).

3.3.1 Model Layer 1

A mass-balance analysis with solid- and dissolved-phase partitioning for the contaminants from the source area, assuming that the infiltrating precipitation contains residual source leachate or background contamination and that dispersion in the Layer 1 is negligible, yields the following expression for the time-dependent leachate concentration in the Layer 1:

$$\frac{dC_A}{dt} = \left[\frac{Q_1}{S_A V_{wA} + K_{dA} W_{sA}}\right] [CU_1 - C_A] - \lambda_A C_A \qquad (1)$$

where:

CU_1 is the contaminant concentration in infiltrating precipitation (μg/L)

Q_1 is the infiltration rate (L/day)

C_A is the aqueous concentration in Layer 1 (μg/L)

S_A is the soil saturation fraction in Layer 1 (dimensionless)

V_{wA} is the void volume in Layer 1 (L)

K_{dA} is the aqueous/solid phase distribution coefficients in Layer 1 (L/kg)

W_{sA} is the dry weight of soil in Layer 1 (kg)

λ_A is the first-order chemical decay rate in Layer 1 (day^{-1})

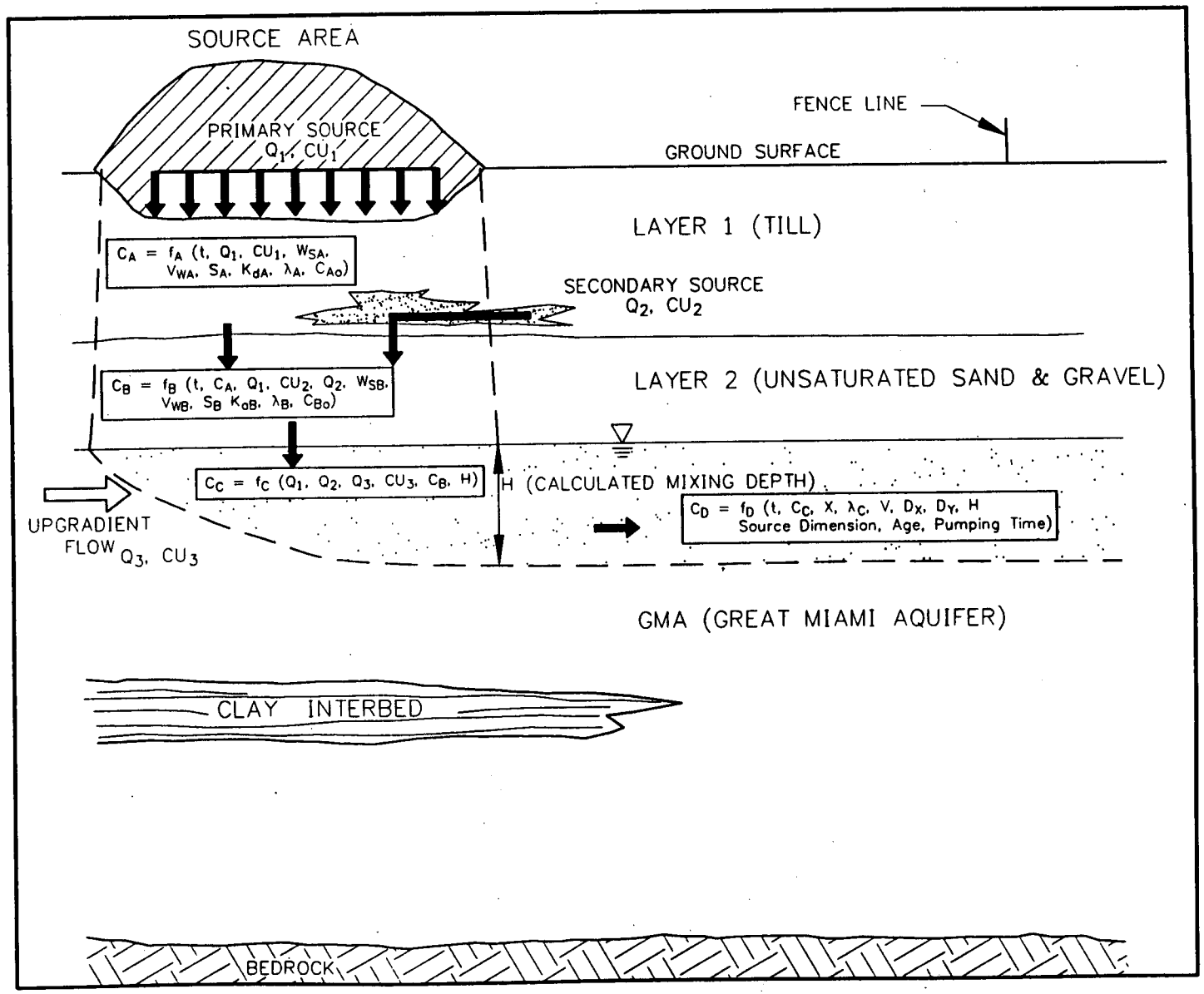


FIGURE 3-2
REPRESENTATIVE MODEL CROSS SECTION WITH MODEL PARAMETERS

For an initial condition of $C_A = C_{Ao}$, this equation may be solved via direct integration to yield the following solution:

$$C_A = \frac{CU_1 - \{CU_1 - [1 + (S_A V_{WA} + K_{dA} W_{sA})(\lambda_A / Q_1)] C_{Ao}\} \exp\left[- \frac{Q_1 + (S_A V_{WA} + K_{dA} W_{sA})\lambda_A}{S_A V_{WA} + K_{dA} W_{sA}} t \right]}{[1 + (S_A V_{WA} + K_{dA} W_{sA})(\lambda_A / Q_1)]} \quad (2)$$

3.3.2 Model Layer 2

Using a similar mass-balance/mass-partitioning approach, a general case for model Layer 2 which includes a time-dependent source loading term (C_A as described by Eq. (2)) and a secondary source may be written in the following differential equation:

$$\frac{dC_B}{dt} + \frac{K_2}{K_1} C_B = \frac{K_3}{K_1} + \frac{K_4}{K_1} \exp[-K_5 t] \quad (3)$$

In which:

$$K_1 = S_B V_{wB} + K_{dB} W_{sB}$$

$$K_2 = Q_1 + Q_2 + (S_B V_{wB} + K_{dB} W_{sB}) \lambda_B$$

$$K_3 = Q_1 CU_1 \; / \; [1 + (S_A V_{wA} + K_{dA} W_{sA})(\lambda_A / Q_1)] + Q_2 CU_2$$

$$K_4 = Q_1 C_{Ao} - Q_1 CU_1 \; / \; [1 + (S_A V_{wA} + K_{dA} W_{sA})(\lambda_A / Q_1)]$$

$$K_5 = [Q_1 + (S_A V_{wA} + K_{dA} W_{sA})\lambda_A] / (S_A V_{wA} + K_{dA} W_{sA})$$

And where:

CU_2 is the contaminant leachate concentration of the secondary source (μg/L)

C_B is the aqueous concentration in Layer 2 (μg/L)

Q_2 is the perched water inflow rate of the secondary source (L/day)

S_B is the soil saturation fraction in Layer 2 (dimensionless)

V_{wB} is the void volume in Layer 2 (L)

K_{dB} is the aqueous/solid phase distribution coefficients in Layer 2 (L/kg)

W_{sB} is the dry weight of soil in Layer 2 (kg)

λ_B is the first-order chemical decay rate in Layer 2 (day^{-1})

This equation is of the following general form:

$$C'_B + p(t)C_B = r(t)$$

where: $p(t) = K_2/K_1$

$$r(t) = \frac{k_3}{k_1} + \frac{k_4}{k_1}\exp[-k_5 t]$$

The above equation has a general solution as follows:

$$C_B = \exp[-h]\left[\int \exp(h)\, r(t)\, dt + K\right]$$

where: $h = \int p(t)dt$ and K is a constant of integration

This equation may be solved for the initial condition of $C_B = C_{Bo}$ using the preceding integrating factor approach or the method of undetermined coefficients to yield the following:

$$C_B = \frac{K_3}{K_2} + \frac{K_4}{K_2 - K_1 K_5}\exp(-K_5 t) + \left[C_{Bo} - \frac{K_3}{K_2} - \frac{K_4}{K_2 - K_1 K_5}\right]\exp\left(-\frac{K_2 t}{K_1}\right) \quad (4)$$

Special Cases

In addition to this standard form of the solution (i.e., Eq. (4)), the following two special cases were also considered and included in ECTran:

- For a constant-concentration in Layer 1 (i.e., $C_A = CU_1$), the equation for Layer 2 becomes:

$$C_B = \frac{Q_1 CU_1 + Q_2 CU_2 - \{Q_1 CU_1 + Q_2 CU_2 - K_2 C_{Bo}\}\exp\left(-\frac{K_2 t}{K_1}\right)}{K_2} \quad (5)$$

- In the case of $K_2 = K_1K_5$ (e.g., when both Layer 1 and Layer 2 are identical and $Q_2=0$), the solution of Eq. (3) and thus the equation for Layer 2 leachate concentration becomes:

$$C_B = \frac{K_3}{K_2} + \left[C_{Bo} - \frac{K_3}{K_2} + \frac{K_4}{K_1}t\right] \exp(-K_5 t) \tag{6}$$

3.3.3 Underlying Saturated Zone

Based on the mass balance in the underlying saturated zone, the following equation is derived:

$$C_C = \frac{CU_3Q_3 + C_B(Q_1+Q_2)}{Q_1+Q_2+Q_3} \tag{7}$$

Where: C_c is the aqueous concentration in underlying saturated zone (μg/L)
CU_3 is the contaminant concentration in upgradient groundwater flow (μg/L)
Q_3 is the upgradient groundwater flow rate through the saturated mixing zone underlying the source area (L/day).

This equation does not consider the portion of contaminant that can be adsorbed to soil and therefore gives a very conservative estimation of the dissolved phase concentrations. Equation (7) is also known as the Summer's model (from several sources including EPA, 1983).

In order to compute Q_3, the thickness of the mixing zone in the aquifer, which represents the vertical extent of the contamination in the model, must be determined. It is usually selected based on the minimum of the following three possible values:

- The thickness of the entire saturated zone.
- The lowest position of detected contaminants of concern.
- The mixing zone depth calculated by the following equation (Salhotra et al., 1990):

$$H = B[1 - \exp(-V_{zo}L / (BV_x))] + (2\alpha_v L)^{1/2} \tag{8}$$

where: H is the mixing zone thickness (ft)
B is the total saturated zone thickness (i.e., thickness of the upper GMA) (ft)

V_p is the vertical seepage velocity (ft/yr)

L is the length of the source area in the groundwater flow direction (ft)

V_x is the horizontal seepage velocity (ft/yr)

α_v is the vertical dispersivity (ft)

Since H is usually less than B, the mixing zone depth concept was found to be the most appropriate to be used for the FEMP site. This approach is also more conservative than the fixed top layer thickness used in the current SWIFT groundwater fate and transport model.

3.3.4 Downgradient Transport

A simplified version of a general solution to a three-dimensional contaminant advection/dispersion/sorption/decay equation was used to simulate solute transport. It provides an estimate of the contaminant concentration at a receptor location or discharge area downgradient of the source area under different source-loading conditions.

The basic equation, a modified version of a general constant-source equation developed by Domenico (1987), for the plume centerline is as follows:

$$C(X, t, Co) = \frac{Co}{2} \exp\left\{\left(\frac{X}{2\,(D_x/V)}\right)\left[1 - \left(1 + \frac{4\lambda_C D_x}{V_2}\right)^{1/2}\right]\right\}$$

$$erfc\left[\frac{X - Vt\left(1 + \frac{4\lambda_C D_x}{V^2}\right)^{1/2}}{2(D_x t)^{1/2}}\right] erf\left[\frac{Y}{4\left(\frac{D_y}{V} X\right)^{1/2}}\right] \qquad (9)$$

where: C is the downgradient concentration along the plume centerline caused by C_o (μg/L)

C_o is the constant groundwater concentration at/below the source (μg/L)

X is the distance downgradient from the source(ft)

V is the retarded contaminant velocity (ft/year)

t is the elapsed time since the beginning of the constant source loading (years)

D_x is the principle value of the dispersion tensor in the x (longitudinal) direction (ft^2/year)

Y is the source dimension in the y (lateral) direction (ft)

D_y is the principle value of the dispersion tensor in the y (lateral) direction (ft^2/year)

λ_c is the chemical decay rate ($years^{-1}$)

In the preceding expression, erf and erfc are the error function and the complimentary error function, respectively. Vertical dispersion was not considered in equation (9) in order to provide a more conservative estimate of the exposure point concentration. The contaminant velocity is determined as the groundwater interstitial pore velocity divided by the retardation factor. The retardation factor (R_d) can be estimated using the distribution coefficient (K_{dc}), the soil bulk density (ρ), and porosity or volumetric water content (θ) of the soil as:

$$R_d = 1 + \frac{\rho K_{dc}}{\theta}$$

In cases where the net recharge, outside the source area (i.e., recharge that directly percolates into and dilutes the downgradient contaminant plume), is significant, the effective decay rate in the downgradient area can be increased to λ_c*, as follows

$$\lambda_c^* = \lambda_c + \frac{q}{B\theta}$$

Where q is the annual infiltration rate in the downgradient area (ft/year); and θ is the volumetric water content in the underlying saturated zone.

Although derived for a constant source loading condition, Equation (9) can be applied using superposition to simulate the time-dependent source loading. For a time-dependent source, the concentration at a downgradient location at a given time T can be estimated using the following procedure. First the continuous function of the time-dependent source concentration C_c [i.e., Eq. (7)] is approximated by a series of step impulses which simplifies the solution and is usually also more conservative than the original function as shown in Figure 3-3. In Figure 3-3, it is also assumed that the source area has been contaminated with a concentration S_0 for a time period ("Age") before the initial time t_0. This contaminant concentration has convected to the area downgradient of the source area by dispersion/sorption/decay. Therefore, the contaminant concentration S_0 in this time period is also treated as an impulse.

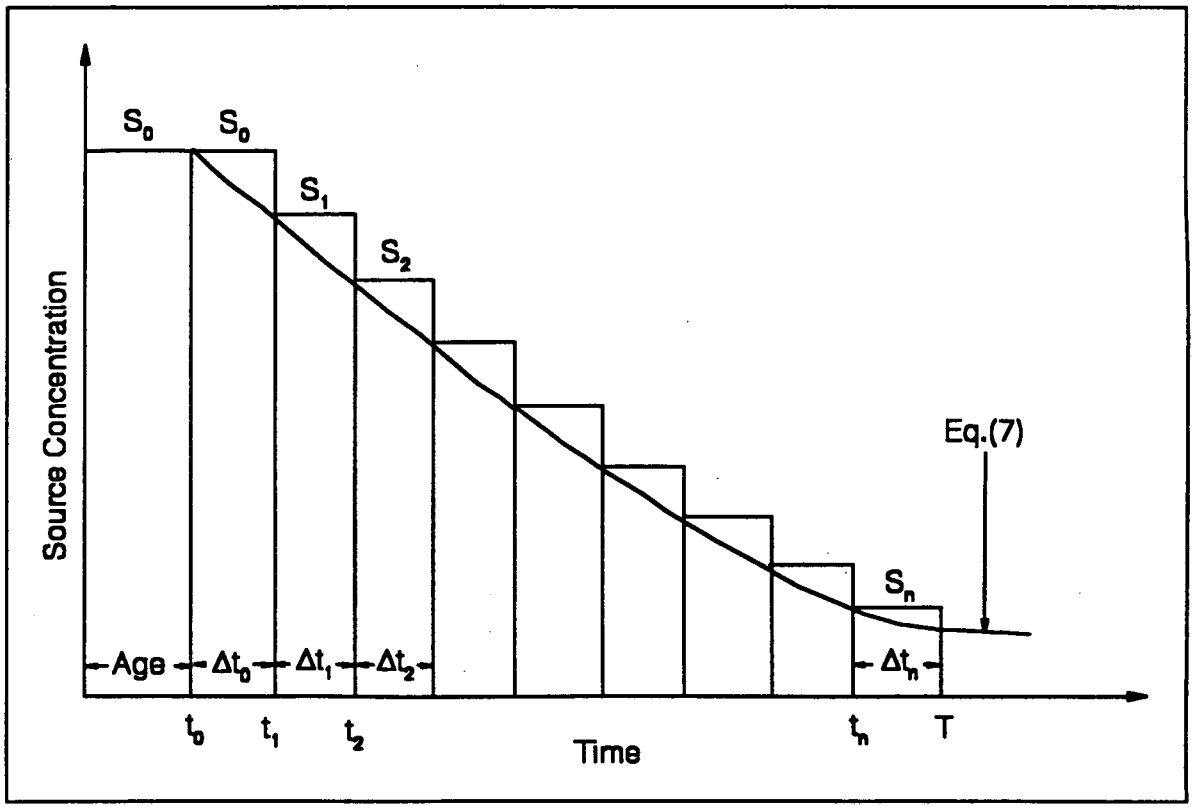


FIGURE 3-3
CONCEPTUAL MODEL OF THE SOURCE CONCENTRATION

The concentration at X feet downgradient of the source at time T can therefore be estimated by superposition of constant source solutions [Eq. (9)] for all impulses prior to time T as follows:

$$
\begin{aligned}
C_D(x, T) &= C(X, T-t_o+Age, S_o) - C(X, T-t_o, S_o) + \sum_{i=0}^{n} [C(X, T-t_i, S_i) - C(X, T-t_i-\Delta t_i, S_i)] \\
&= C(X, T-t_o+Age, S_o) - C(X, T-t_o, S_o) \\
&\quad + C(X, T-t_0, S_0) - C(X, T-t_0 - \Delta t_0, S_0) \\
&\quad +\ldots+ C(X, T-t_n, S_n) - C(X, T-t_n - \Delta t_n, S_n)
\end{aligned}
\tag{10}
$$

where: S_i is the source concentration of the ith impulse

t_i is the starting time of the ith impulse

Δt_i is the time interval for the ith impulse

$T-t_n-\Delta t_n = 0$

C_D (X, T) is the combined effects of n + 1 impulses

In the preceding equation (i.e., Eq. (9)), C (X, t, S) is the concentration at X caused by a constant source with concentration S for a duration of t. Therefore, C(X,t,S) needs to be applied twice to determine each single impulse's net lasting effect at time T. This approach is similar to the procedure used in the Expert ROKEY Computer System (McClymont and Schivarte, 1987). The Expert ROKEY Computer System is a saturated-zone contaminant fate and transport model with an expert system that assists the user to estimate necessary hydrogeological and chemical parameters for the model. The source loading from the unsaturated zone must be specified by the user in the Expert ROKEY.

If a groundwater pumping system is designed to prevent the movement of contaminated groundwater to the downgradient area, the Eq. (10) may be modified. For instance, if the pumping starts at t_0 and stops at t_j as shown in Figure 3-4, the S_i, i from 0 to j-1 , will have no impact on the downgradient area. Therefore, Eq. (10) will be rewritten as:

$$
\begin{aligned}
C_D(x, T) &= C(X, T-t_o+Age, S_o) - C(X, T-t_o, S_o) + \sum_{i=j}^{n} [C(X, T-t_i, S_i) - C(X, T-t_i-\Delta t_i, S_i)] \\
&= C(X, T-t_o+Age, S_o) - C(X, T-t_o, S_o) + C(X, T-t_j, S_j) - C(X, T-t_j - \Delta t_j, S_j) \\
&\quad + C(X, T-t_{j+1}, S_{j+1}) - C(X, T-t_{j+1} - \Delta t_{j+1}, S_{j+1}) \\
&\quad +\ldots+ C(X, T-t_n, S_n) - C(X, T-t_n - \Delta t_n, S_n)
\end{aligned}
\tag{11}
$$

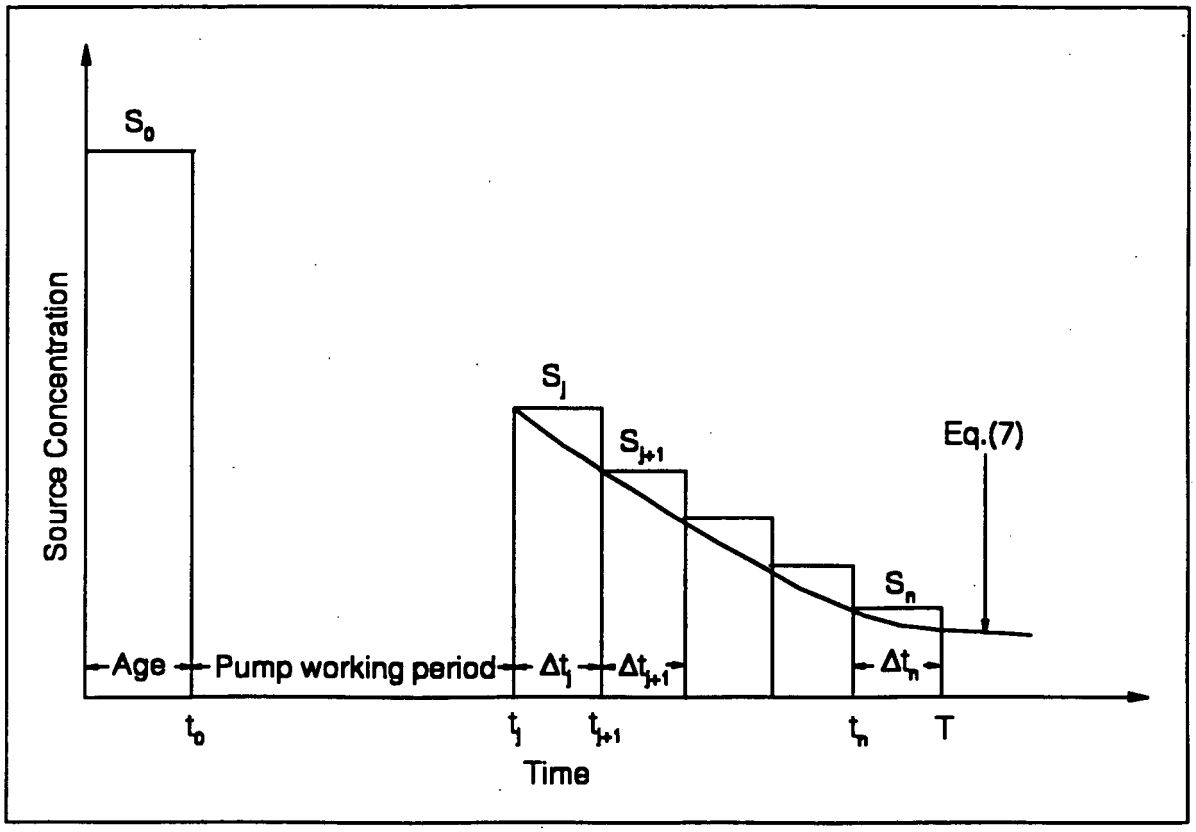


FIGURE 3-4
CONCEPTUAL MODEL OF THE SOURCE CONCENTRATION WITH HYDRAULIC BARRIER SYSTEM

3.4 SPREADSHEET IMPLEMENTATION

Several advantages of a spreadsheet-based model over a traditional "pre/post-processors and stand-alone program approach" are apparent. Because the simulation is implemented by a spreadsheet, the model input and output data are contained in the same file. It is extremely easy for the user to change values of any specific input parameters, and the effects of various input values can be seen on the computer screen. The graphical and statistical capability provided by the spreadsheet makes presentation of the model results very efficient and flexible. A spreadsheet in Excel (i.e., ECTran) was developed to code the equations described in Section 3.3. This section describes the spreadsheet coding, input/output format, and example output of the ECTran model.

3.4.1 Coding

The coding for equations in Layer 1 and underlying saturated zone was straightforward, (i.e., the Eqs (2) and (7) are directly coded in Excel). For layer 2, the **IF** function in Excel was used to take care of the special cases specified in Section 3.3.2. The Excel functions, such as **ERF**, **ERFC** and **SUMPRODUCT**, were used to code equations (9), (10) and (11) for downgradient transport calculations. The **ERF** and **ERFC** functions compute the error function and the complimentary error function, respectively. The **SUMPRODUCT** function returns the sum of the products of the specified arrays.

It is important for the ECTran model to maintain consistency among all the inter-related model parameters. Therefore, some of the model parameters are automatically calculated and protected in the spreadsheet. Other intermediate calculations are performed in spreadsheet cells outside the main table as shown in Table 3-1. These cells were also protected and hidden from the user. For example, a column in the spreadsheet was specified to compute the following term in Eq. (8):

$$F(t_i)=erfc\left[\frac{X-V\,t_i\left(1+\frac{4\lambda_c D_x}{V^2}\right)^{1/2}}{2(D_x t_i)^{1/2}}\right]$$

TABLE 3-1

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BROWN & ROOT ENVIRONMENTAL

SCREENING-LEVEL EXCEL-CRYSTAL BALL TRANSPORT (ECTran) MODEL

SITE:

INVESTIGATOR:

DATE:

CONTAMINANT:		CHEMICAL X	
KOC (L/KG):	*	WATER CRITERIA (UG/L):	*
HALF LIFE (YRS):		CONSTANT SOURCE LEACHATE (UG/L):	*
LAYER 1:	*	INITIAL LAYER 1 SOIL CONC. (MG/KG):	*
LAYER 2:	*	INITIAL LAYER 2 SOIL CONC. (MG/KG):	*
GMA:	*		

UNSAT. SOURCE AREA:		LAYER 1 (GLACIAL OVERBURDEN)		LAYER 2 (SAND & GRAVEL)		GREAT MIAMI AQUIFER (SAT. S. & G.)			
						B (FT):	*	Vzo (FT/YR):	*
LENGTH (FT):	*	FOC (KG/KG):	*	FOC (KG/KG):	*	GW Q3 (L/DAY)	**	FOC (KG/KG):	*
WIDTH (FT):	*	Kd (L/KG):	**	Kd (L/KG):	**	GW V.(FT/YR):	*	Kd (L/KG):	**
		SATURATION:	*	SATURATION:	*	H (FT):	**	RETARDATION:	**
POROSITY:	*	THICKNESS (FT):	*	THICKNESS (FT):	*	EFF. POROSITY	*	q (FT/YR) :	*
DENSITY (G/CM3):	*	DECAY (1/DAY):	**	DECAY (1/DAY):	**	DISPERSIVITY:		DECAY (1/YR):	**
INFILT. (FT/YR):	*	CAo (UG/L):	*	CBo (PPB):	*	Az(FT):	*	CU3 (PPB):	*
		CU1 (PPB):	*	CU2 (PPB):	*	Ax (FT):	*	P&T(YEARS):	*
AGE (YEARS):	*	Q1 (L/DAY):	**	Q2 (L/DAY):	*	Ay (FT):	*	DISTANCE TO F.L.(FT):	*

TIME INTERVAL (YRS) *	LAYER 1 LEACHATE CONC.	LAYER 2 LEACHATE CONC.	SOURCE AREA CONC.	FENCE LINE CONC.
ELAPSED TIME - YRS DAYS	(UG/L)	(UG/L)	(UG/L)	(UG/L)
Time	Calculated C_A	Calculated C_B	Calculated C_C	Calculated C_D
MAXIMUM:				

Notes:

* Required Input Parameters

** Automatically Calculated Parameters

The value of each cell in the column varies with t_i (elapsed time) and t_i ranges from 0 to the T with a increment Δt_i. The product, between each of S_i (i.e., S_0, S_1,...,S_n), $F(t_i)$ and a constant will give $C(X,t,S_i)$. The constant is the following remaining terms in Eq.(8):

$$\frac{1}{2}\exp\left\{\left(\frac{X}{2(D_x/V)}\right)\left[1-\left(1+\frac{4\lambda_c D_x}{V^2}\right)^{1/2}\right]\right\} erf\left[\frac{Y}{4\left(\frac{D_y}{V}X\right)^{1/2}}\right]$$

Finally, the Excel function **SUMPRODUCT** computes the $C_0(x,T)$ in Eq. (10) through summation of the products from t_0 to T or computes the $C_0(x,T)$ in Eq. (11) through summation of the products from t_i to T when the pump system exists.

In a previous version of this model (Chiou and Hubbard, 1992), which was implemented on SuperCalc5, a separate FORTRAN program (Appendix B) was required to perform calculations described in Eqs (9), (10), and (11). The linkage between the main spreadsheet and the external executable file was accomplished using macro commands in the spreadsheet. With Excel this external FORTRAN program was no longer necessary due the unique functions available within the spreadsheet.

3.4.2 Input/Output Format

Table 3-1 shows the format of the input/output table used by ECTran. This table is designed for both easy data input/revision processes and clear/complete output presentations. Table 3-1 also briefly explains the types of information included and the purpose of each portion of the format. The necessary input parameters used to calculate all the other information in the table are identified. These parameters will be discussed in Section 4.

3.4.3 Example Output

Three examples are presented here to demonstrate the capabilities and possible uses of the ECTran model during a typical RI/FS process for a hypothetical hazardous waste site.

Concentrations calculated by ECTran model in Layer 1, Layer 2, underlying saturated zone and downgradient transport under a constant source loading at a initially clean site are shown in Table 3-2 and Figure 3-5. This example presents the baseline conditions that need to be studied during the RI process. On the other hand, the next two examples will present the effect of remedial actions studied during the FS.

Model predicted concentrations for the same site used in the previous example, with the source loading being removed after 10 years, are shown in Table 3-3 and Figure 3-6. In this case the model parameter "Age" was specified as 10 years. In order to determine long-term residual impact at the downgradient exposure point, a longer time interval (i.e., 250 years) was simulated in this example.

Source loading removal and pumping of contaminated groundwater around the source area are both simulated in the third example. Model results are shown in Table 3-4 and Figure 3-7. In this case the model parameter "Age" was still specified as 10 years while the parameter "P&T" was specified as 20 years. The same time interval as in the second example was simulated in this example. As indicated by the last two examples, both source removal and pumping are required for the hypothetical site to ensure that the groundwater contaminant concentrations will be less than the given water criteria at the fence line.

3.5 MONTE CARLO SIMULATION

Unavoidably, uncertainties in the model input parameters will create uncertainties in the model outputs. Monte Carlo simulations can be used to assess the uncertainties of model predictions, based on the probability distributions of the model input parameters. The concept of a Monte Carlo simulation is to run a predicting model repeatedly with varying sets of possible input parameters. All the individual results can then be statistically analyzed to generate probability distributions of the "true" result. For performing Monte Carlo simulations, the uncertainties of input parameters may best be expressed in terms of probability density functions. These functions of input parameters should be statistically analyzed individually and be consistent with available observed data. Values of every model parameter to be studied in the Monte Carlo simulation should then be randomly generated according to these probability density functions before each individual simulation run.

Monte Carlo simulation requires a sufficiently large number of runs to achieve accuracy, which means that the ECTran model can typically be run numerous times. All the governing analytical transport equations implemented in ECTran are very efficient. Each individual run of ECTran can be completed within just a

4775

TABLE 3-2

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SCREENING-LEVEL EXCEL-CRYSTAL BALL TRANSPORT (ECTran) MODEL

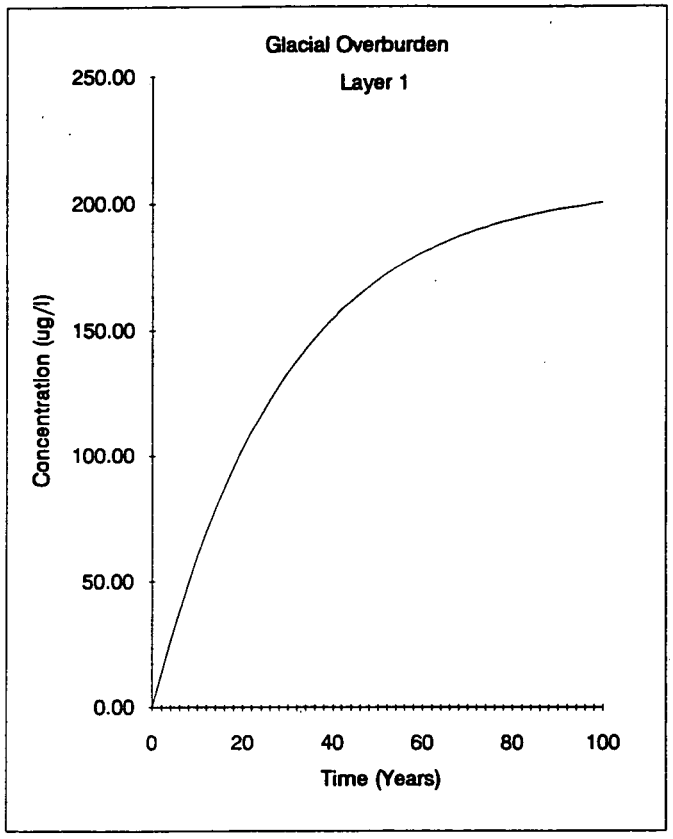
SITE:	HYPOTHETICAL, FEMP, FERNALD, OH	CONTAMINANT:	CHEMICAL X		
	BASELINE	KOC (L/KG):	45.00	WATER CRITERIA (UG/L):	3.00E+00
		HALF LIFE (YRS):		CONSTANT SOURCE LEACHATE (UG/L):	2.07E+02
		LAYER 1:	4.47E+09	INITIAL LAYER 1 SOIL CONC. (MG/KG):	0.00E+00
INVESTIGATOR:	CAR	LAYER 2:	4.47E+09	INITIAL LAYER 2 SOIL CONC. (MG/KG):	0.00E+00
DATE:	8/7/93	GMA:	4.47E+09		

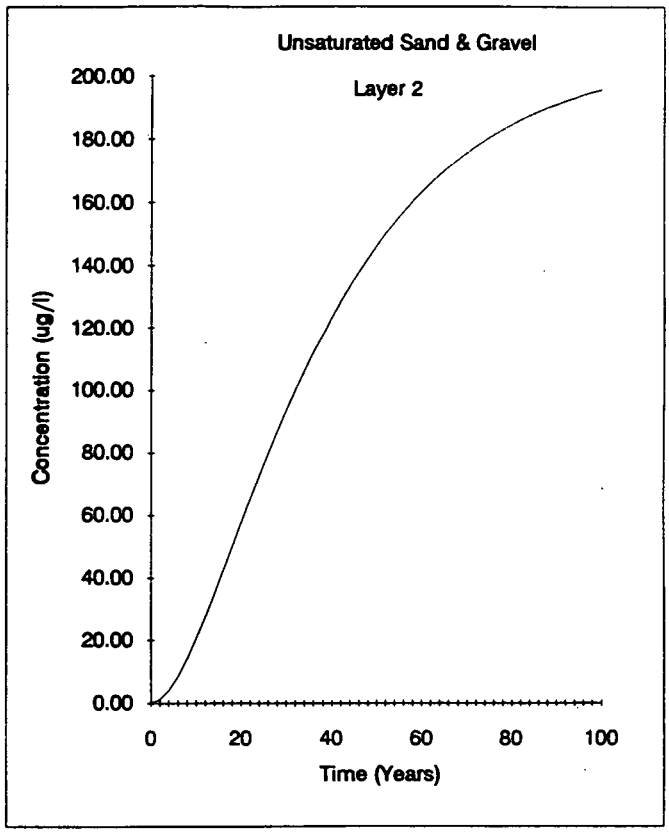
UNSAT. SOURCE	AREA:	LAYER 1 (GLACIAL OVERBURDEN)		LAYER 2 (SAND & GRAVEL)		GREAT MIAMI AQUIFER (SAT. S. & G.)			
						B (FT):	67	Vzo (FT/YR):	11.5445
LENGTH (FT):	250	FOC (KG/KG):	0.04	FOC (KG/KG):	0.0329	GW Q3 (L/DAY)	3.26E+04	FOC (KG/KG):	0.0329
WIDTH (FT):	230	Kd (L/KG):	1.8	Kd (L/KG):	1.481	GW. V.(FT/YR):	575.00	Kd (L/KG):	1.4805
		SATURATION:	0.45	SATURATION:	0.25	H (FT):	12.7100	RETARDATION:	11.5412
POROSITY:	0.34	THICKNESS (FT):	10.00	THICKNESS (FT):	5.00	EFF. POROSITY	0.25	q (FT/YR) :	0
DENSITY (G/CM3):	1.78	DECAY (1/DAY):	4.25E-13	DECAY (1/DAY):	4.25E-13	DISPERSIVITY:		DECAY (1/YR):	1.6E-10
INFILT. (FT/YR):	1.15	CAo (UG/L):	0.00E+00	CBo (PPB):	0.00E+00	Az(FT):	0.12	CU3 (PPB):	0
		CU1 (PPB):	207	CU2 (PPB):	0.00E+00	Ax (FT):	100.00	P&T(YEARS):	0
AGE (YEARS):	0	Q1 (L/DAY):	5.13E+03	Q2 (L/DAY):	0.00E+00	Ay (FT):	33.33	DISTANCE TO F.L.(FT):	275

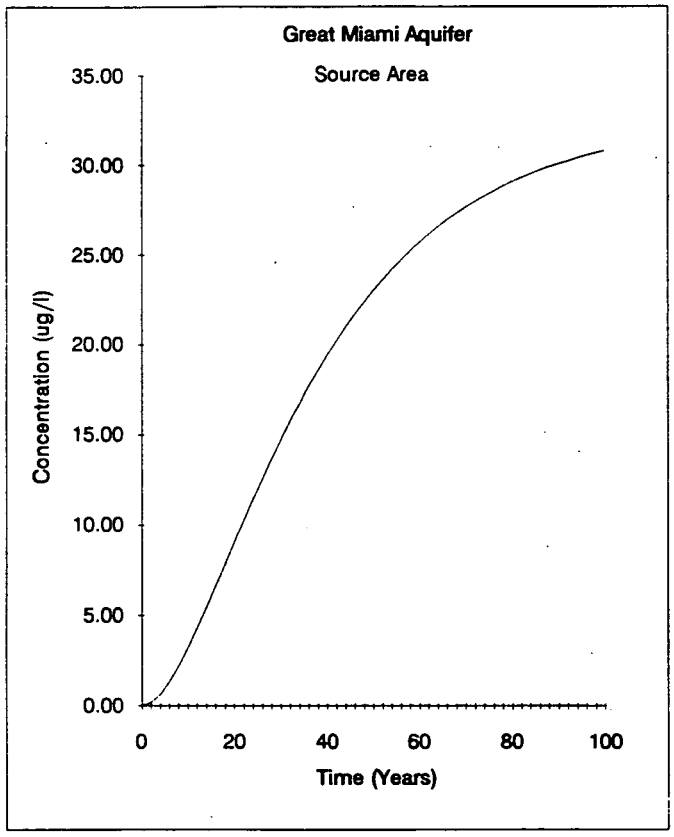
TIME INTERVAL (YRS)	2	LAYER 1 LEACHATE CONC.	LAYER 2 LEACHATE CONC.	SOURCE AREA CONC.	FENCE LINE CONC.
ELAPSED TIME - YRS	DAYS	(UG/L)	(UG/L)	(UG/L)	(UG/L)
0	0	0.00	0.00	0.00	0.00
2	730	13.71	1.11	0.17	0.00
4	1460	26.52	4.11	0.65	0.01
6	2190	38.48	8.56	1.35	0.07
8	2920	49.64	14.12	2.22	0.20
10	3650	60.07	20.50	3.23	0.43
12	4380	69.80	27.44	4.32	0.75
14	5110	78.89	34.77	5.47	1.16
16	5840	87.38	42.33	6.66	1.64
18	6570	95.31	49.98	7.86	2.18
20	7300	102.71	57.63	9.07	2.77
22	8030	109.62	65.21	10.26	3.40
24	8760	116.07	72.64	11.43	4.05
26	9490	122.09	79.89	12.57	4.72
28	10220	127.72	86.91	13.68	5.40
30	10950	132.97	93.69	14.74	6.08
32	11680	137.88	100.20	15.77	6.75
34	12410	142.46	106.44	16.75	7.41
36	13140	146.73	112.39	17.69	8.05
38	13870	150.72	118.06	18.58	8.68
40	14600	154.45	123.44	19.42	9.29
42	15330	157.93	128.55	20.23	9.87
44	16060	161.19	133.39	20.99	10.43
46	16790	164.22	137.96	21.71	10.97
48	17520	167.06	142.28	22.39	11.49
50	18250	169.70	146.35	23.03	11.98
52	18980	172.17	150.18	23.63	12.44
54	19710	174.48	153.79	24.20	12.88
56	20440	176.63	157.19	24.73	13.30
58	21170	178.65	160.38	25.24	13.69
60	21900	180.53	163.37	25.71	14.07
62	22630	182.28	166.18	26.15	14.42
64	23360	183.92	168.82	26.57	14.75
66	24090	185.45	171.30	26.95	15.06
68	24820	186.87	173.61	27.32	15.36
70	25550	188.21	175.79	27.66	15.63
72	26280	189.45	177.82	27.98	15.89
74	27010	190.62	179.72	28.28	16.14
76	27740	191.70	181.51	28.56	16.37
78	28470	192.71	183.18	28.82	16.58
80	29200	193.66	184.74	29.07	16.78
82	29930	194.54	186.20	29.30	16.97
84	30660	195.37	187.56	29.51	17.15
86	31390	196.14	188.84	29.72	17.31
88	32120	196.86	190.04	29.90	17.47
90	32850	197.53	191.15	30.08	17.61
92	33580	198.16	192.20	30.24	17.75
94	34310	198.74	193.17	30.40	17.88
96	35040	199.29	194.08	30.54	17.99
98	35770	199.80	194.94	30.67	18.10
100	36500	200.28	195.73	30.80	18.21
MAXIMUM:		200.28	195.73	30.80	18.21

32

FIGURE 3-5


Glacial Overburden
Layer 1
Concentration (ug/l)
250.00
200.00
150.00
100.00
50.00
0.00
0
20
40
60
80
100
Time (Years)


Unsaturated Sand & Gravel
Layer 2
Concentration (ug/l)
200.00
180.00
160.00
140.00
120.00
100.00
80.00
60.00
40.00
20.00
0.00
0
20
40
60
80
100
Time (Years)


Great Miami Aquifer
Source Area
Concentration (ug/l)
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
0
20
40
60
80
100
Time (Years)

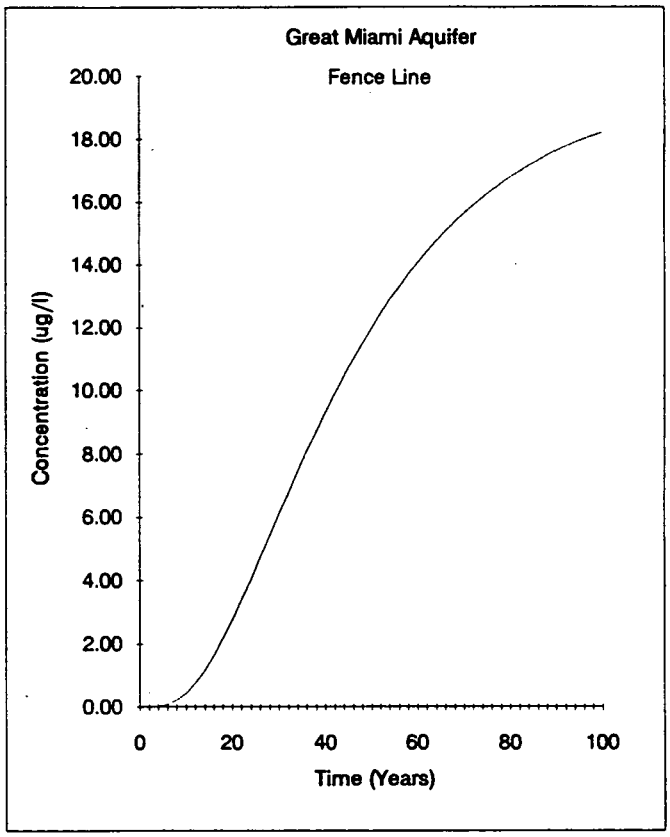

Great Miami Aquifer
Fence Line
Concentration (ug/l)
20.00
18.00
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
0
20
40
60
80
100
Time (Years)

TABLE 3-3

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BROWN & ROOT ENVIRONMENTAL

SCREENING-LEVEL EXCEL-CRYSTAL BALL TRANSPORT (ECTran) MODEL

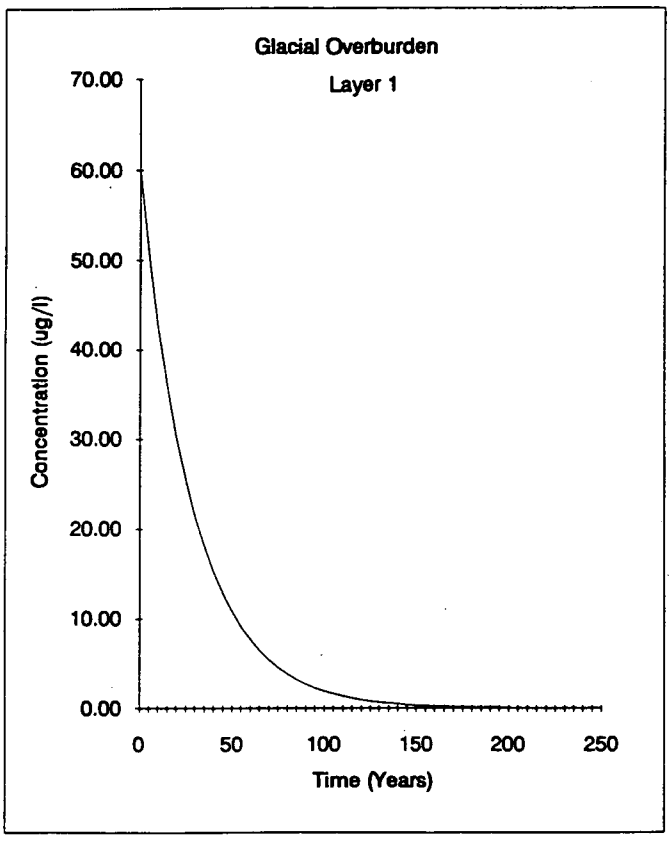
SITE:	HYPOTHETICAL, FEMP, FERNALD, OH
	AGE = 10 YRS; SOURCE REMOVED
	RESIDUAL CONTAMINATION IN LAYER 1 & 2
	PUMPING = 0 YRS
INVESTIGATOR:	CAR
DATE:	8/7/93

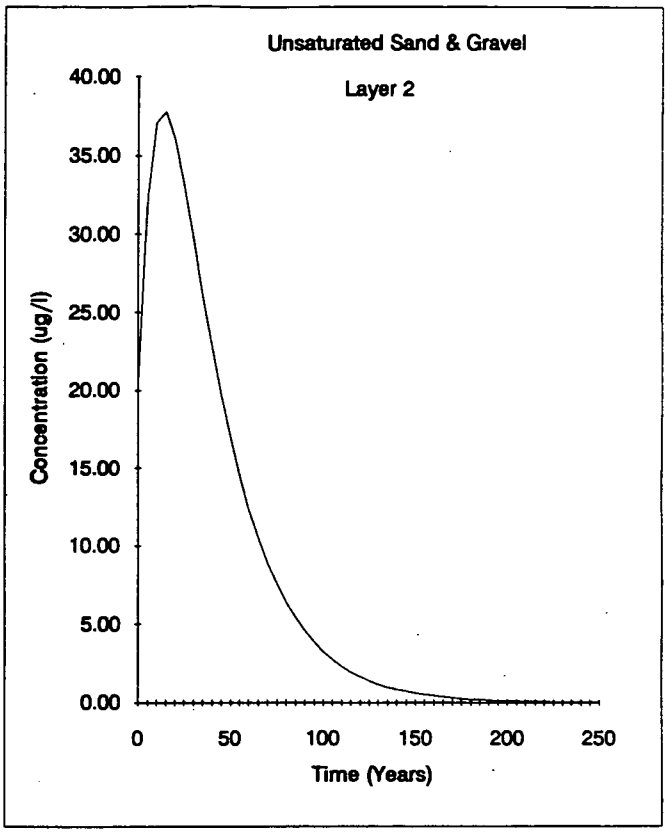
CONTAMINANT:		CHEMICAL X	
KOC (L/KG):	45.00	WATER CRITERIA (UG/L):	3.00E+00
HALF LIFE (YRS):		CONSTANT SOURCE LEACHATE (UG/L):	0.00E+00
LAYER 1:	4.47E+09	INITIAL LAYER 1 SOIL CONC. (MG/KG):	1.08E-01
LAYER 2:	4.47E+09	INITIAL LAYER 2 SOIL CONC. (MG/KG):	3.03E-02
GMA:	4.47E+09		

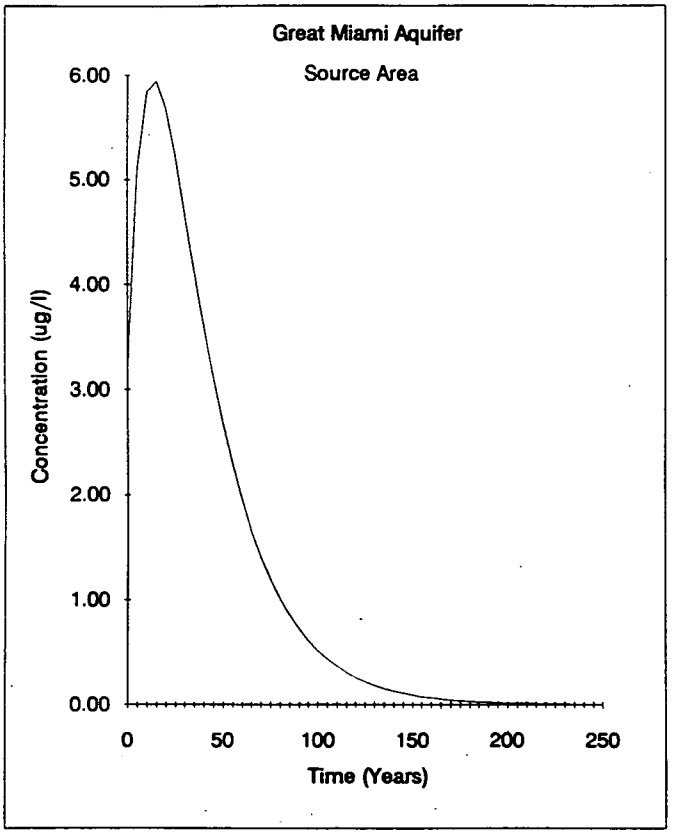
UNSAT. SOURCE	AREA:	LAYER 1 (GLACIAL OVERBURDEN)		LAYER 2 (SAND & GRAVEL)		GREAT MIAMI AQUIFER (SAT. S. & G.)			
						B (FT):	67	Vzo (FT/YR):	11.5445
LENGTH (FT):	250	FOC (KG/KG):	0.04	FOC (KG/KG):	0.0329	GW Q3 (L/DAY)	3.26E+04	FOC (KG/KG):	0.0329
WIDTH (FT):	230	Kd (L/KG):	1.8	Kd (L/KG):	1.481	GW V.(FT/YR):	575.00	Kd (L/KG):	1.4805
		SATURATION:	0.45	SATURATION:	0.25	H (FT):	12.7100	RETARDATION:	11.5412
POROSITY:	0.34	THICKNESS (FT):	10.00	THICKNESS (FT):	5.00	EFF. POROSITY	0.25	q (FT/YR) :	0
DENSITY (G/CM3):	1.78	DECAY (1/DAY):	4.25E-13	DECAY (1/DAY):	4.25E-13	DISPERSIVITY:		DECAY (1/YR):	1.6E-10
INFILT. (FT/YR):	1.15	CAo (UG/L):	6.01E+01	CBo (PPB):	2.05E+01	Az(FT):	0.12	CU3 (PPB):	0
		CU1 (PPB):	0	CU2 (PPB):	0.00E+00	Ax (FT):	100.00	P&T(YEARS):	0
AGE (YEARS):	10	Q1 (L/DAY):	5.13E+03	Q2 (L/DAY):	0.00E+00	Ay (FT):	33.33	DISTANCE TO F.L.(FT):	275

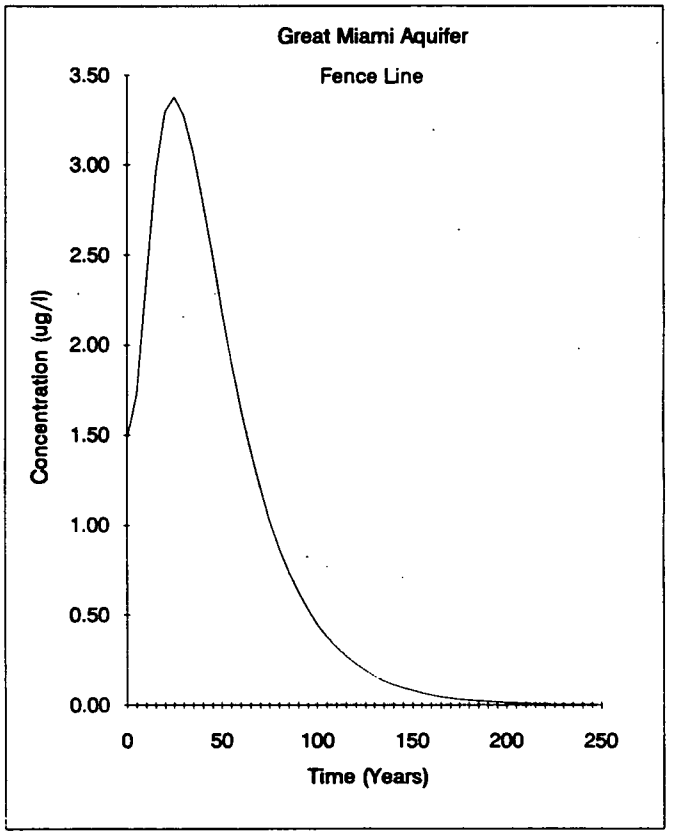
TIME INTERVAL (YRS)	5	LAYER 1 LEACHATE CONC.	LAYER 2 LEACHATE CONC.	SOURCE AREA CONC.	FENCE LINE CONC.
ELAPSED TIME - YRS	DAYS	(UG/L)	(UG/L)	(UG/L)	(UG/L)
0	0	60.06	20.49	3.22	1.48
5	1825	50.60	32.34	5.09	1.73
10	3650	42.63	37.13	5.84	2.36
15	5475	35.91	37.75	5.94	2.96
20	7300	30.26	36.05	5.67	3.30
25	9125	25.49	33.15	5.22	3.38
30	10950	21.48	29.75	4.68	3.28
35	12775	18.09	26.25	4.13	3.06
40	14600	15.25	22.90	3.60	2.78
45	16425	12.84	19.80	3.12	2.48
50	18250	10.82	17.02	2.68	2.18
55	20075	9.12	14.56	2.29	1.90
60	21900	7.68	12.41	1.95	1.64
65	23725	6.47	10.55	1.66	1.41
70	25550	5.45	8.95	1.41	1.20
75	27375	4.59	7.58	1.19	1.03
80	29200	3.87	6.41	1.01	0.87
85	31025	3.26	5.42	0.85	0.74
90	32850	2.75	4.58	0.72	0.63
95	34675	2.31	3.86	0.61	0.53
100	36500	1.95	3.26	0.51	0.45
105	38325	1.64	2.75	0.43	0.38
110	40150	1.38	2.32	0.36	0.32
115	41975	1.17	1.96	0.31	0.27
120	43800	0.98	1.65	0.26	0.23
125	45625	0.83	1.39	0.22	0.19
130	47450	0.70	1.17	0.18	0.16
135	49275	0.59	0.99	0.16	0.14
140	51100	0.49	0.83	0.13	0.11
145	52925	0.42	0.70	0.11	0.10
150	54750	0.35	0.59	0.09	0.08
155	56575	0.30	0.50	0.08	0.07
160	58400	0.25	0.42	0.07	0.06
165	60225	0.21	0.35	0.06	0.05
170	62050	0.18	0.30	0.05	0.04
175	63875	0.15	0.25	0.04	0.03
180	65700	0.13	0.21	0.03	0.03
185	67525	0.11	0.18	0.03	0.02
190	69350	0.09	0.15	0.02	0.02
195	71175	0.08	0.13	0.02	0.02
200	73000	0.06	0.11	0.02	0.01
205	74825	0.05	0.09	0.01	0.01
210	76650	0.04	0.08	0.01	0.01
215	78475	0.04	0.06	0.01	0.01
220	80300	0.03	0.05	0.01	0.01
225	82125	0.03	0.05	0.01	0.01
230	83950	0.02	0.04	0.01	0.01
235	85775	0.02	0.03	0.01	0.00
240	87600	0.02	0.03	0.00	0.00
245	89425	0.01	0.02	0.00	0.00
250	91250	0.01	0.02	0.00	0.00
MAXIMUM:		60.06	37.75	5.94	3.38

FIGURE 3-6


Glacial Overburden
Layer 1
Concentration (ug/l)
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
0
50
100
150
200
250
Time (Years)


Unsaturated Sand & Gravel
Layer 2
Concentration (ug/l)
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
0
50
100
150
200
250
Time (Years)


Great Miami Aquifer
Source Area
Concentration (ug/l)
6.00
5.00
4.00
3.00
2.00
1.00
0.00
0
50
100
150
200
250
Time (Years)


Great Miami Aquifer
Fence Line
Concentration (ug/l)
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
0
50
100
150
200
250
Time (Years)

4775

TABLE 3-4

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BROWN & ROOT ENVIRONMENTAL

SCREENING-LEVEL EXCEL-CRYSTAL BALL TRANSPORT (ECTran) MODEL

SITE:	HYPOTHETICAL, FEMP, FERNALD, OH
	AGE = 10 YRS; SOURCE REMOVED
	RESIDUAL CONTAMINATION IN LAYER 1 & 2
	PUMPING = 20 YRS
INVESTIGATOR:	CAR
DATE:	8/7/93

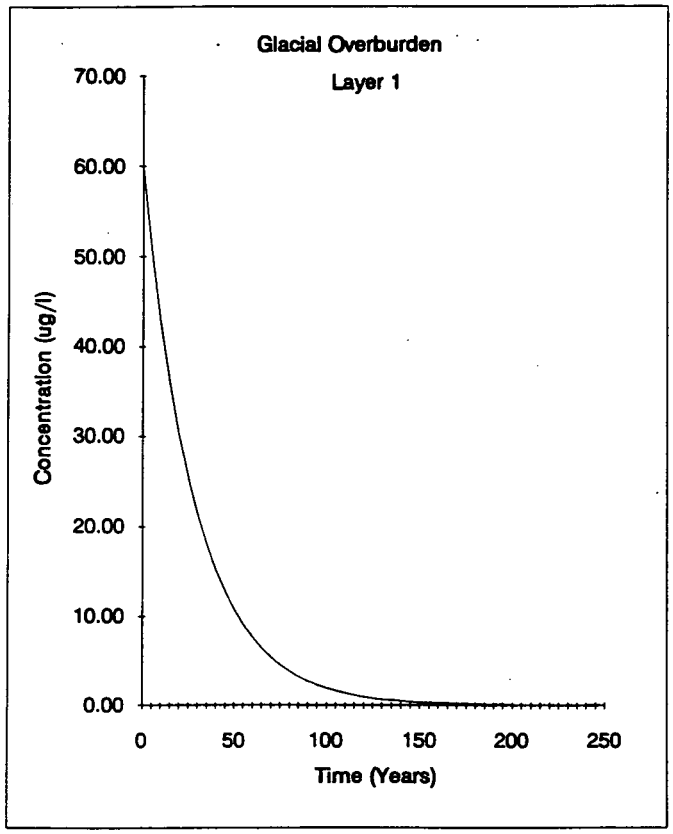
CONTAMINANT:		CHEMICAL X	
KOC (L/KG):	45.00	WATER CRITERIA (UG/L):	3.00E+00
HALF LIFE (YRS):		CONSTANT SOURCE LEACHATE (UG/L):	0.00E+00
LAYER 1:	4.47E+09	INITIAL LAYER 1 SOIL CONC. (MG/KG):	1.08E-01
LAYER 2:	4.47E+09	INITIAL LAYER 2 SOIL CONC. (MG/KG):	3.03E-02
GMA:	4.47E+09		

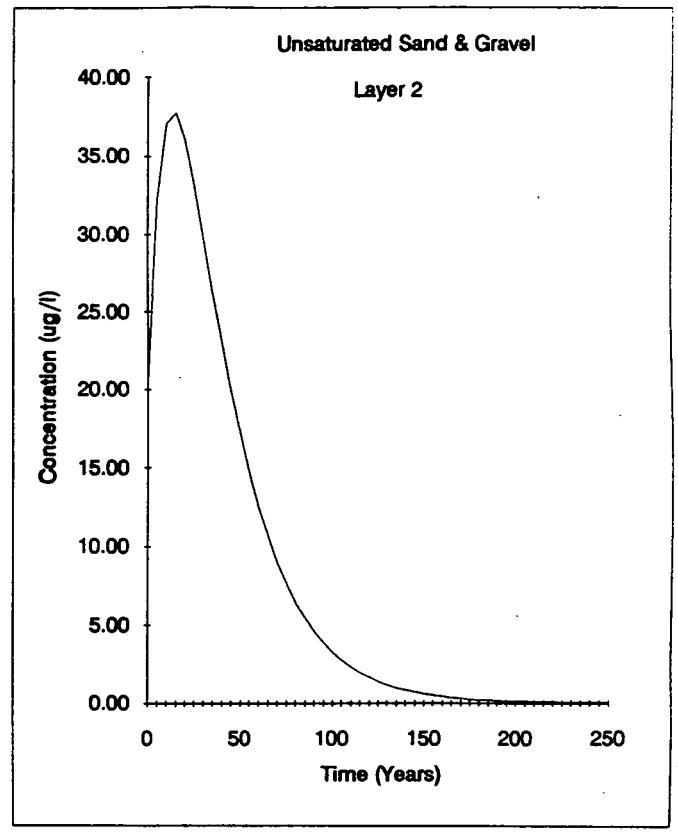
UNSAT. SOURCE	AREA:	LAYER 1 (GLACIAL OVERBURDEN)		LAYER 2 (SAND & GRAVEL)		GREAT MIAMI AQUIFER (SAT. S. & G.)			
						B (FT):	67	Vzo (FT/YR):	11.5445
LENGTH (FT):	250	FOC (KG/KG):	0.04	FOC (KG/KG):	0.0329	GW Q3 (L/DAY)	3.26E+04	FOC (KG/KG):	0.0329
WIDTH (FT):	230	Kd (L/KG):	1.8	Kd (L/KG):	1.481	GW V.(FT/YR):	575.00	Kd (L/KG):	1.4805
		SATURATION:	0.45	SATURATION:	0.25	H (FT):	12.7100	RETARDATION:	11.5412
POROSITY:	0.34	THICKNESS (FT):	10.00	THICKNESS (FT):	5.00	EFF. POROSITY	0.25	q (FT/YR) :	0
DENSITY (G/CM3):	1.78	DECAY (1/DAY):	4.25E-13	DECAY (1/DAY):	4.25E-13	DISPERSIVITY:		DECAY (1/YR):	1.6E-10
INFILT. (FT/YR):	1.15	CAo (UG/L):	6.01E+01	CBo (PPB):	2.05E+01	Az(FT):	0.12	CU3 (PPB):	0
		CU1 (PPB):	0	CU2 (PPB):	0.00E+00	Ax (FT):	100.00	P&T(YEARS):	20
AGE (YEARS):	10	Q1 (L/DAY):	5.13E+03	Q2 (L/DAY):	0.00E+00	Ay (FT):	33.33	DISTANCE TO F.L.(FT):	275

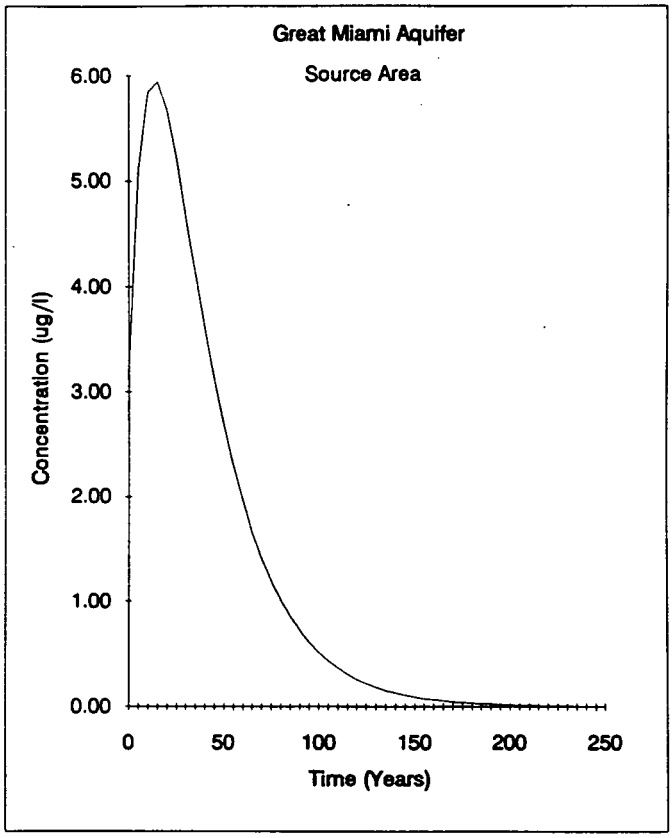
TIME INTERVAL (YRS)	5	LAYER 1 LEACHATE CONC.	LAYER 2 LEACHATE CONC.	SOURCE AREA CONC.	FENCE LINE CONC.
ELAPSED TIME - YRS	DAYS	(UG/L)	(UG/L)	(UG/L)	(UG/L)
0	0	60.06	20.49	3.22	1.48
5	1825	50.60	32.34	5.09	0.85
10	3650	42.63	37.13	5.84	0.36
15	5475	35.91	37.75	5.94	0.17
20	7300	30.26	36.05	5.67	0.08
25	9125	25.49	33.15	5.22	1.59
30	10950	21.48	29.75	4.68	2.50
35	12775	18.09	26.25	4.13	2.70
40	14600	15.25	22.90	3.60	2.61
45	16425	12.84	19.80	3.12	2.40
50	18250	10.82	17.02	2.68	2.14
55	20075	9.12	14.56	2.29	1.88
60	21900	7.68	12.41	1.95	1.63
65	23725	6.47	10.55	1.66	1.40
70	25550	5.45	8.95	1.41	1.20
75	27375	4.59	7.58	1.19	1.02
80	29200	3.87	6.41	1.01	0.87
85	31025	3.26	5.42	0.85	0.74
90	32850	2.75	4.58	0.72	0.63
95	34675	2.31	3.86	0.61	0.53
100	36500	1.95	3.26	0.51	0.45
105	38325	1.64	2.75	0.43	0.38
110	40150	1.38	2.32	0.36	0.32
115	41975	1.17	1.96	0.31	0.27
120	43800	0.98	1.65	0.26	0.23
125	45625	0.83	1.39	0.22	0.19
130	47450	0.70	1.17	0.18	0.16
135	49275	0.59	0.99	0.16	0.14
140	51100	0.49	0.83	0.13	0.11
145	52925	0.42	0.70	0.11	0.10
150	54750	0.35	0.59	0.09	0.08
155	56575	0.30	0.50	0.08	0.07
160	58400	0.25	0.42	0.07	0.06
165	60225	0.21	0.35	0.06	0.05
170	62050	0.18	0.30	0.05	0.04
175	63875	0.15	0.25	0.04	0.03
180	65700	0.13	0.21	0.03	0.03
185	67525	0.11	0.18	0.03	0.02
190	69350	0.09	0.15	0.02	0.02
195	71175	0.08	0.13	0.02	0.02
200	73000	0.06	0.11	0.02	0.01
205	74825	0.05	0.09	0.01	0.01
210	76650	0.04	0.08	0.01	0.01
215	78475	0.04	0.06	0.01	0.01
220	80300	0.03	0.05	0.01	0.01
225	82125	0.03	0.05	0.01	0.01
230	83950	0.02	0.04	0.01	0.01
235	85775	0.02	0.03	0.01	0.00
240	87600	0.02	0.03	0.00	0.00
245	89425	0.01	0.02	0.00	0.00
250	91250	0.01	0.02	0.00	0.00
MAXIMUM:		60.06	37.75	5.94	2.70

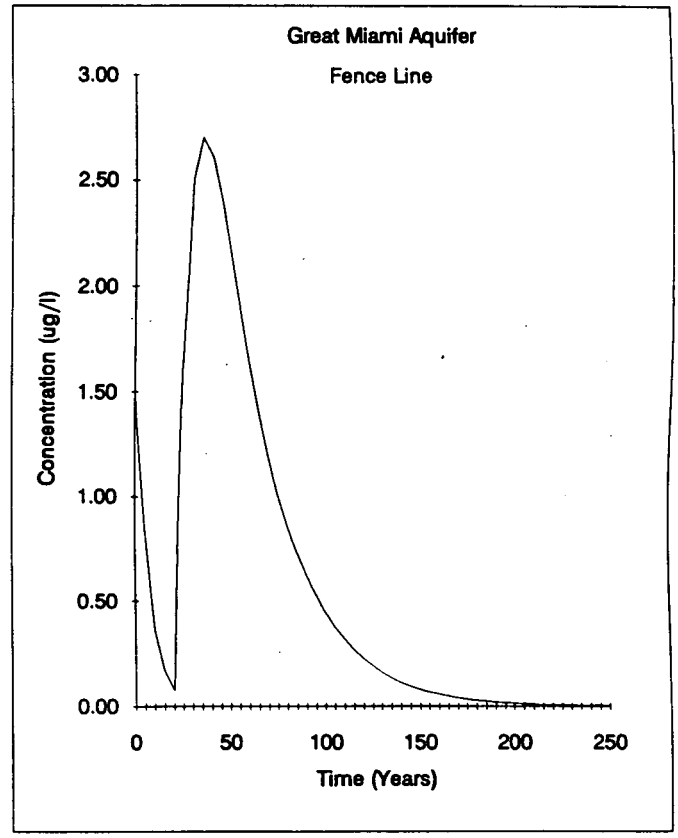
36

FIGURE 3-7


Glacial Overburden
Layer 1
Concentration (ug/l)
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
0
50
100
150
200
250
Time (Years)


Unsaturated Sand & Gravel
Layer 2
Concentration (ug/l)
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
0
50
100
150
200
250
Time (Years)


Great Miami Aquifer
Source Area
Concentration (ug/l)
6.00
5.00
4.00
3.00
2.00
1.00
0.00
0
50
100
150
200
250
Time (Years)


Great Miami Aquifer
Fence Line
Concentration (ug/l)
3.00
2.50
2.00
1.50
1.00
0.50
0.00
0
50
100
150
200
250
Time (Years)

few seconds. Therefore, Monte Carlo simulation can be very efficiently performed with ECTran. On the other hand, SWIFT and ODAST, which require more than 30 hours for a typical application at FEMP, are not suggested to be used in a Monte Carlo simulation.

3.5.1 Implementation

For a spreadsheet without specially designed capabilities, it is very difficult to repeat and summarize computations with automatically changing parameters. Fortunately, a software package called Crystal Ball is available which can work within Excel to facilitate Monte Carlo simulation. Crystal Ball allows different probability distributions, such as normal, Poisson, binomial and exponential, to be defined for each uncertain cell in the Excel spreadsheet and then generates random numbers from the given probability distributions. Crystal Ball uses these random numbers to compute the formulas in the forecast cells. This process continues with the forecast formulas being recalculated over and over until the required number of individual simulations is reached. Also, while the simulation is running, Crystal Ball charts the forecast results in an easy-to-understand graphical format. Finally, Crystal Ball will give the statistics that describe the forecast results. As described, Crystal Ball significantly extends the forecasting capability of Excel.

ECTran utilizes Crystal Ball during the Monte Carlo simulation applications. For example, selected stratigraphy, hydrogeology, and contaminant parameters can be analyzed separately or simultaneously to quantify the probability of groundwater concentrations at an exposure point exceeding given criteria.

The sensitivity of the groundwater concentrations to the input parameters may also be approximated in terms of the correlation coefficients between the outputs and inputs.

3.5.2 Examples

A Monte Carlo simulation in ECTran based on the third example presented in Section 3.4.3 (i.e., remediation with source removal and pumping) was performed. The infiltration rate, saturation rates, foc values, and groundwater velocity in the model were treated as random variables simultaneously with specific probability functions. For this demonstrative example, 500 simulations were automatically run by ECTran. The resulting maximum groundwater contaminant concentrations at the source area and the fence line in the GMA were statistically analyzed and a summary report was generated by the model.

Although the previously predicted maximum concentration at the fence line was acceptable, the Monte Carlo simulation concluded that, with about 40 percent possibility, this maximum groundwater contaminant

concentration may actually exceed the water criteria given the uncertainties in model parameters. Therefore, it was determined necessary to extend the pumping time in the source area to 30 years. A second Monte Carlo simulation was conducted for this new pumping time with the same uncertainties associated with the model parameters. Results of this analysis indicate that there is less than a 5 percent possibility that the maximum fence line groundwater contaminant concentration will exceed the water criteria.

Complete summary reports of the first and second Monte Carlo simulations are included in Appendices A.1 and A.2, respectively.

4.0 DATA REQUIREMENT

As a screening model, several types of data are still required for the ECTran model to realistically simulate a site. Necessary data includes contaminant, geochemical and hydrogeological information at the study area. Preferably, site-specific data is determined by field tests or laboratory analyses and used as input for the model. In some cases, when site-specific values are not available when the model is applied, the input data can be estimated from literature values. Other information such as the risk assessment scenario and remedial alternative can also be incorporated and analyzed by the ECTran model.

4.1 CONTAMINANT AND GEOCHEMICAL INFORMATION

Radionuclides, inorganic and organic contaminants are all present at the FEMP. The data necessary to model radionuclides includes radioactive decay half-lives and soil- and contaminant-specific distribution coefficients (K_d). For the organic contaminants, soil and groundwater biodegradation and chemical decay half-lives and the contaminant-specific organic carbon partition coefficient (K_{oc}) or octanol-water partition coefficient (K_{ow}) are necessary model input. For the inorganic contaminants, soil- and contaminant-specific K_ds are required.

Information regarding the initial/current levels of contamination in each model layer and future source loading rates should also be defined. Chemical-specific acceptable concentration levels are also provided in cleanup goal development applications.

4.2 HYDROGEOLOGICAL INFORMATION

Several aquifer and soil parameters are necessary in the ECTran model. They include porosity, bulk density, saturation rate, fraction of organic content (FOC), hydraulic conductivity, hydraulic gradient, travel distance to downgradient exposure points, groundwater velocity, infiltration rate, dispersion coefficient, and vertical seepage velocity.

A majority of these parameters have been estimated by field measurements at the FEMP. For instance, hydraulic conductivity values were estimated by a pump test in the South Plume and numerous slug tests throughout the facility. Hydraulic gradients can be calculated from groundwater contour maps which were

developed from monthly field measurements. Porosity, bulk density, saturation rate, and foc can be acquired from the results of geotechnical and laboratory analyses.

Other input parameters can be estimated using other hydrological models. For example, the HELP model can be used to estimate the infiltration rate and the degree of saturation or moisture content of the unsaturated zones.

4.3 RISK ASSESSMENT SCENARIO INFORMATION

For many fate and transport modeling tasks the results of the modeling are used to determine the potential risk of the contaminants in the groundwater to humans, wildlife, and the environment. To assess the effects of the groundwater contaminants on the potential receptors, the model must be flexible enough to calculate the contaminant concentrations at each potential exposure point defined in the risk assessment scenario. A risk assessment scenario is the combination of the potential migration and exposure pathways and the protocol for risk calculations. Usually an acceptable chemical-specific groundwater concentration for a receptor are defined in the scenario. These criteria are usually either the Maximum Concentration Limits (MCLs) or the incremental cancer risk-based concentrations which can be calculated based on chemical-specific cancer slope factors.

For model applications at the FEMP to support risk assessment, there are three potential groundwater exposure scenarios. They include using perched groundwater, GMA groundwater under the contaminant source area, or GMA groundwater downgradient at the FEMP property line as drinking or irrigation water. The criteria used for the modeling will usually be the incremental cancer risk-based concentrations. These values can be more conservative than the MCLs and account for the combined effect of contaminants.

4.4 REMEDIAL ALTERNATIVE INFORMATION

Remedial alternatives constitute the proposed actions to be performed on contaminant source areas to mitigate potential impacts on human health, wildlife, and environment. Several alternatives which are currently evaluated at the FEMP include capping, source reduction and removal, soil washing, and hydraulic recovery and barrier. All of these alternatives' effectiveness can be investigated with the ECTran model. The capping alternative can be simulated in the ECTran model by reducing the infiltration rate. Source removal can be accomplished with the model by reducing the source leachate concentration or initial

concentrations in soil layers. The impact of saturated zone containment or pumping on the downgradient groundwater concentrations can be investigated by using the pumping option of the ECTran model.

5.0 COMPARISON AND VERIFICATION WITH SWIFT AND ODAST

As described in Sections 2.0 and 3.0, the ECTran model can simulate contaminant transport through both the vadose and saturated zones. In previous modeling at the FEMP site two separate models were used to estimate the contaminant migration through these zones and they are ODAST and SWIFT (DOE, 1993a), respectively. The following sections compare results from these two different modeling approaches. Also the advantages and disadvantages of using the two different modeling schemes are described.

It is important to note that the overall purpose of the model comparsions discussed in this section is to demonstrate the relative conservativeness between the two modeling approaches (i.e., ECTran and current ODAST/SWIFT). Because the current groundwater flow and transport model developed with SWIFT code is under improvements (DOE, 1993b), the accuracy or correctness of either model are not the main focus of this section.

5.1 MODEL RESOLUTION

A model's accuracy and usefulness is highly dependent on the resolution of the model. The resolution of a model is dependent upon the characteristics of the natural system to be modeled and the required modeling results. Vertical and areal coverages allowed in the model are the two most important resolution characteristics. For instance an aquifer's vertical resolution may be represented in the model using either a general single-layer structure or a detailed multi-layer structure. The model using the general single-layer structure would estimate only a single contaminant result for the entire depth of the aquifer. This type of model would be best suited for a homogeneous aquifer system. In comparison the model which uses the detailed multi-layer structure could simulate layer-specific contaminant concentrations which would be more comparable to the natural aquifer system. This type of model would be better suited for a heterogeneous aquifer system.

The goal during the screening model development was to create a single flexible model which could adequately estimate the maximum contaminant concentrations in the vadose and saturated zones underlying any given source area in the FEMP. To accommodate this goal, the model was created so that concentrations could be calculated in two separate vadose zone layers and at two separate saturated zone locations (i.e., under the source area and a down gradient location which is usually at the fence line). The

saturated thickness used in the ECTran model was the mixing depth. This thickness is usually smaller than the thickness used for the top layer in the current SWIFT model. The current SWIFT model has two model layers in the Upper Great Miami Aquifer which has an about 65 to 75 feet saturated thickness. The current top SWIFT model layer is 40 feet (in which about 35 feet is saturated). Using Equation (8) in Section 3, calculated groundwater mixing depths at the FEMP are usually between 10 and 20 feet. Therefore, with the mixing depth approach, the ECTran model provides higher resolution than the current SWIFT model in the saturated zone. ECTran, thus, gives more conservative estimations of the maximum groundwater contaminant concentrations. Due to the differences between the mixing depth used in ECTran and the fixed top layer thickness in current SWIFT model alone, the maximum groundwater concentrations estimated by ECTran are expected to be at least 2 to 4 times higher than corresponding concentrations by the current SWIFT model.

There are also limitations to having a simple model as compared to a very rigid, detailed model. The ECTran model uses uniform flow equations, considers only one source at a time, areal coverage limited to one specific region, and the model represents the aquifer as a single, continuous, homogeneous layer. In comparison the SWIFT model uses nonuniform flow equations, can consider multiple sources at one time, the areal coverage of the model is almost limitless, and the aquifer can be separated into discrete grid blocks each having its own properties to account for the heterogeneities in the aquifer.

5.2 MODEL RESULT

In general, different models may simulate the same system slightly differently. The differences are usually due to the simplifications and assumptions in the conceptual models, governing equations, numerical methods, and amount of detail used by each model. A comparison can be made to quantify the differences between the ECTran model results and the ODAST and SWIFT models results. So that the comparison is equal, the same input should be used for each of the models. Table 5-1 summarizes site characteristics for comparing two OU2 waste units that were used for the three models of interest. It is re-emphasized that significant differences between the two modeling approaches are expected. Therefore, the purpose of these comparsions is to demonstrate and quantify the relative conservativeness. The accuracy or correctness of either model are not the main focus of the comparsions.

TABLE 5-1

SUMMARY OF MODELING CHARACTERISTICS
FOR TWO OU2 WASTE UNITS

Parameter	Solid Waste Landfill	Inactive Fly Ash Pile
Source Leachate Conc.[1] (ug/L)	57,000	502
Source Area (ft^2)	42,400	130,800
Porosity	0.34	0.34
Layer 1 K_d[2] (L/kg)	1.80	1.80
Layer 2 K_d[2] (L/kg)	1.48	1.48
Aquifer K_d[2] (L/kg)	1.48	1.48
Infiltration Rate (ft/yr)	1.06	1.06
Layer 1 Thickness (ft)	20	5
Layer 2 Thickness (ft)	30	25
Aquifer Thickness[3] (ft)	65 (9.03)	72 (18.87)

(1) Uranium concentration estimated in the previous RI report (DOE, 1992).

(2) K_d value used in the previous RI report. The area-specific K_d values are currently under laboratory study.

(3) The aquifer thickness presented is an approximation of the Upper Great Miami Aquifer thickness. The values in parentheses are the calculated mixing depths used in the ECTran model. Thickness of the top layer in the current SWIFT model is 40 ft.

The data summarized in Table 5-1 was used in the ECTran, ODAST, and SWIFT models. A comparison of the ECTran and ODAST model's results is presented in Figures 5-1 and 5-2. From Figures 5-1 and 5-2 it can be seen that the ECTran and ODAST models compare fairly well for Inactive Flyash Pile Waste Site and not as well for the Solid Waste Landfill Site. The reason for the difference is that the two waste units have different source characteristics. The Inactive Flyash Pile has a very long depletion time for the source due to the presence of a large amount of contaminant mass, small α (decay constant), and long T_o (time for complete depletion of source). With these characteristics, the source of the Inactive Flyash Pile waste unit acts like as a constant source, which is the same way ECTran models the source loading. In contrast, the Solid Waste Landfill has a very short depletion time for the source due to a limited amount of contaminant mass, large α (decay constant), and short T_o (time for complete depletion of the source). A source with these characteristics will deplete quickly and is not directly comparable to a constant source.

A comparison of the ECTran and SWIFT model's results is presented in Figures 5-3 and 5-4. From the figures it is obvious that the ECTran model is more conservative than the SWIFT model. For the Inactive Flyash Pile the ECTran concentrations are approximately five (5) times greater than the SWIFT predicted concentrations. In comparison the ECTran results for the Solid Waste Landfill vary from approximately 5 to 155 times greater than the SWIFT results. The differences between the results are due to both the thicknesses of model layers and the source depletion characteristics. After reviewing the comparison between the ECTran model and the current ODAST and SWIFT models it is obvious that the ECTran model is more conservative than the other models. Therefore, the ECTran model can be used safely as a screening model but the model may over estimate the final (e.g., after 1,000 years from the current time) contaminant concentrations in the aquifer. These final concentrations should be estimated using the more complex ODAST/SWIFT model combination which considers depletion of the source term.

Although not directly related to ECTran model development and application, it is also important to note that the current SWIFT groundwater fate and transport model is currently under improvement activities (DOE, 1993b). One of the improvement tasks is to increase the vertical resolution by dividing the current top layer into two (2) separated model layers. After this improvement, it is expected that maximum concentrations estimated by SWIFT model will increase by two (2) to four (4) times. The difference between ECTran and ODAST/SWIFT model will then be insignificant within a five-hundred-year time frame for the major contaminant (i.e., uranium) in most of the source areas at the FEMP because of the existing amount of contaminant.

FIGURE 5-1

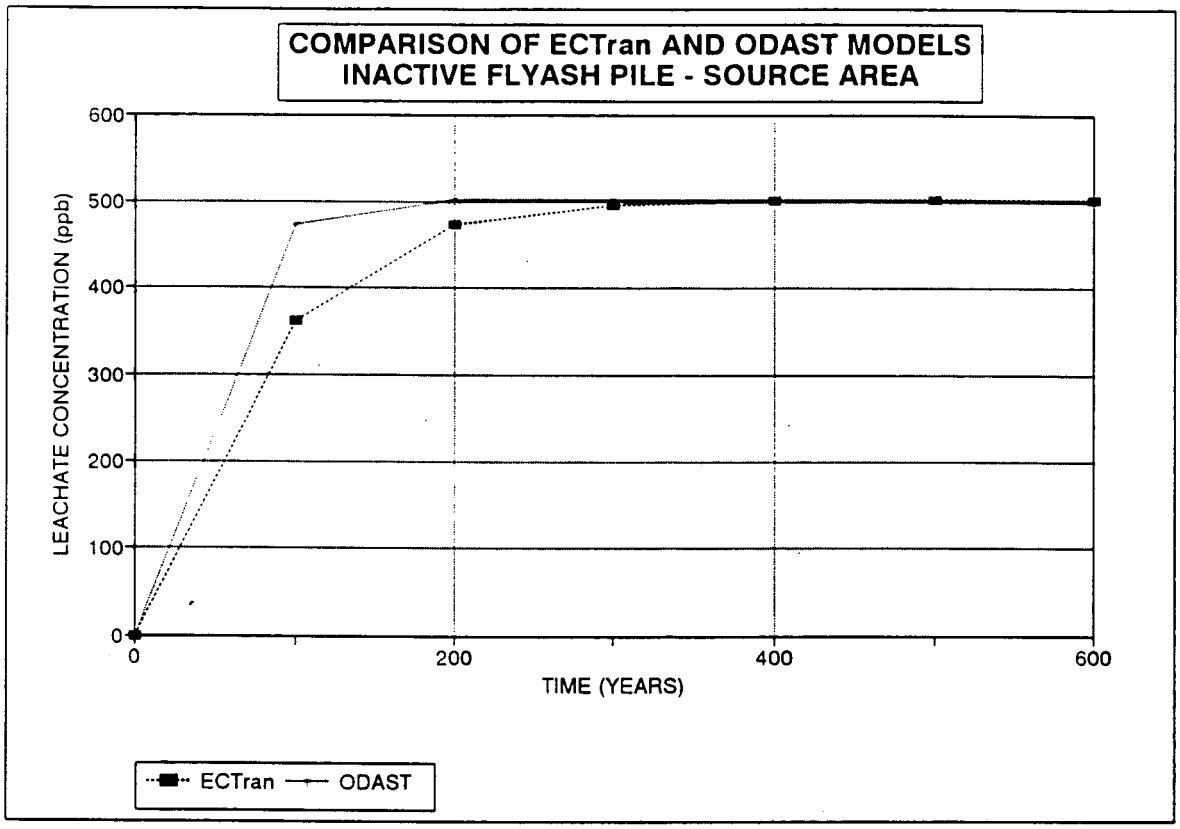


FIGURE 5-2

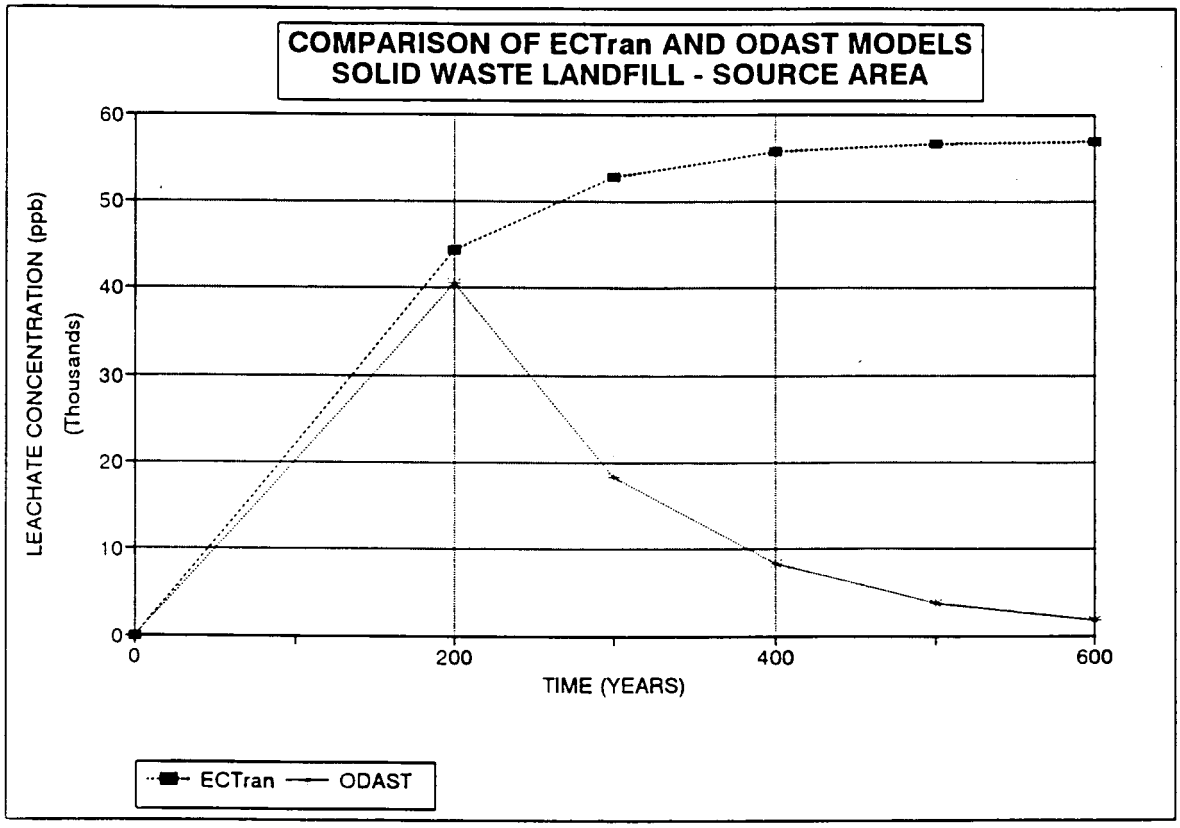


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FIGURE 5-3

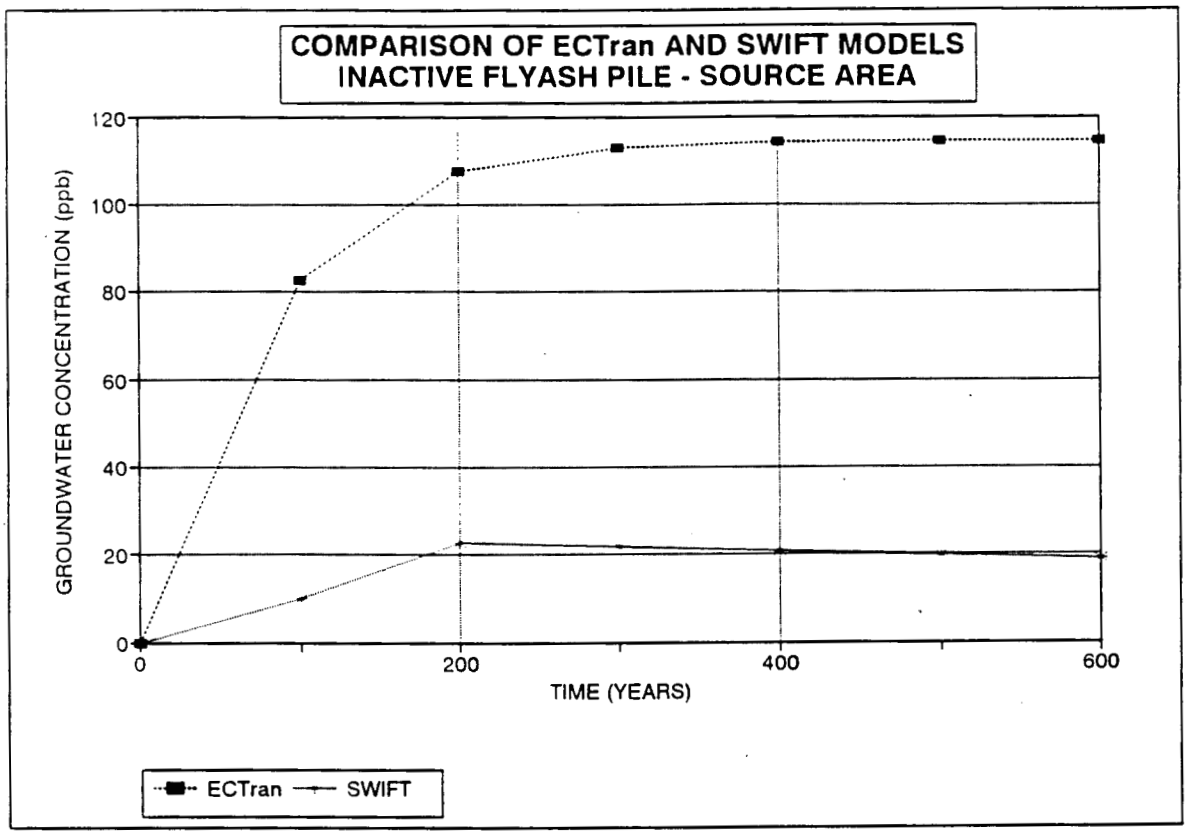
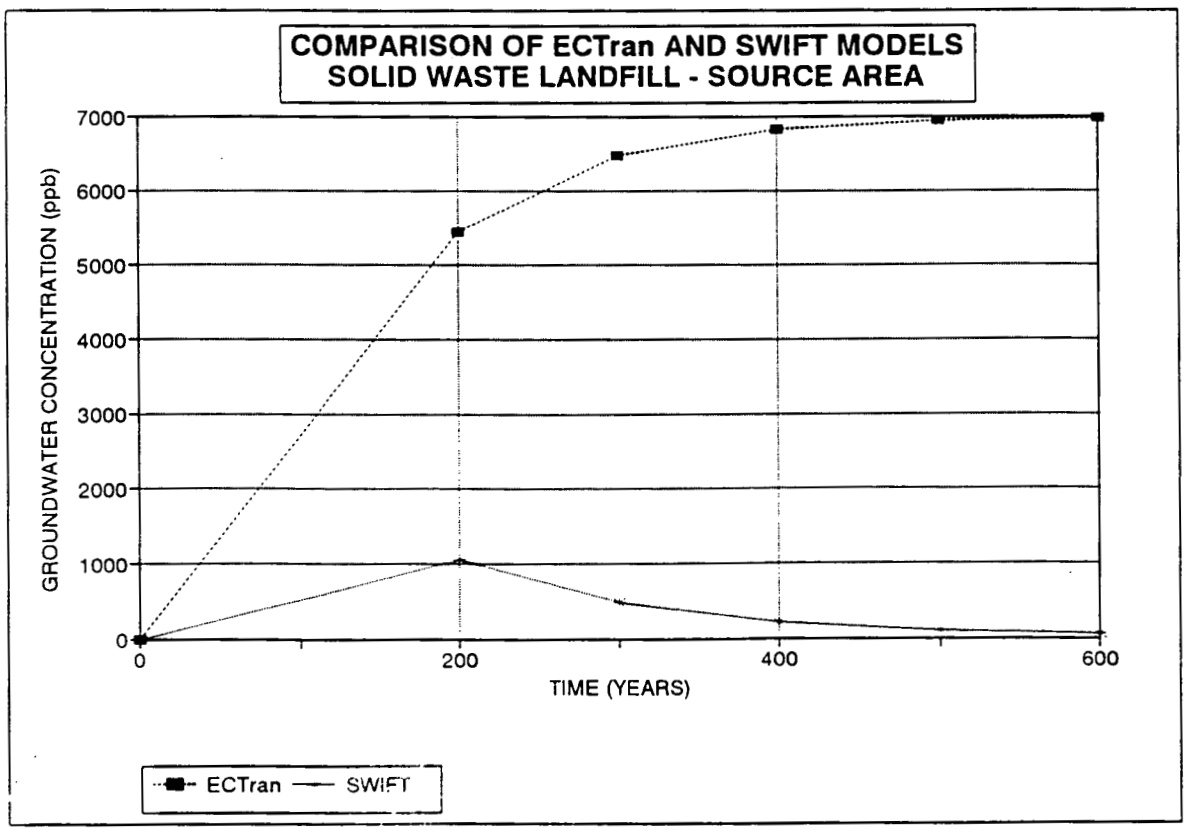


FIGURE 5-4



5.3 MODEL RUN TIME

The model run times for the ODAST/SWIFT model combination are very lengthy, approximately 30 hours using a 486/50 PC to simulate a single Uranium transport scenario for 1,000 years. The required run time for some other contaminants are even longer (e.g., 3 days for technetium). Because of this lengthy run time, a screening model (i.e., the ECTran model) was developed. The run times for the ECTran model vary depending on the particular case scenario but are independent of chemicals simulated. Generally ECTran requires between 4 seconds (for single simulations) to 30 minutes (for automatic Monte Carlo simulations and interactive simulations for model calibrations or cleanup goal developments) to run. This run time range is far less than ODAST/SWIFT model combination run time. Therefore, by using the ECTran model a greater amount of runs can be made and many more case scenarios and chemicals of concern can be investigated.

6.0 APPLICATION

This section discusses potential uses of the ECTran as a screening model during the RI/FS processes at the FEMP. As stated earlier, the primary objective of the proposed screening model is to efficiently support the current ODAST and SWIFT models in tasks where large numbers of long-term modeling runs are required. These tasks may include: transport model calibrations for specific contaminants and source areas; initial contaminants of concern (COC) screening; working cleanup goal developments; preliminary comparisons between remedial alternatives; and parameter sensitivity analyses. ECTran can also be utilized to perform stochastical modeling which ODAST and SWIFT were not designed for.

6.1 EXAMPLES OF PREVIOUS APPLICATIONS

Spreadsheet-based fate and transport models, using the same governing equations as ECTran, have been applied in other RCRA and CERCLA projects. These projects were located in U.S. EPA Regions III, VI, and X. The modeling tasks included the following types: developing soil cleanup goals; ACL demonstrations; estimating groundwater cleanup times; and identifying potential contaminant source areas. Most of the sites, for which these modeling tasks were conducted, usually had insufficient information to support more complex fate and transport models. The reasons for the insufficient site information usually are that the hydrogeological and contamination conditions are too complicated or the project is still in its early stages.

Some of the previous applications are presented in one of the attached papers (Appendix C.1, Chiou and Hubbard, 1992). Other applications such as parameter sensitivity analyses using these models were also frequently conducted. The other attached paper (Appendix C.2, Chiou et al., 1992) summarizes some of the typical sensitivity analyses conducted during cleanup goal development processes.

6.2 PROPOSED APPLICATIONS AT FEMP

Considering the capabilities and limitations of ODAST, SWIFT, and ECTran models, possible applications of ECTran are identified. These applications should be able to streamline and enhance the qualities of the fate and transport modeling tasks required in the RI/FS processes at the FEMP. The following subsections describe the proposed ECTran applications.

6.2.1 Working PRG Development

The ECTran model could be used at the FEMP to develop Working Preliminary Remediation Goals (WPRGs). The prefix "Working" is used to describe PRG since the goals which are developed by the ECTran model will be preliminary and considered as "ballpark numbers." The purpose for developing WPRGs using ECTran is to assist the FS process in evaluating remedial alternatives in a timely and cost-effective manner, before all the contaminant and hydrogeological data for detailed designs is available. The FS team may require these WPRGs since at the FEMP each Operable Unit is conducting the RI and FS in parallel in order to "fast track" their completions. This situation is a detriment to the FS team since they have to develop remediation strategies without the benefit of having the complete RI results. However, by estimating the WPRGs using ECTran, the FS team can determine what contaminants will have a major impact on remediation and identify and resolve potential difficulties for selecting the final remedial alternative earlier.

The ECTran model is well suited for developing WPRGs since there are numerous contaminants and exposure scenarios to be investigated in the early stages of the FS. WPRGs can be determined for any number of contaminants, exposure scenarios, and risk-based groundwater or soil criteria. The ECTran model can be used to calculate WPRGs more than 300 times quicker than the ODAST and SWIFT models. Applications of the model will also allow the FS team to investigate several possible remediation strategies without relying on the complex models.

A typical WPRG development procedure for a contaminant consists of: (1) calibrating the source leachate concentration against the available groundwater contaminant concentrations in 1000 and 2000 series monitoring wells; (2) using the calibration results to determine the current contaminant concentrations in Layers 1 and 2 which can be subsequently used as the initial conditions for these layers during WPRG development; (3) estimate WPRGs based on a chosen remediation strategy (e.g., source removal/reduction or capping); (4) for source removal, the Layer 2, Layer 1, and source leachate concentrations would be modified, in that order, until the modeled maximum contaminant concentration at the exposure point equals the risk-based criteria; (5) for capping alternative, the infiltration rate would be reduced until the modeled maximum contaminant concentration at the exposure point equals the risk-based criteria; and (6) A sensitivity analysis on pertinent model parameters could also be performed in order to assess the effects of these parameters on WPRGs.

6.2.2 Scoping and Cross-Verification

In addition to WPRG development, ECTran can be applied for individual contaminant source areas during the initial stages of the following tasks:

- Transport model calibrations
- ACL demonstrations
- Sensitivity analyses of model parameters
- COC screening

Due to ECTran's short run time, large numbers of simulations can be run when the uncertainties associated with model parameters are still high. Results of these preliminary runs can then be used to select specific or a smaller range of values for each model parameter to be assigned in the ODAST and SWIFT models. Therefore, the number of necessary ODAST and SWIFT model runs, which will require very long run times, can be significantly reduced.

Because of the conservative nature of the ECTran model, it can be used to screen out contaminants that are very unlikely to cause future impact on the groundwater from the pathways simulated by the model. Therefore, the number of contaminants which need to be further studied by ODAST and SWIFT can be reduced.

When both ECTran and ODAST/SWIFT modeling results for the same case scenario are available, cross-verification can also be conducted. During cross-verification the predicted levels and occurring times of the maximum groundwater concentration can be compared. Although exactly the same results are not expected from these two different models, the cross-verification process can ensure that the models have been applied properly when similar results are obtained from both models.

6.2.3 Stochastical Modeling

With the Monte Carlo simulation capability, ECTran can be used to perform stochastical/probabilistical groundwater contaminant fate and transport modeling. The uncertainty associated with the model predictions can be quantified. Also, the probability of success of a given remedial alternative can be estimated.

7.0 REFERENCES

Chiou, J. D., R. J. Hubbard, and A. E. Hubbard, 1992, "Important Factors in Cleanup Goal Development for Contaminated Soil and Groundwater - Sensitivity Analyses by Model Simulations," in Proceedings of Water Environment Federation 65th Annual Conference & Exposition, New Orleans, Louisiana, pp. 235-246.

Chiou, J. D. and R. J. Hubbard, 1992, "Development and Application of a Spreadsheet-Based Multimedia Contaminant Fate and Transport Model," in Proceedings of Solving Groundwater Problems with Models, The fifth international conference on the use of models to analyze and find working solutions to groundwater problems, Dallas, Texas, pp. 623-637.

Domenico, P. A., 1987, "An Analytical Model for Multidimensional Transport of a Decaying Contaminant Species," J. Hydrol., Vol. 91, pp. 49-58.

Fetter, C. W., 1989, Applied Hydrogeology, Second Ed., Charles E. Merill Publishing Company, Columbus, Ohio.

Freeze, R. A. and J. A. Cherry, 1979, Groundwater, Prentice-Hall, New York.

Huyakorn, P. S., M. J. Ungs, L. A. Mulkey, and E. A. Sudicky, 1987, "A Three-Dimensional Analytical Method for Predicting Leachate Migration," *Groundwater*, Volume 25, No. 5, September-October.

McClymont, G. L., and F. W. Schivartz, 1987, "Development and Application of an Expert System in Contaminant Hydrogeology - The Expert ROKEY Computer System," prepared for National Hydrology Research Institute, Environment Canada, Alberta Environmental Research Trust.

Salhotra, A. M., P Mineant, S. Sharp-Hansen, and T. Allison, 1990, "Multimedia Exposure Assessment Model (Multimed) for the Evaluating the Land Disposal of Wastes - Model Theory," EPA Contract No. 68-03-3513 and No. 68-03-6304, U.S. EPA, Athens, GA.

U.S. Department of Energy (DOE), October 1992, *Remedial Investigation for Operable Unit 2*, RI/FS, FEMP, Fernald, Ohio.

4775

U.S. Department of Energy (DOE), April 1993, *Groundwater Modeling Report--Summary of Model Development*, Prepared by IT Corporation and FERMCO, FEMP, Fernald, Ohio.

U.S. Department of Energy (DOE), April 1993, *Groundwater Modeling Evaluation Report and Improvement Plan*, Prepared by PARSONS and FERMCO, FEMP, Fernald, Ohio.

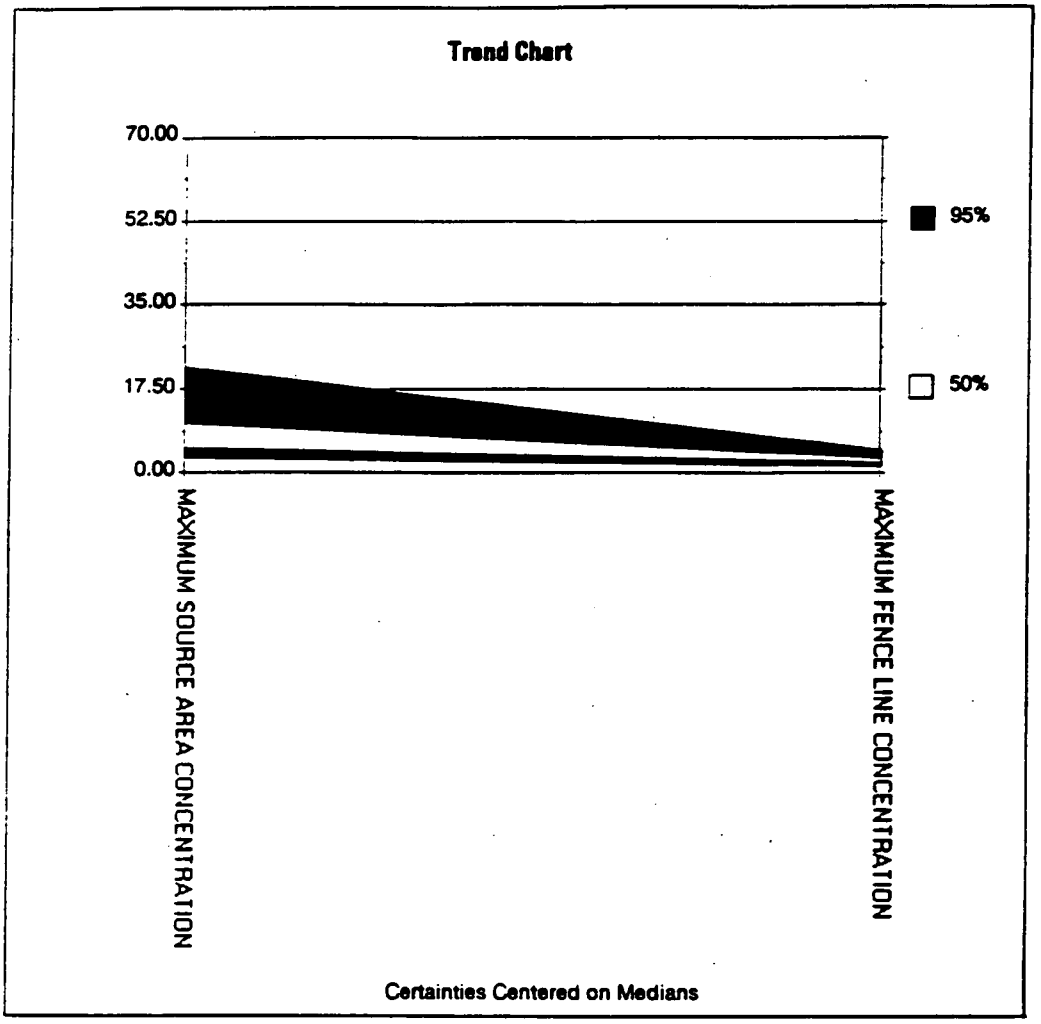
U.S. Environmental Protection Agency (EPA), 1983, "Rapid Assessment of Potential Ground-Water Contamination Under Emergency Response Conditions," Office of Health and Environmental Assessment, Washington, D.C., November 1983, EPA-600/8-83-030.

Walton, W. C., 1970, Groundwater Resource Evaluation, McGraw-Hill.

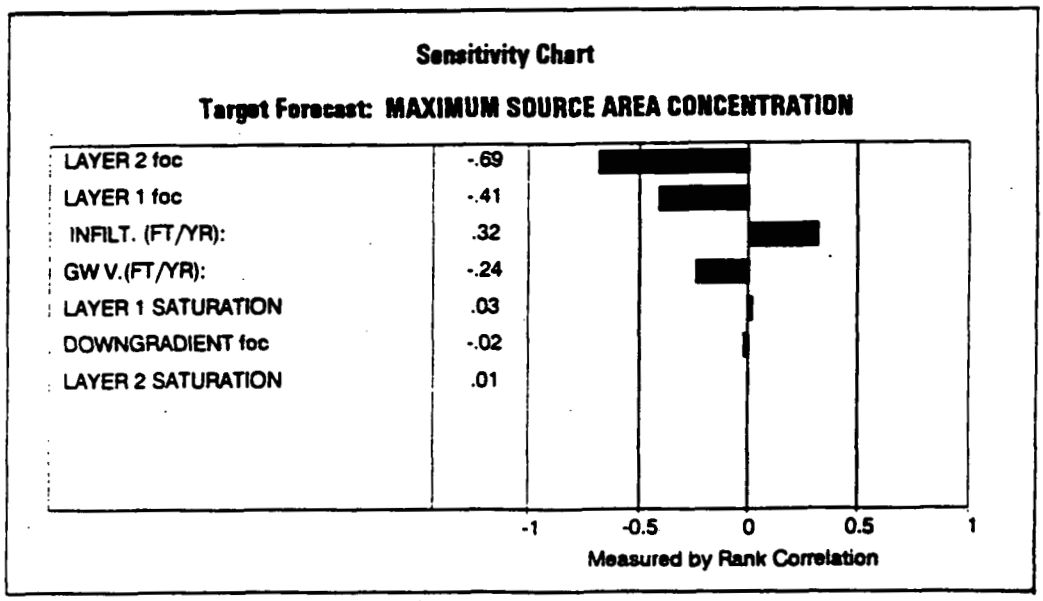
APPENDIX A.1

MONTE CARLO SIMULATION REPORT
20 YEARS PUMPING

Crystal Ball Report
Simulation started on 8/6/93 at 16:46:48
Simulation stopped on 8/6/93 at 17:21:36



This trend chart displays the certainty ranges of the concentrations at the source area and fence line. The bands of certainty narrow down from the maximum source area concentration to the maximum fence line concentration. This indicates that the maximum source area concentration is higher than that of the maximum fence line concentration and the standard deviation of the source area concentration is greater than that of the fence line concentration.



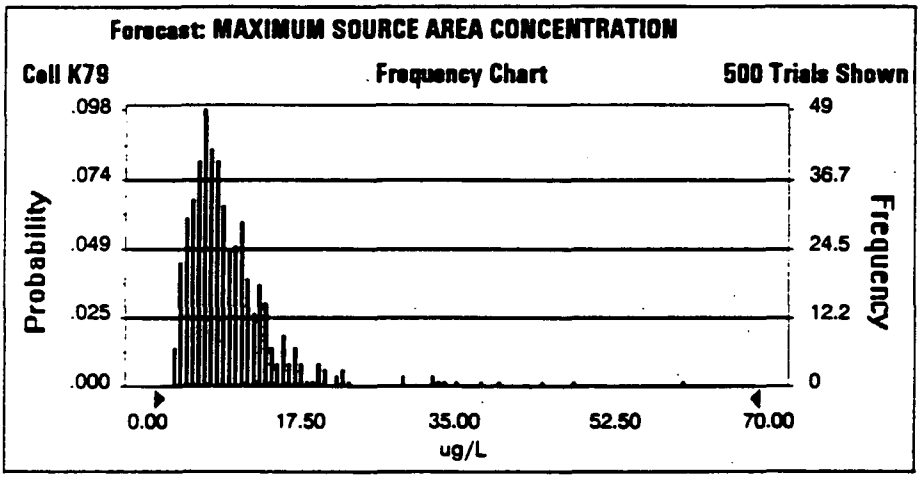
The sensitivity chart shows which variables are the most important or least important ones in the model. In this example, there are seven variables listed in the sensitivity chart. The first variable, Layer 2 foc, has the highest sensitivity ranking and can be considered the most important variable in the model. Therefore, the value of Layer 2 foc should be carefully selected in order to compute the correct maximum source area concentration. Since the rank correlation between Layer 2 foc and maximum source area concentration is negative, it indicates that the increase of the value of foc will make the maximum source area concentration smaller. The last variable, Layer 2 saturation, has the lowest sensitivity ranking and is the least important variable in the model. The effect of this variable on the maximum source area concentration is not as great as the other variables.

Forecast: MAXIMUM SOURCE AREA CONCENTRATION **Cell: K79**

Summary:

Display Range is from 0.00 to 70.00 ug/L
Entire Range is from 2.24 to 61.39 ug/L
After 500 Trials, the Std. Error of the Mean is 0.28

Statistics:	Value
Trials	500
Mean	9.00
Median (approx.)	7.43
Mode (approx.)	6.09
Standard Deviation	6.20
Variance	38.46
Skewness	3.51
Kurtosis	21.81
Coeff. of Variability	0.69
Range Minimum	2.24
Range Maximum	61.39
Range Width	59.15
Mean Std. Error	0.28



This figure shows the frequency distribution of the maximum source area concentration. In 500 trials, the minimum value of the maximum source area concentration is 2.24 ug/l and the maximum value of it is 61.39 ug/l. The most frequently simulated value of the maximum source area concentration is about 6.09 ug/l, which appears 49 times in 500 trials.

Forecast: MAXIMUM SOURCE AREA CONCENTRATION (cont'd) **Cell: K79**

Percentiles:

Percentile	ug/L (approx.)
0%	2.24
10%	4.05
25%	5.46
50%	7.43
75%	10.58
90%	14.76
100%	61.39

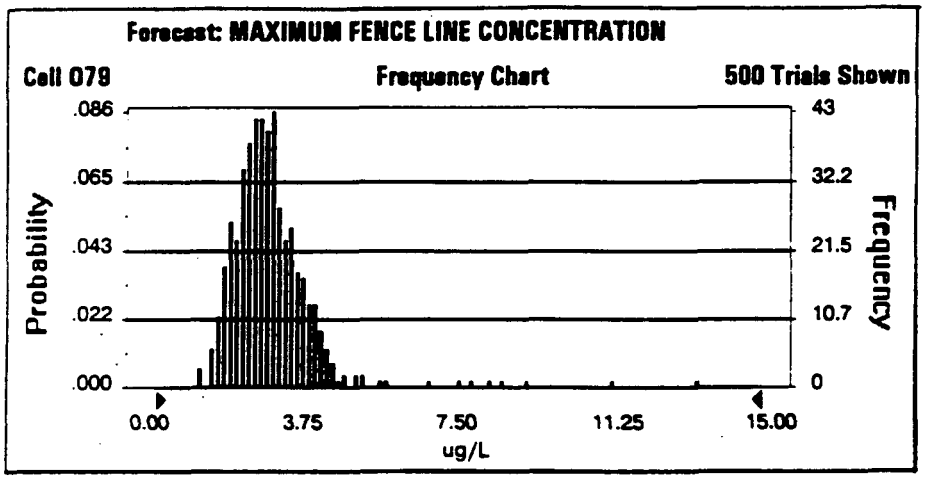
End of Forecast

Forecast: MAXIMUM FENCE LINE CONCENTRATION **Cell: O79**

Summary:

Display Range is from 0.00 to 15.00 ug/L
Entire Range is from 1.16 to 13.48 ug/L
After 500 Trials, the Std. Error of the Mean is 0.05

Statistics:	Value
Trials	500
Mean	2.89
Median (approx.)	2.72
Mode (approx.)	2.94
Standard Deviation	1.13
Variance	1.27
Skewness	3.82
Kurtosis	28.78
Coeff. of Variability	0.39
Range Minimum	1.16
Range Maximum	13.48
Range Width	12.33
Mean Std. Error	0.05



This figure shows the frequency distribution of the maximum fence line concentration. In 500 trials, the minimum value of the maximum fence line concentration is 1.16 ug/l and the maximum value of it is 13.48 ug/l. The most frequently simulated value of the maximum fence line concentration is about 2.94 ug/l, which appears 43 times in 500 trials.

Forecast: MAXIMUM FENCE LINE CONCENTRATION (cont'd) **Cell: O79**

Percentiles:

Percentile	ug/L (approx.)
0%	1.16
10%	1.88
25%	2.26
50%	2.72
75%	3.28
90%	3.87
100%	13.48

End of Forecast

4775

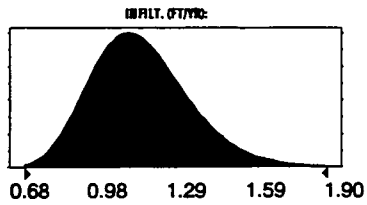
Assumptions

Assumption: INFILT. (FT/YR): **Cell: C20**

Lognormal distribution with parameters:

Mean	1.15
Standard Dev.	0.20

Selected range is from 0.00 to +Infinity
Mean value in simulation was 1.16

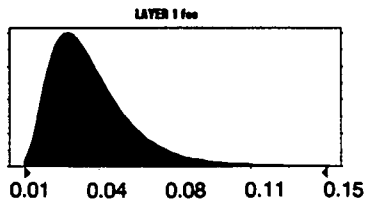


Assumption: LAYER 1 foc **Cell: F15**

Lognormal distribution with parameters:

Mean	0.04
Standard Dev.	0.02

Selected range is from 0.00 to +Infinity
Mean value in simulation was 0.04

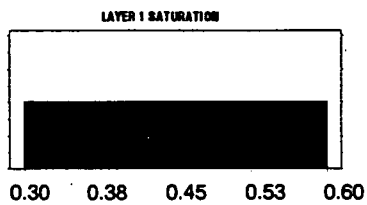


Assumption: LAYER 1 SATURATION **Cell: F17**

Uniform distribution with parameters:

Minimum	0.30
Maximum	0.60

Mean value in simulation was 0.45

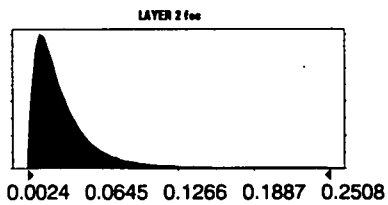


Assumption: LAYER 2 foc **Cell: I15**

Lognormal distribution with parameters:

Mean	0.0329
Standard Dev.	0.0300

Selected range is from 0.0000 to +Infinity
Mean value in simulation was 0.0311

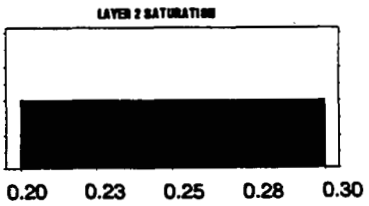


Assumption: LAYER 2 SATURATION **Cell: I17**

Uniform distribution with parameters:

Minimum	0.20
Maximum	0.30

Mean value in simulation was 0.25

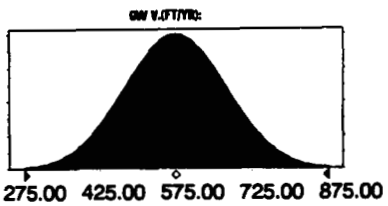


Assumption: GW V.(FT/YR): **Cell: L16**

Normal distribution with parameters:

Mean	575.00
Standard Dev.	100.00

Selected range is from -Infinity to +Infinity
Mean value in simulation was 573.75

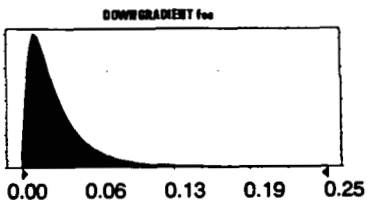


Assumption: DOWNGRADIENT foc **Cell: P15**

Lognormal distribution with parameters:

Mean	0.03
Standard Dev.	0.03

Selected range is from 0.00 to +Infinity
Mean value in simulation was 0.03



End of Assumptions

APPENDIX A.2

MONTE CARLO SIMULATION REPORT
30 YEARS PUMPING

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BROWN & ROOT ENVIRONMENTAL

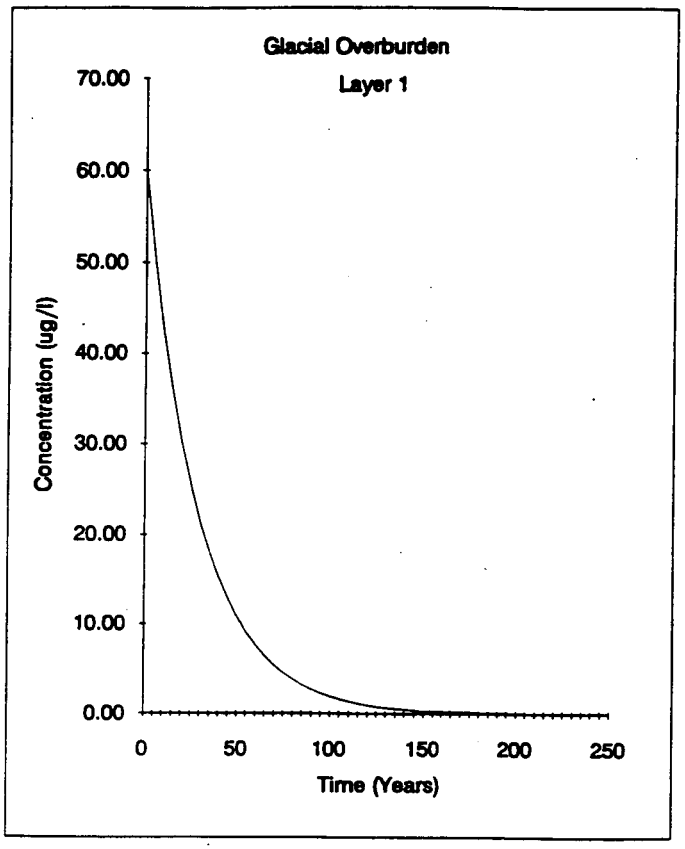
SCREENING-LEVEL EXCEL-CRYSTAL BALL TRANSPORT (ECTran) MODEL

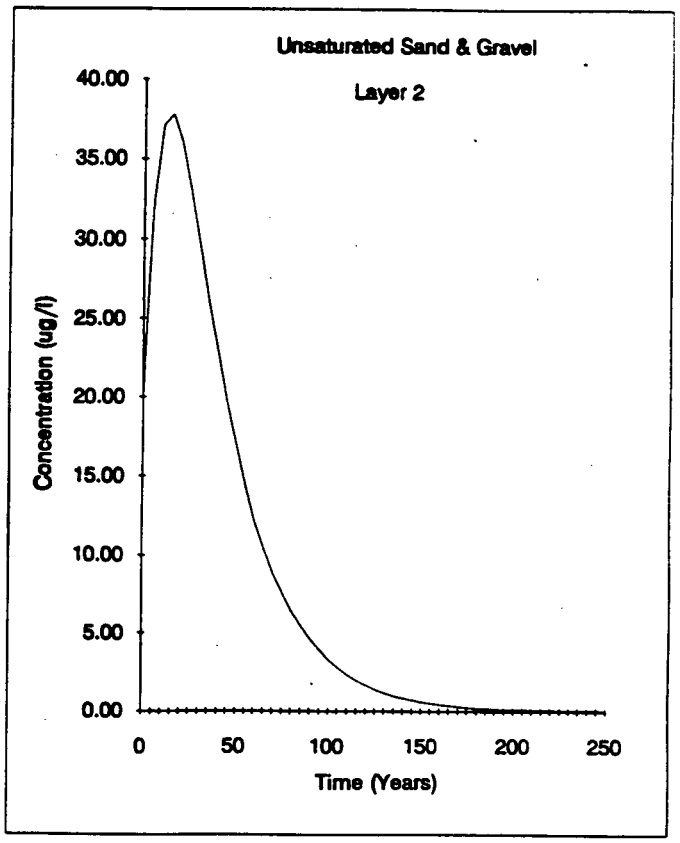
SITE:	HYPOTHETICAL, FEMP, FERNALD, OH
	AGE = 10 YRS; SOURCE REMOVED
	RESIDUAL CONTAMINATION IN LAYER 1 & 2
	PUMPING = 30 YRS
INVESTIGATOR:	CAR
DATE:	8/7/93

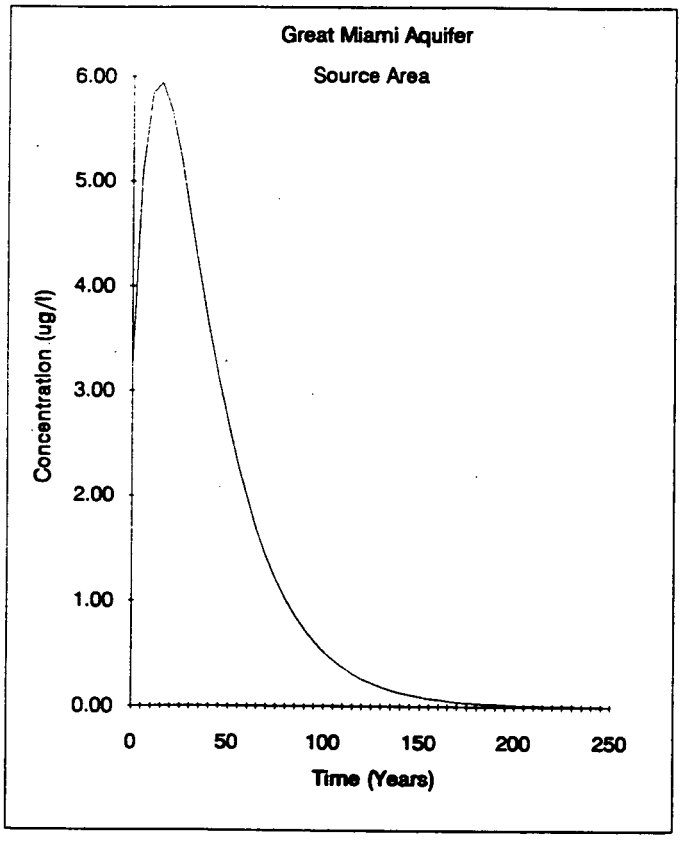
CONTAMINANT:		CHEMICAL X	
KOC (L/KG):	45.00	WATER CRITERIA (UG/L):	3.00E+00
HALF LIFE (YRS):		CONSTANT SOURCE LEACHATE (UG/L):	0.00E+00
LAYER 1:	4.47E+09	INITIAL LAYER 1 SOIL CONC. (MG/KG):	1.08E-01
LAYER 2:	4.47E+09	INITIAL LAYER 2 SOIL CONC. (MG/KG):	3.03E-02
GMA:	4.47E+09		

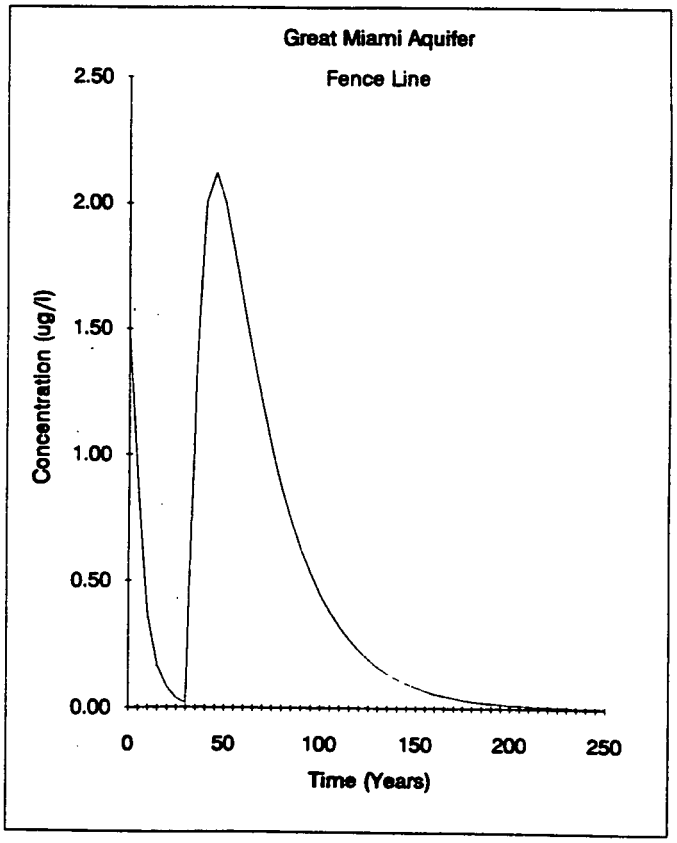
UNSAT. SOURCE AREA:		LAYER 1 (GLACIAL OVERBURDEN)		LAYER 2 (SAND & GRAVEL)		GREAT MIAMI AQUIFER (SAT. S. & G.)			
						B (FT):	67	Vzo (FT/YR):	11.5445
LENGTH (FT):	250	FOC (KG/KG):	0.04	FOC (KG/KG):	0.0329	GW Q3 (L/DAY)	3.26E+04	FOC (KG/KG):	0.0329
WIDTH (FT):	230	Kd (L/KG):	1.8	Kd (L/KG):	1.481	GW V.(FT/YR):	575.00	Kd (L/KG):	1.4805
		SATURATION:	0.45	SATURATION:	0.25	H (FT):	12.7100	RETARDATION:	11.5412
POROSITY:	0.34	THICKNESS (FT):	10.00	THICKNESS (FT):	5.00	EFF. POROSITY	0.25	q (FT/YR) :	0
DENSITY (G/CM3):	1.78	DECAY (1/DAY):	4.25E-13	DECAY (1/DAY):	4.25E-13	DISPERSIVITY:		DECAY (1/YR):	1.6E-10
INFILT. (FT/YR):	1.15	CAo (UG/L):	6.01E+01	CBo (PPB):	2.05E+01	Az(FT):	0.12	CU3 (PPB):	0
		CU1 (PPB):	0	CU2 (PPB):	0.00E+00	Ax (FT):	100.00	P&T(YEARS):	30
AGE (YEARS):	10	Q1 (L/DAY):	5.13E+03	Q2 (L/DAY):	0.00E+00	Ay (FT):	33.33	DISTANCE TO F.L.(FT):	275

TIME INTERVAL (YRS) 5		LAYER 1 LEACHATE CONC.	LAYER 2 LEACHATE CONC.	SOURCE AREA CONC.	FENCE LINE CONC.
ELAPSED TIME - YRS	DAYS	(UG/L)	(UG/L)	(UG/L)	(UG/L)
0	0	60.06	20.49	3.22	1.48
5	1825	50.60	32.34	5.09	0.85
10	3650	42.63	37.13	5.84	0.36
15	5475	35.91	37.75	5.94	0.17
20	7300	30.26	36.05	5.67	0.08
25	9125	25.49	33.15	5.22	0.04
30	10950	21.48	29.75	4.68	0.02
35	12775	18.09	26.25	4.13	1.29
40	14600	15.25	22.90	3.60	2.00
45	16425	12.84	19.80	3.12	2.12
50	18250	10.82	17.02	2.68	2.01
55	20075	9.12	14.56	2.29	1.81
60	21900	7.68	12.41	1.95	1.60
65	23725	6.47	10.55	1.66	1.39
70	25550	5.45	8.95	1.41	1.19
75	27375	4.59	7.58	1.19	1.02
80	29200	3.87	6.41	1.01	0.87
85	31025	3.26	5.42	0.85	0.74
90	32850	2.75	4.58	0.72	0.63
95	34675	2.31	3.86	0.61	0.53
100	36500	1.95	3.26	0.51	0.45
105	38325	1.64	2.75	0.43	0.38
110	40150	1.38	2.32	0.36	0.32
115	41975	1.17	1.96	0.31	0.27
120	43800	0.98	1.65	0.26	0.23
125	45625	0.83	1.39	0.22	0.19
130	47450	0.70	1.17	0.18	0.16
135	49275	0.59	0.99	0.16	0.14
140	51100	0.49	0.83	0.13	0.11
145	52925	0.42	0.70	0.11	0.10
150	54750	0.35	0.59	0.09	0.08
155	56575	0.30	0.50	0.08	0.07
160	58400	0.25	0.42	0.07	0.06
165	60225	0.21	0.35	0.06	0.05
170	62050	0.18	0.30	0.05	0.04
175	63875	0.15	0.25	0.04	0.03
180	65700	0.13	0.21	0.03	0.03
185	67525	0.11	0.18	0.03	0.02
190	69350	0.09	0.15	0.02	0.02
195	71175	0.08	0.13	0.02	0.02
200	73000	0.06	0.11	0.02	0.01
205	74825	0.05	0.09	0.01	0.01
210	76650	0.04	0.08	0.01	0.01
215	78475	0.04	0.06	0.01	0.01
220	80300	0.03	0.05	0.01	0.01
225	82125	0.03	0.05	0.01	0.01
230	83950	0.02	0.04	0.01	0.01
235	85775	0.02	0.03	0.01	0.00
240	87600	0.02	0.03	0.00	0.00
245	89425	0.01	0.02	0.00	0.00
250	91250	0.01	0.02	0.00	0.00
MAXIMUM:		60.06	37.75	5.94	2.12

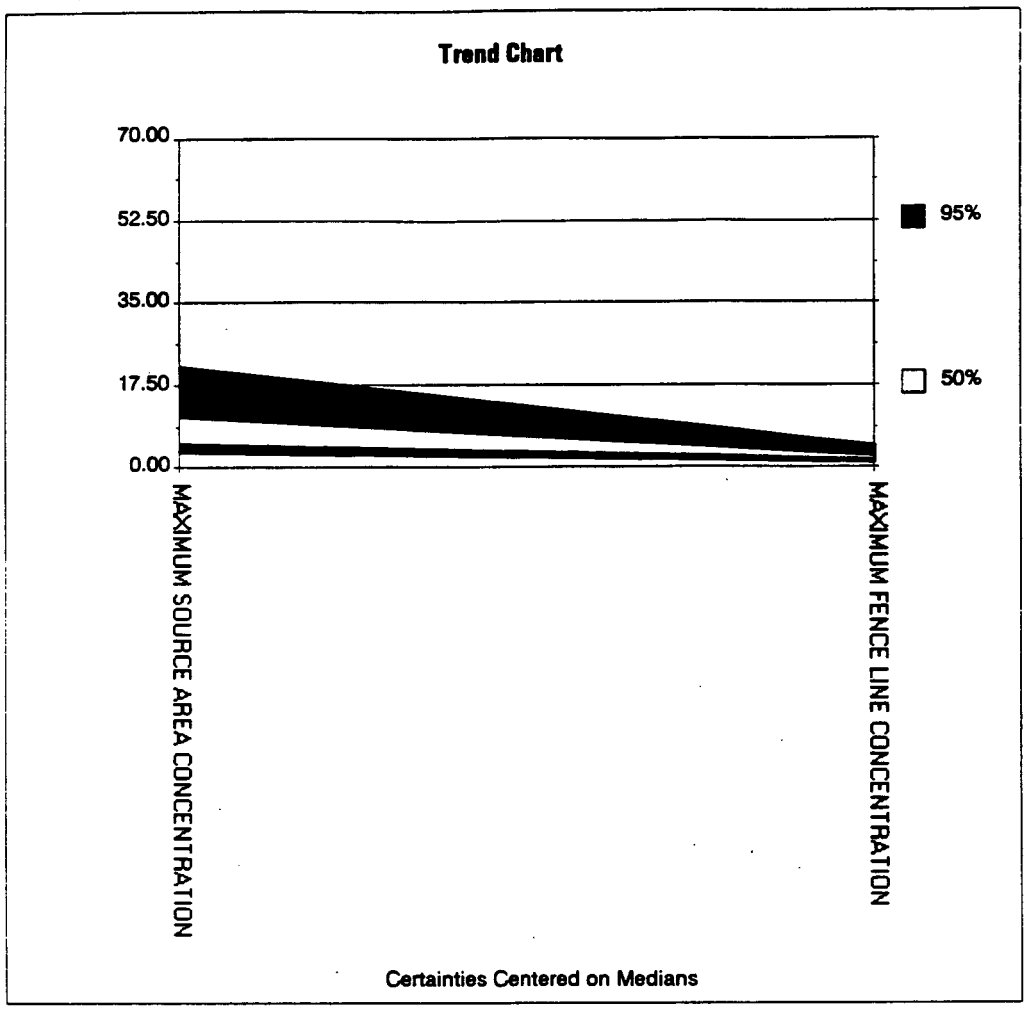

Glacial Overburden
Layer 1
Concentration (ug/l)
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
0
50
100
150
200
250
Time (Years)

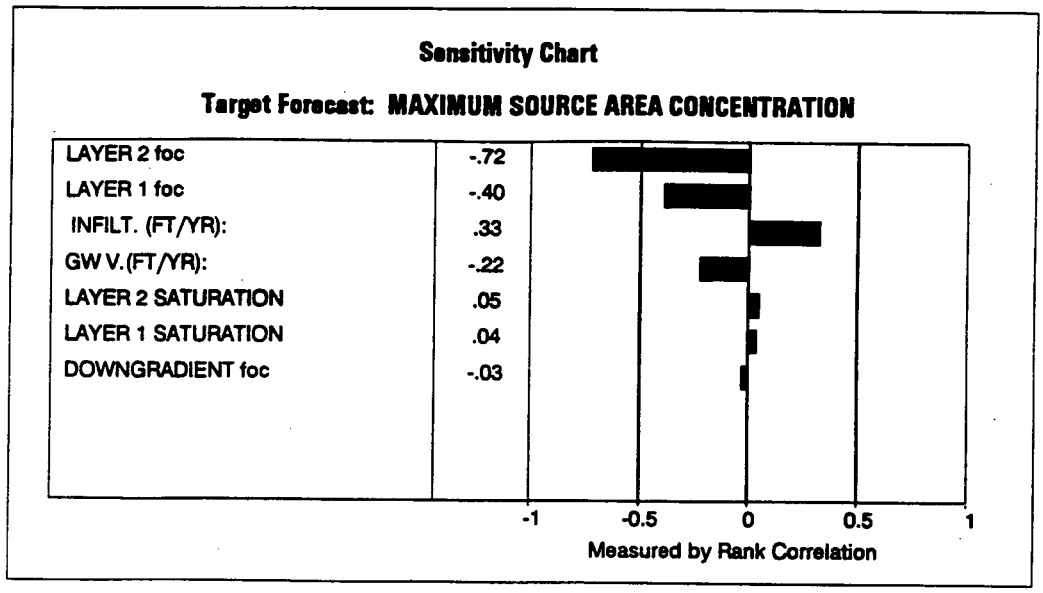

Unsaturated Sand & Gravel
Layer 2
Concentration (ug/l)
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
0
50
100
150
200
250
Time (Years)


Great Miami Aquifer
Source Area
Concentration (ug/l)
6.00
5.00
4.00
3.00
2.00
1.00
0.00
0
50
100
150
200
250
Time (Years)


Great Miami Aquifer
Fence Line
Concentration (ug/l)
2.50
2.00
1.50
1.00
0.50
0.00
0
50
100
150
200
250
Time (Years)

Crystal Ball Report
Simulation started on 8/7/93 at 8:10:26
Simulation stopped on 8/7/93 at 8:30:00



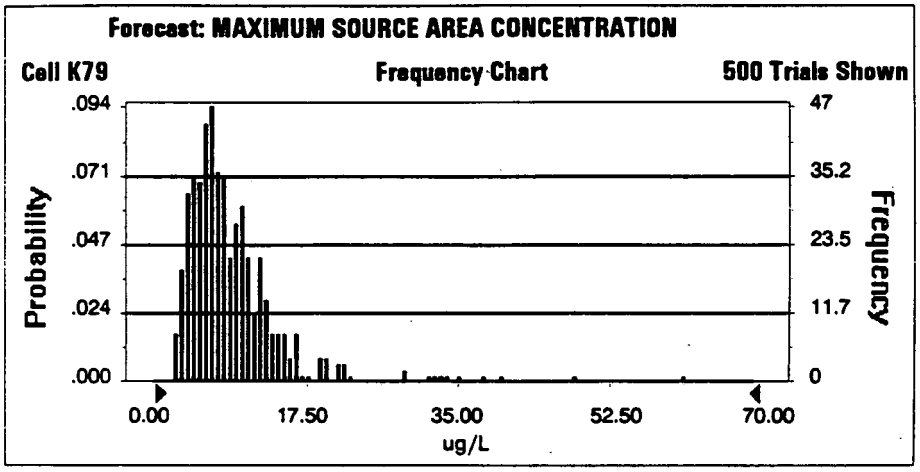

Sensitivity Chart
Target Forecast: MAXIMUM SOURCE AREA CONCENTRATION
LAYER 2 foc
-.72
LAYER 1 foc
-.40
INFILT. (FT/YR):
.33
GW V.(FT/YR):
-.22
LAYER 2 SATURATION
.05
LAYER 1 SATURATION
.04
DOWNGRADIENT foc
-.03
-1
-0.5
0
0.5
1
Measured by Rank Correlation

Forecast: MAXIMUM SOURCE AREA CONCENTRATION **Cell: K79**

Summary:

Display Range is from 0.00 to 70.00 ug/L
Entire Range is from 2.17 to 61.39 ug/L
After 500 Trials, the Std. Error of the Mean is 0.27

Statistics:	Value
Trials	500
Mean	9.02
Median (approx.)	7.58
Mode (approx.)	6.02
Standard Deviation	5.99
Variance	35.83
Skewness	3.45
Kurtosis	22.31
Coeff. of Variability	0.66
Range Minimum	2.17
Range Maximum	61.39
Range Width	59.22
Mean Std. Error	0.27



Forecast: MAXIMUM SOURCE AREA CONCENTRATION (cont'd) **Cell: K79**

Percentiles:

Percentile	ug/L (approx.)
0%	2.17
10%	4.09
25%	5.49
50%	7.58
75%	10.69
90%	14.34
100%	61.39

End of Forecast

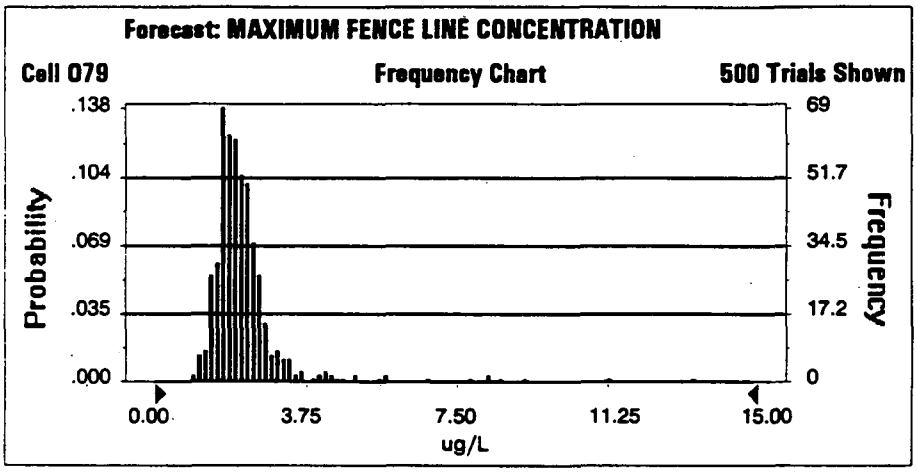
4775

Forecast: MAXIMUM FENCE LINE CONCENTRATION **Cell: O79**

Summary:

Display Range is from 0.00 to 15.00 ug/L
Entire Range is from 1.02 to 13.48 ug/L
After 500 Trials, the Std. Error of the Mean is 0.05

Statistics:	Value
Trials	500
Mean	2.28
Median (approx.)	2.06
Mode (approx.)	1.70
Standard Deviation	1.14
Variance	1.29
Skewness	5.01
Kurtosis	37.68
Coeff. of Variability	0.50
Range Minimum	1.02
Range Maximum	13.48
Range Width	12.47
Mean Std. Error	0.05



71

Forecast: MAXIMUM FENCE LINE CONCENTRATION (cont'd) **Cell: O79**

Percentiles:

Percentile	ug/L (approx.)
0%	1.02
10%	1.56
25%	1.75
50%	2.06
75%	2.42
90%	2.93
100%	13.48

End of Forecast

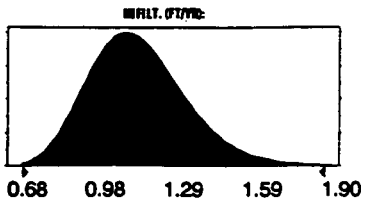
Assumptions

Assumption: INFILT. (FT/YR): **Cell: C20**

Lognormal distribution with parameters:

Mean	1.15
Standard Dev.	0.20

Selected range is from 0.00 to +Infinity
Mean value in simulation was 1.16

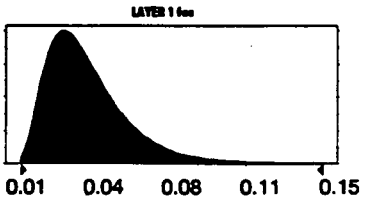


Assumption: LAYER 1 foc **Cell: F15**

Lognormal distribution with parameters:

Mean	0.04
Standard Dev.	0.02

Selected range is from 0.00 to +Infinity
Mean value in simulation was 0.04

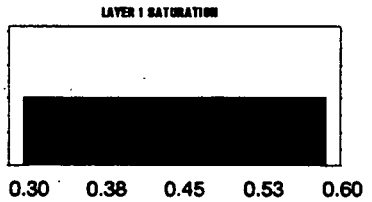


Assumption: LAYER 1 SATURATION **Cell: F17**

Uniform distribution with parameters:

Minimum	0.30
Maximum	0.60

Mean value in simulation was 0.45

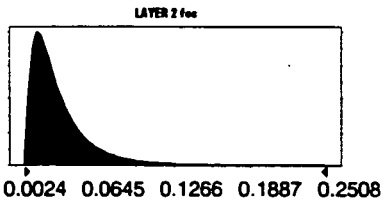


Assumption: LAYER 2 foc **Cell: I15**

Lognormal distribution with parameters:

Mean	0.0329
Standard Dev.	0.0300

Selected range is from 0.0000 to +Infinity
Mean value in simulation was 0.0312



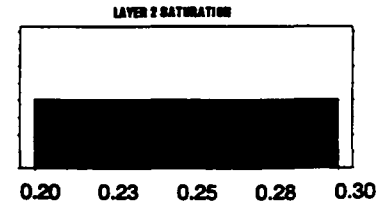
73

Assumption: LAYER 2 SATURATION **Cell: I17**

Uniform distribution with parameters:

Minimum	0.20
Maximum	0.30

Mean value in simulation was 0.25

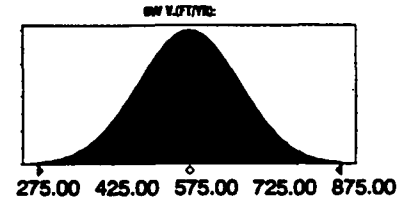


Assumption: GW V.(FT/YR): **Cell: L16**

Normal distribution with parameters:

Mean	575.00
Standard Dev.	100.00

Selected range is from -Infinity to +Infinity
Mean value in simulation was 570.89

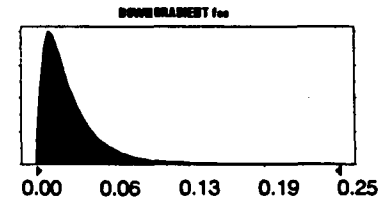


Assumption: DOWNGRADIENT foc **Cell: P15**

Lognormal distribution with parameters:

Mean	0.03
Standard Dev.	0.03

Selected range is from 0.00 to +Infinity
Mean value in simulation was 0.03



End of Assumptions

APPENDIX B

FORTRAN IMPLEMENTATION OF DOWNGRADIENT TRANSPORT

```
      IMPLICIT REAL*8 (A-H, L, O-Z)
      DIMENSION CO(55),TCO(55)
C-----------------------------------------------
      OPEN(UNIT=10,FILE='SOURCE.DAT',STATUS='OLD')
      OPEN(UNIT=11,FILE='EXPO.DAT',STATUS='NEW')
C-----------------------------------------------
      READ(10,*) V,RF,DIST,Y,HL,AX,AGE,PTY
      READ(10,*) (TCO(J),CO(J),J=1,51)
C-----------------------------------------------
      DT1 = TCO(2)-TCO(1)
      DT = DT1
      CAGE = CO(1)
      DO 400 I=1,51
        IF((TCO(I)+DT).LE.PTY) THEN
          CO(I) = 0.0
        ELSE IF(TCO(I).LT.PTY) THEN
          DT1 = DT - (PTY - TCO(I))
        ENDIF
400   CONTINUE
C-----------------------------------------------
      AY=AX/3.
      V=V/RF
      DX=AX*V
      DY=AY*V
      IF(HL.GT.0.D0) THEN
        LAMDA=DLOG(2.D0)/HL
      ELSE
        LAMDA=0.D0
      ENDIF
      TIME=0.0D0
      X3=DERF(Y/(4.0D0*DSQRT(DY/V*DIST)))*
     1  EXP((DIST/(2.0D0*DX/V))*
     2  (1.0D0-DSQRT(1.0D0+(4.0D0*LAMDA*DX)/(V**2.D0))))
      print *, 'Please wait!  Calculating exposure point concentration.'
300   C500=0.0D0
      IF(TIME.LE.PTY) GO TO 200
      DO 100 I=1,51
        IF(CO(I).EQ.0.0) GO TO 100
        IF(TCO(I).LT.(TIME-DT)) THEN
          IF(TCO(I).GE.PTY) THEN
            T1 = TIME - TCO(I)
            T2 = TIME - TCO(I) - DT
          ELSE IF((TCO(I)+DT).GT.PTY) THEN
            T1 = TIME - PTY
            T2 = TIME - PTY - DT1
          ENDIF
          X1=DERF((DIST-V*T1*DSQRT(1.D0+(4.D0*LAMDA*DX)/(V**2.D0)))
     1      /(2.D0*DSQRT(DX*T1)) )
          X2=DERF((DIST-V*T2*DSQRT(1.D0+(4.D0*LAMDA*DX)/(V**2.D0)))
     1      /(2.D0*DSQRT(DX*T2)) )
          CX = CO(I)*X3/2.D0*(X2-X1)
          C500 = C500 + CX
        ELSE IF(TCO(I).GE.(TIME-DT).AND.TCO(I).LT.TIME) THEN
          IF(TCO(I).GE.PTY) THEN
```

```
        T1 = TIME - TCO(I)
        ELSE IF((TCO(I)+DT).GT.PTY) THEN
          T1 = TIME - PTY
        ENDIF
        X1=DERF((DIST-V*T1*DSQRT(1.D0+(4.D0*LAMDA*DX)/(V**2.D0)))
     1    /(2.D0*DSQRT(DX*T1)) )
        CX = CO(I)*X3/2*(1-X1)
        C500 = C500 + CX
      ELSE
        GO TO 200
      ENDIF
100   CONTINUE
200   T1 = TIME + AGE
      T2 = TIME
      X1=DERF((DIST-V*T1*DSQRT(1.D0+(4.D0*LAMDA*DX)/(V**2.D0)))
     1  /(2.D0*DSQRT(DX*T1)) )
      X2=DERF((DIST-V*T2*DSQRT(1.D0+(4.D0*LAMDA*DX)/(V**2.D0)))
     1  /(2.D0*DSQRT(DX*T2)) )
      CX = CAGE*X3/2.D0*(X2-X1)
      C500 = C500 + CX
      WRITE(11,2000) TIME,C500
      TIME = TIME + DT
      IF(TIME.LE.DT*50.) GO TO 300
      STOP
900   FORMAT(4X,7D9.3)
1000  FORMAT(4X,D9.3,D9.3)
2000  FORMAT(F11.3,2X,E12.4)
      END
C
      FUNCTION DERF(X)
C
      IMPLICIT REAL*8 (A-H, O-Z)
      DIMENSION A(5)
      DATA A/0.254829592D0,-0.284496736D0,1.421413741D0,-1.453152027D0,
     *1.061405429D0/,P/0.3275911D0/
      SP1=0.0D0
      IF(DABS(X).GT.5.0D0) GO TO 6
      IF(X) 2,4,2
 4    SP1=1.0D0
      GO TO 6
 2    SP=DABS(X)
      T=1.0D0/(1.0D0+P*SP)
      SP1=0.0D0
      DO 1 I=1,5
 1    SP1=SP1+A(I)*T**I
      SP1=SP1*DEXP(-SP**2.)
 6    DERF = 1.0D0-SP1
      IF(X.LT.0.0D0) DERF = -DERF
      RETURN
      END
```

APPENDIX C.1

PREVIOUS APPLICATIONS

DEVELOPMENT AND APPLICATION OF A SPREADSHEET-BASED MULTIMEDIA CONTAMINANT FATE AND TRANSPORT MODEL

Jyh-Dong Chiou and Robert J. Hubbard

HALLIBURTON NUS Environmental Corporation
Pittsburgh, Pennsylvania

INTRODUCTION

A spreadsheet-based, multimedia, contaminant fate and transport model was developed to support screening-level risk assessment, cleanup goal development, and Alternate Concentration Limit determination for hazardous waste treatment, storage, and disposal facilities. This paper discusses various components of the model used to simulate contaminant washout from a source area, downgradient solute transport, and estimation of receptor concentrations under various types of exposure scenarios. A spreadsheet was used to implement and link various simulation modules and to simplify the model input, interactive execution, and output presentation processes. The model guides the user regarding the influence of various parameters on the contaminant concentration at the point of exposure and, therefore, focuses remedial measures or data collection efforts.

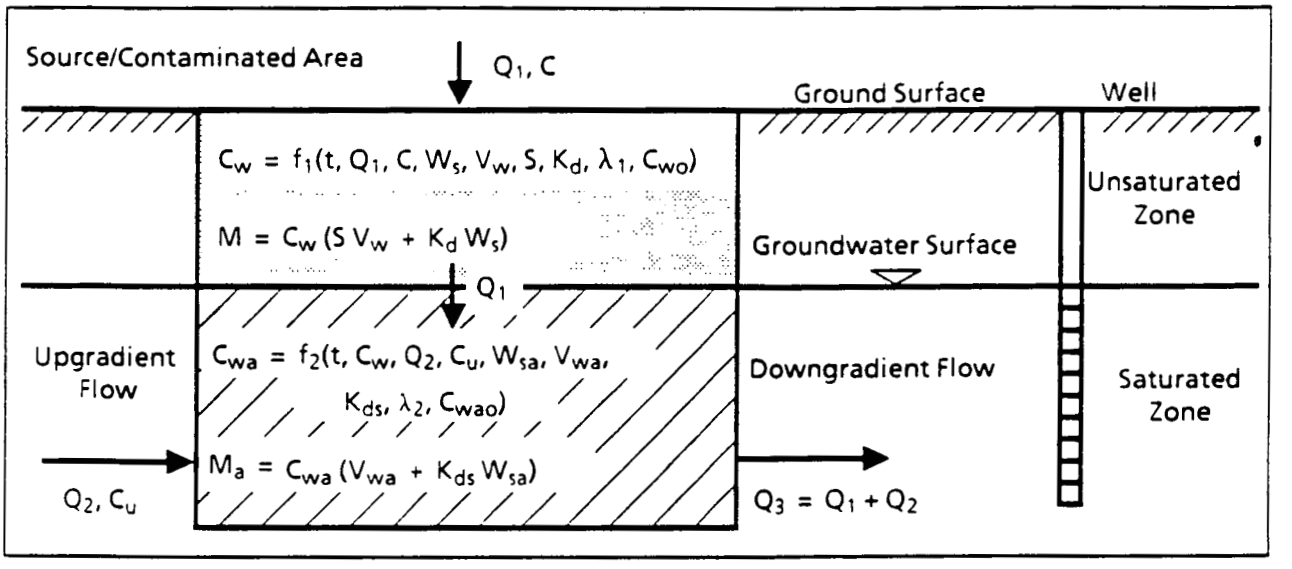
MODEL DEVELOPMENT

Contaminant Source Module

A system of analytical models which describe various aspects of source loading and contaminant washout from both the unsaturated and saturated zones was configured via straightforward mass balances. Although several simplifying assumptions were made, the model can simulate very complex source-loading scenarios, as shown in Figure 1. For example, any combination of the following aspects of source loading and contaminant washout may be simulated:

- Surface infiltration and percolation
- Contaminant loading via infiltration
- Sorption in the unsaturated zone
- Upgradient groundwater flow
- Contaminant loading via upgradient flow
- Sorption in the saturated zone
- Zone-specific contaminant decay rates
- Zone-specific initial contaminant concentrations
- Constant or time varying concentration in the unsaturated zone

FIGURE 1: CONCEPTUAL MODEL OF THE SOURCE AREA



Variables used to describe/quantify these processes are shown in Figure 1 and are defined as follows:

- C is the contaminant concentration in infiltrating precipitation (mg/L)
- Q_1 is the infiltration rate (L/day)
- C_w is the aqueous concentration in the unsaturated zone (mg/L)
- C_{wo} is the initial value of C_w (mg/L)
- S is the saturation fraction (dimensionless)
- M is the total mass of contaminant in the unsaturated zone (mg)
- W_s is the weight of soil in the unsaturated zone (kg)
- V_w is the void volume in the unsaturated zone (L)
- C_u is the contaminant concentration in upgradient groundwater (mg/L)
- Q_2 is the upgradient groundwater flow rate (L/day)
- C_{wa} is the aqueous concentration in the saturated zone (mg/L)
- C_{wao} is the initial value of C_{wa} (mg/L)
- M_a is the total mass of contaminant in the saturated zone below the source (mg)
- V_{wa} is the void volume in the saturated zone (L)
- W_{sa} is the weight of soil in the saturated zone (kg)
- Q_3 is the combined downgradient flow $[Q_1 + Q_2]$ (L/day)
- λ_1, λ_2 are the first-order decay rates in the unsaturated and saturated zone (day^{-1})
- K_d, K_{ds} are the aqueous/solid phase distribution coefficients in the unsaturated and saturated zone, respectively (L/kg)
- t is time (days)

Unsaturated Zone

A mass balance for the wash out of contaminants from an unsaturated source area, assuming that the infiltrating precipitation contains background contamination and that dispersion in the unsaturated zone is negligible, yields the following expression for the time-dependent concentration in the unsaturated zone:

$$\frac{dC_w}{dt} = \left[\frac{Q_1}{SV_w - K_d W_s}\right] * \left[C - C_w\right] - \lambda_1 C_w \qquad (1)$$

For an initial condition of $C_w = C_{wo}$, this equation may be solved via direct integration to yield the following solution:

$$C_w = \frac{C - \left\{C - \left[1 + \left(SV_w + K_d W_s\right)\left(\lambda_1/Q_1\right)\right] C_{wo}\right\} \exp\left[-\frac{Q_1 + \left(SV_w + K_d W_s\right)\lambda_1}{SV_w + K_d W_s} t\right]}{\left[1 + \left(SV_w + K_d W_s\right)\left(\lambda_1/Q_1\right)\right]} \qquad (2)$$

Saturated Zone

Using a similar approach, a general case for the saturated zone which includes a time-dependent source loading term (C_w as described above) and an upgradient contribution as a result of background contamination may be written in the following form:

$$\frac{dC_{wa}}{dt} + \frac{K_2}{K_1} C_{wa} = \frac{K_3}{K_1} + \frac{K_4}{K_1} \exp\left[-K_5 t\right] \qquad (3)$$

Where:

$K_1 = V_{wa} + K_{ds} W_{sa}$
$K_2 = Q_3 + (V_{wa} + K_{ds} W_{sa}) \lambda_2$
$K_3 = Q_1 C / [1 + (SV_w + K_d W_s)(\lambda_1/Q_1)] + Q_2 C_u$
$K_4 = Q_1 C_{wo} - Q_1 C / [1 + (SV_w + K_d W_s)(\lambda_1/Q_1)]$
$K_5 = [Q_1 + (SV_w + K_d W_s)\lambda_1]/(SV_w + K_d W_s)$

This equation is of the general form:

$$C'_{wa} + p(t) C_{wa} = r(t)$$

and has a general solution as follows:

$$C_{wa} = \exp[-h] \cdot [\int \exp(h) r(t)\, dt + K]$$

Where: $h = \int p(t) dt$ and K is a constant of integration

This equation may be solved for the initial condition of $C_{wa} = C_{wao}$ using the preceding integrating factor approach or the method of undetermined coefficients to yield the following:

$$C_{wa} = \frac{K_3}{K_2} + \frac{K_4}{K_2 - K_1 K_5} \exp\left(-K_5 t\right) + \left[C_{wao} - \frac{K_3}{K_2} - \frac{K_4}{K_2 - K_1 K_5}\right] \exp\left(-\frac{K_2 t}{K_1}\right) \qquad (4)$$

Special Cases

In addition to this standard form of the solution, the following two special cases were also considered:

- For a constant-concentration unsaturated zone (i.e., $C_w = C$), the saturated zone equation becomes:

$$C_{wa} = \frac{Q_1C + Q_2C_u - \left\{Q_1C + Q_2C_u - K_2C_{wao}\right\}\exp\left(-\frac{K_2t}{K_1}\right)}{K_2} \quad (5)$$

- In the case of $K_2 = K_1K_5$, the solution of Eq. (3) and thus the saturated zone equation becomes:

$$C_{wa} = \frac{K_3}{K_2} + \left[C_{wao} - \frac{K_3}{K_2} + \frac{K_4}{K_1}t\right]\exp\left(-K_5t\right) \quad (6)$$

Downgradient Solute Transport Module

A simplified version of a general solution to a three-dimensional advection/dispersion/sorption/decay equation was used to simulate solute transport. It provides an estimate of the contaminant concentration at a receptor location or discharge area downgradient of the source area under different source-loading conditions. As a result of the complexity of this model, a separate, executable FORTRAN program was required to perform the calculations. The linkage between the main spreadsheet and this executable file was accomplished using macro commands in the spreadsheet.

The basic equation, a modified version of a general constant-source equation developed by Domenico (1987), for the plume centerline is as follows:

$$C(X, t, Co) = \frac{Co}{2}\exp\left\{\left(\frac{X}{2\left(D_x/V\right)}\right)\left[1-\left(1+\frac{4\lambda_3D_x}{V^2}\right)^{1/2}\right]\right\}$$

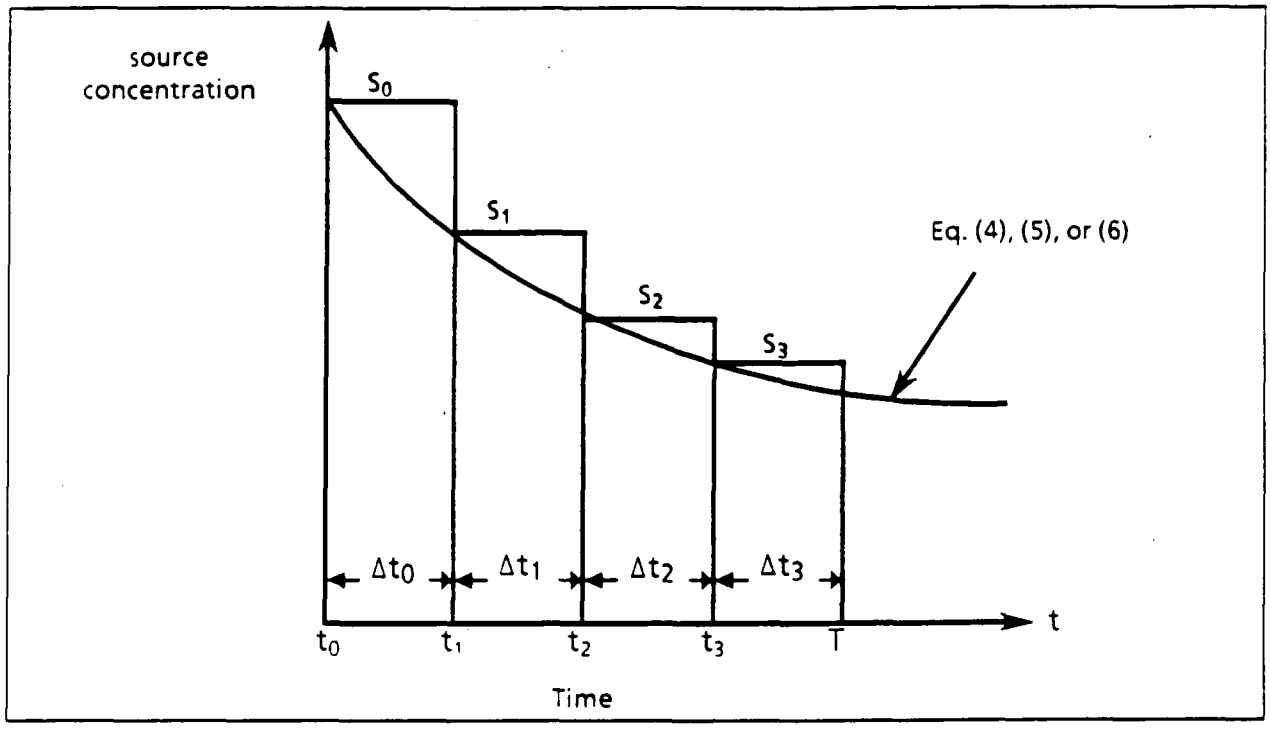
$$\operatorname{erfc}\left[\frac{X - Vt\left(1+\frac{4\lambda_3D_x}{V^2}\right)^{1/2}}{2\left(D_xt\right)^{1/2}}\right]\operatorname{erf}\left[\frac{Y}{4\left(\frac{D_y}{V}X\right)^{1/2}}\right] \quad (7)$$

Where:
- C = the downgradient concentration along the plume centerline (mg/L)
- C_o = the constant groundwater concentration at/below the source (mg/L)
- X = the distance downgradient of the source (ft)
- V = the contaminant velocity (ft/year)
- t = elapsed time since the beginning of the source loading (years)
- D_x = the principle value of the dispersion tensor in the x (longitudinal) direction (ft^2/year)
- Y = source dimension in the y (lateral) direction (ft)
- D_y = the principle value of the dispersion tensor in the y (lateral) direction (ft^2/year)
- λ_3 = decay rate ($years^{-1}$)

In the preceding expression, erf and erfc are the error function and the complimentary error function, respectively. Vertical dispersion was not considered in equation (7) in order to provide a conservative estimate of the exposure point concentration. The contaminant velocity is determined as the groundwater interstitial pore velocity divided by the retardation factor. The retardation factor can be estimated using the distribution coefficient (K_d) and the bulk density and porosity of the soil. Equation (7) was applied using superposition to simulate the time-dependent source loading. For this

time-dependent source, the concentration at a downgradient location at a given time T can be estimated using the following procedure. First the continuous function of the time-dependent source concentration [Eq. (4), (5), or (6)] is approximated by a series of step impulses which simplifies the solution and is also more conservative than the original function as shown in Figure 2.

FIGURE 2: CONCEPTUAL MODEL OF THE SOURCE CONCENTRATION



The concentration at X feet downgradient of the source at time T can therefore be estimated by superposition of constant source solutions [Eq. (7)] for all impulses prior to time T as follows:

$$C(x,T) = \sum_{i=0}^{n} \left[C\left(X, T-t_i, S_i\right) - C\left(X, T-t_i - \Delta t_i, S_i\right) \right]$$

$$= C\left(X, T-t_0, S_0\right) - C\left(X, T-t_0 - \Delta t_0, S_0\right) +$$

$$C\left(X, T-t_1, S_1\right) - C\left(X, T-t_1 - \Delta t_1, S_1\right) + \ldots +$$

$$C\left(X, T-t_n, S_n\right) - C\left(X, T-t_n - \Delta t_n, S_n\right) \qquad (8)$$

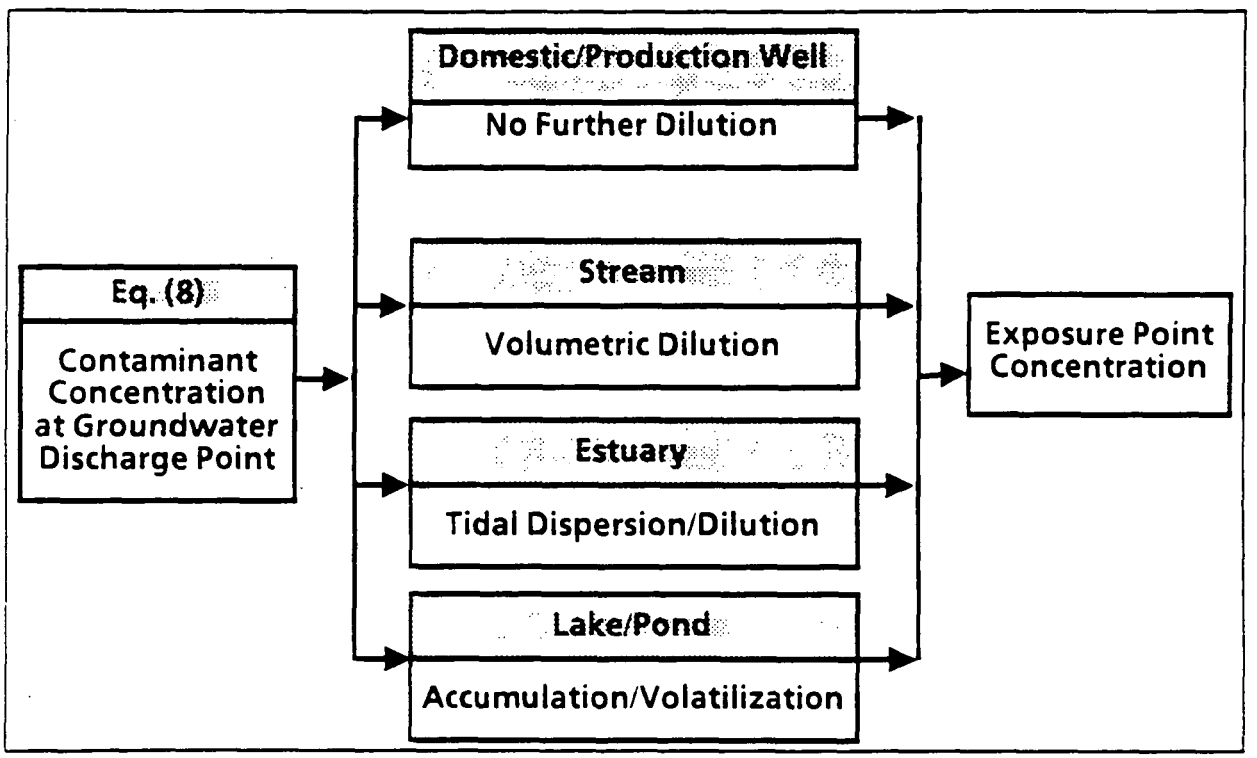
Where: S_i is the source concentration of the ith impulse; t_i is the starting time of the ith impulse; Δt_i is the time interval for the ith impulse; $T-t_n-\Delta t_n = 0$; and C (X, T) is the combined effects of n + 1 impulses. In the preceding equation, C (X, t, S) [i.e., Eq. (7)] is the concentration at X caused by a constant source with concentration S for a duration of t. Therefore, C(X,t,S) needs to be applied twice to determine each single impulse's net lasting effect at time T. This approach is similar to the procedure used in the Expert ROKEY Computer System (McClymont and Schivarte, 1987). The Expert ROKEY Computer System is a saturated-zone contaminant fate and transport model with an expert

system that assists the user to estimate necessary hydrogeological and chemical parameters for the model. The source loading from the unsaturated zone must be specified by the user.

Discharge/Exposure Module

Analytical models for estimating contaminant concentrations at four different types of exposure points were developed and incorporated into the spreadsheet. They include direct use of groundwater, as well as groundwater discharge into a flowing stream, a closed lake/pond, or a tidally affected water body. As shown in Figure 3, the discharge/exposure module of the model estimates the dilution caused by mixing of contaminated groundwater with surface water and, thus, the contaminant concentration at an appropriate exposure point.

FIGURE 3: TYPES OF EXPOSURE POINT AND ASSOCIATED ATTENUATION IMPLEMENTED



Although the basic equations for estimating dilution factors in streams, estuarys, and lakes (Thomann and Mueller, 1987) are simple, it is usually necessary to modify or combine several equations, based on the site-specific conditions, to obtain the final dilution model. Therefore, details or a generalized approach regarding the development of the dilution factors used in this module will not be described in this paper.

MODEL PARAMETER ESTIMATION

Table 1 is an example of the output generated using the developed model for a direct groundwater use scenario. Values of input parameters that must be specified by the user are circled. These parameters can be estimated based on site-specific conditions such as the extent of source contamination (i.e., LENGTH and WIDTH); soil characteristics (i.e., POROSITY, DENSITY, and FOC); hydrogeologic information (i.e., GW VEL., DISTANCE, DISPERSIVITY, and THICKNESS); water budget information generated using models such as the Hydrologic Evaluation of Landfill Performance (HELP) Model (i.e., INFILT. and SATURATION); contaminant concentration (i.e., CWAO); and background contamination (i.e., C and CU). As one of the user-specified input values, the upgradient groundwater flow velocity (GW VEL.) can be estimated by the following equation:

GW VEL. = average GW gradient x average hydraulic conductivity/POROSITY (9)

The longitudinal dispersivity (Ax) is usually taken as 1/10 of the DISTANCE, where the transverse dispersivity (Ay) is equal to 1/3 of the longitudinal value. The rest of the parameters in Table 1, as well as some parameters used in Figure 1 and Equations (4) and (7) are internally calculated automatically by the spreadsheet, using the following equations and the user-specified parameters (proper conversions of units):

Contaminant source model parameters shown in Figure 1:

- Q_1 = INFILT. x LENGTH x WIDTH
- V_w = POROSITY x LENGTH x WIDTH x THICKNESS (unsaturated zone)
- K_d = KOC x FOC (unsaturated zone)
- W_s = DENSITY x LENGTH x WIDTH x THICKNESS (unsaturated zone)
- M = C_w x (SATURATION x V_w + K_d x W_s)
- C_{w0} = CLEAN-UP GOAL / K_d
- Q_2 = GW VEL. x WIDTH x THICKNESS (saturated zone) x POROSITY
- V_{wa} = POROSITY x LENGTH x WIDTH x THICKNESS (saturated zone)
- K_{ds} = KOC x FOC (saturated zone)

- W_{sa} = DENSITY x LENGTH x WIDTH x THICKNESS (saturated zone)
- M_a = C_{wa} x (V_{wa} + K_{ds} x W_{sa})
- Q_3 = Q_1 + Q_2
- λ = DECAY RATE = -ln(0.5) / HALF LIFE (zone specific)

Downgradient solute transport module parameters used in Equation (7):

- RETARDATION = 1 + DENSITY x KD / POROSITY
- C_0 = S_0, S_1, S_2, or S_3 as shown in Figure 2.
- X = DISTANCE (distance from the downgradient edge of the source area to the exposure point)
- GW V. = Q_3/ (POROSITY x WIDTH x THICKNESS)
- V = GW V. / RETARDATION
- Y = WIDTH
- D_x = V x DISPERSIVITY (Ax) = V x 0.1 x DISTANCE
- D_y = V x DISPERSIVITY (Ay) = D_x / 3
- λ_3 = DECAY RATE = -ln(0.5) / HALF LIFE (zone specific)

4775

TABLE 1: EXAMPLE OF MODEL OUTPUT

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HALLIBURTON NUS ENVIRONMENTAL CORPORATION
SCREENING-LEVEL MULTIMEDIA CONTAMINANT FATE AND TRANSPORT MODEL
EXPOSURE SCENARIO #1: TIME VARYING SOURCE AND DIRECT USE OF GROUNDWATER

SITE: X CHEMICAL SUPERFUND SITE
INVESTGATOR: J. D. CHIOU
DATE: 10-21-91

CONTAMINANT: BENZENE
KOC (L/KG): 65.00
HALF LIFE (YRS):
UNSATURATED: 5.00
SATURATED: 5.00
D.G. PLUME: 5.00

ALLOWABLE EXPOSURE CONC. (UG/L): 5.0
UNSATURATED ZONE SOIL CLEAN UP GOAL (MG/KG): 1.024

SOURCE AREA:		UNSATURATED ZONE		SATURATED ZONE		DOWN GRADIENT AREA / EXPOSURE POINT			
LENGTH (FT):	720	FOC (KG/KG):	.001	FOC (KG/KG):	.0010	Q3 (L/DAY):	1462.40	FOC (KG/KG):	.001
WIDTH (FT):	160	KD (L/KG):	.065	KD (L/KG):	.065	GW V.(FT/YR):	48.09	KD (L/KG):	.065
		SATURATION:	[illegible]	SATURATION:	1.00	DISTANCE (FT):	120.00	RETARDATION:	1.316
POROSITY:	.35	THICKNESS (FT):	7.00	THICKNESS (FT):	7.00	POROSITY:	.35		
DENSITY (G/CM3):	1.7	DECAY (1/DAY):	3.8e-4	DECAY (1/DAY):	3.798e-4	DECAY (1/YR):	1.386e-1		
		CWO (PPB):	4.65e4	CWAO (PPB):	1e2	DISPERSIVITY:			
INFILT. (FT/YR):	.2275	C (PPB):	[illegible]	CU (PPB):	[illegible]	Ax (FT):	112.00		
GW VEL. (FT/YR):	40	Q1 (L/DAY):	245.80	Q2 (L/DAY):	1216.60	Ay (FT):	37.30		

ACCEPT THE GOAL!

ELAPSED TIME - YRS	DAYS	UNSATURATED ZONE CONC. (UG/L)	SATURATED ZONE CONC. (UG/L)	EXPOSURE POINT CONC. (UG/L)	70-YEAR AVERAGE (UG/L)
0	0	46523.08	100.00	.0000	
2	730	34168.82	631.62	.0000	
4	1460	25095.25	846.07	.0000	
6	2190	18431.17	883.06	.0003	
8	2920	13536.75	827.72	.0069	
10	3650	9942.05	730.59	.0600	
12	4380	7301.93	620.57	.2621	
14	5110	5362.89	513.28	.7179	
16	5840	3938.77	416.36	1.4400	
18	6570	2892.82	332.75	2.3340	
20	7300	2124.63	262.85	3.2480	
22	8030	1560.43	205.69	4.0400	
24	8760	1146.06	159.72	4.6140	
26	9490	841.72	123.23	4.9310	
28	10220	618.20	94.56	4.9990	
30	10950	454.04	72.23	4.8560	
32	11680	333.47	54.95	4.5540	
34	12410	244.91	41.66	4.1490	
36	13140	179.88	31.49	3.6870	
38	13870	132.11	23.74	3.2090	
40	14600	97.03	17.85	2.7430	
42	15330	71.26	13.40	2.3090	
44	16060	52.34	10.04	1.9180	
46	16790	38.44	7.50	1.5740	
48	17520	28.23	5.60	1.2780	
50	18250	20.74	4.18	1.0290	
52	18980	15.23	3.11	.8213	
54	19710	11.18	2.32	.6509	
56	20440	8.21	1.72	.5125	
58	21170	6.03	1.28	.4011	
60	21900	4.43	.95	.3123	
62	22630	3.25	.70	.2421	
64	23360	2.39	.52	.1868	
66	24090	1.76	.39	.1436	
68	24820	1.29	.29	.1099	
70	25550	.95	.21	.0839	1.7062
72	26280	.70	.16	.0639	1.7080
74	27010	.51	.12	.0485	1.7093
76	27740	.38	.08	.0367	1.7103
78	28470	.28	.06	.0277	1.7111
80	29200	.20	.05	.0209	1.7115
82	29930	.15	.03	.0157	1.7103
84	30660	.11	.03	.0118	1.7033
86	31390	.08	.02	.0089	1.6836
88	32120	.06	.01	.0066	1.6438
90	32850	.04	.01	.0050	1.5791
92	33580	.03	.01	.0037	1.4890
94	34310	.02	.01	.0028	1.3769
96	35040	.02	.00	.0021	1.2487
98	35770	.01	.00	.0015	1.1118
100	36500	.01	.00	.0011	.9730
MAXIMUM:		46523.08	883.06	4.999	1.7115

Assuming simple hydrolysis and biodegradation, the zone-specific decay rates (i.e. λ_1, λ_2, and λ_3) can also be estimated by the following equations (Huyakorn et al., 1987; Salhotra et al., 1990):

$$\lambda_1 = \left(\frac{\lambda_d \theta_u + \lambda_s K_d \rho_b}{\theta_u + K_d \rho_b} \right) + \lambda_b \tag{10}$$

$$\lambda_2 \text{ (or } \lambda_3) = \left(\frac{\lambda_d \theta + \lambda_s K_{ds} \rho_b}{\theta + K_{ds} \rho_b} \right) + \lambda_b \tag{11}$$

Where:

λ_d = first-order hydrolysis rate constant for the dissolved constituent (day^{-1})
λ_s = first-order hydrolysis rate constant for the sorbed constituent (day^{-1})
λ_b = first-order lumped biodegradation rate (day^{-1})
Θ_u = volumetric water content in the unsaturated zone (dimensionless)
Θ = volumetric water content in the saturated zone (i.e. total porosity)
ρ_b = soil bulk density, g/cm^3

λ_d and λ_s are chemical specific and dependent on the soil and groundwater conditions. The required information and method for estimating λ_d and λ_s are described by Huyakorn (Huyakorn et al., 1987).

Although the contaminant source module assumes a homogeneous unsaturated zone, the use of the HELP Model to determine the infiltration rate and the degree of saturation externally can allow the layered structure of the unsaturated zone to be considered, if necessary. The percolation from the bottom layer and the weighted average of saturation in each layer estimated by the HELP Model can be used as the infiltration rate and the unsaturated zone saturation ratio in this model. The thickness of the saturated zone, which represents the vertical extent of contamination in the model, is usually based on the minimum of the following three possible values:

- The thickness of the entire saturated zone.
- The lowest position of detected contaminants of concern.
- The mixing zone depth calculated by the following equation (Salhotra et al., 1990):

$$H = B\left[1 - \exp\left(-V_{zo} L/(BV_x)\right)\right] + \left(2\,\alpha_v L\right)^{1/2} \tag{12}$$

Where: H is the mixing zone depth (ft); B is the total saturated zone thickness (ft); V_{zo} is the vertical seepage velocity (ft/yr); L is the length of the source area (ft); V_x is the horizontal seepage velocity (ft/yr); and α_v is the vertical dispersivity (ft).

In cases where the net recharge outside the source area percolating directly into and diluting the downgradient contaminant plume is significant, the effective decay rate in the downgradient area can be increased to λ_3*, as follows

$$\lambda_3^* = \lambda_3 + \frac{q}{B\theta} \tag{13}$$

where q is the annual infiltration rate in the downgradient area (ft/year).

With all of the parameters determined (either via direct input or internal calculation), Eqs. (2), (4) [or (5) and (6)], and (8) are then used in the model to calculate C_w, C_{wa}, and C, respectively. Since the model is implemented on a spreadsheet, the graphical capability of the spreadsheet can be directly utilized for presenting the model results. Figure 4 shows the graphical presentations of simulated C_w, C_{wa}, and C for the example in Table 1. Both Table 1 and graphs in Figure 4 are generated by the spreadsheet.

APPLICATION

Three case studies describing instances in which the model has been used to determine cleanup goals are described below.

Cleanup Goal Selection - EPA Superfund Site

The model was used to determine soil cleanup goals at a Superfund site in Virginia. Soil media in localized areas was contaminated in both the saturated and unsaturated zones. The model was run under an interactive approach to determine the maximum unsaturated zone soil concentrations that will result in attainment of the Safe Drinking Water Act Maximum Contaminant Levels (MCLs) at the downgradient edge of the saturated zone beneath the site.

For this particular application, existing contamination was specified based on actual analytical data for saturated zone. The infiltration rate (Q_1) was estimated using the HELP Model, based on local meteorological conditions. Soil mechanical and hydraulic properties, which were determined from samples collected from the site, were used as model inputs to simulate contaminant washout from the unsaturated zone and contaminant transport in the saturated zone. The model was run for 19 different compounds and for various concentrations. Based on the results of the modeling efforts, a variety of potential cleanup scenarios were identified. Remedial alternatives for each scenario were developed for EPA review.

Cleanup Goal Selection - DOD Facility

The model was used to develop cleanup goals for numerous contaminated areas at a DOD facility in Texas based on specific remedial objectives. Figure 5 shows the contaminated zones at the facility and the chemicals of concern. The overall remedial objective was to protect human health and the environment and achieve Applicable, or Relevant and Appropriate Requirements (ARARs) at a location immediately adjacent to a receiving surface water body or at the base boundary. The goals were established based on EPA and TWC (Texas Water Commission) "acceptable" risk levels and assumptions regarding ultimate land uses and contaminant exposure pathways.

Leachate generation, dilution in the aquifer beneath the sites, and downgradient transport, including hydrodynamic dispersion and sorption, were considered to determine soil concentrations that correspond to the groundwater remediation goals at the point of exposure. Although many of the soil contaminants at the various sites are subject to environmental degradation via hydrolysis or microbial degradation, these decay mechanisms were not considered. Model input parameters were determined based on available site information and on professional judgment if site-specific values were not available.

Two other models were used to determine certain input parameters. The groundwater velocity for each site was determined from a calibrated, particle-tracking, groundwater model completed in support of a Remedial Investigation at the facility. This model was used to delineate flow paths and to predict the travel time of a particle from the various sources to the stream or other exposure

FIGURE 4: GRAPHICAL PRESENTATION OF THE MODEL RESULTS

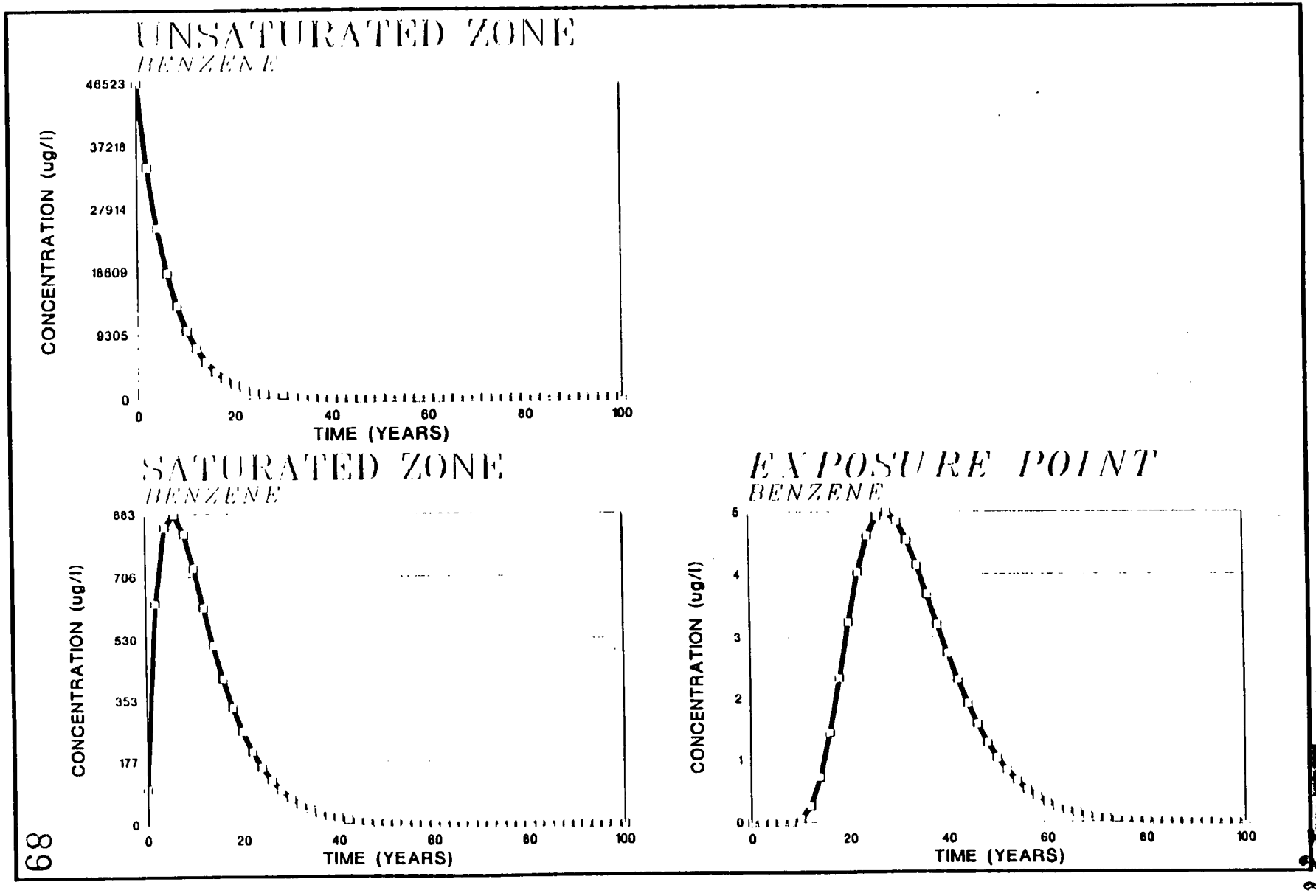
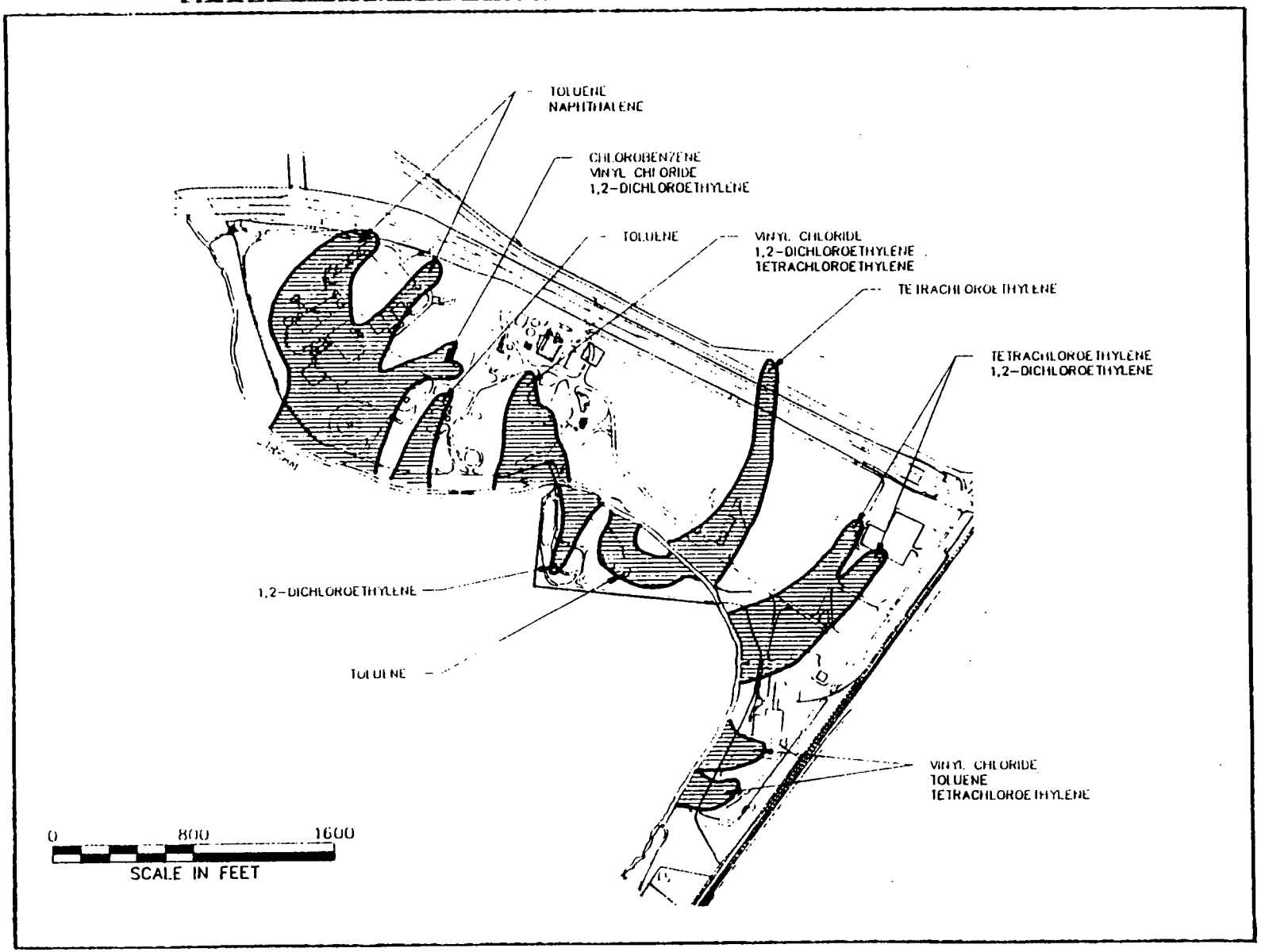


FIGURE 5 SITE MAP AND ROUTE OF CONTAMINANT MIGRATION



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points. The lengths of the flow paths from each site (or discrete site-specific sources) were divided by the simulated travel times to determine an interstitial pore velocity. The annual recnarge (Q_1) for each site was determined using the HELP Model.

Soil remediation goals were determined based on the assumption that the groundwater was either uncontaminated or that it would be restored to acceptable concentrations. Therefore, for model execution, C (the concentration in infiltrating precipitation), C_u (the concentration in upgradient groundwater, and C_{wa} (the concentration in groundwater beneath the site) were all set equal to zero at time t = 0. Furthermore, the concentration in infiltrating precipitation and the upgradient concentration remained at zero throughout the model execution. The saturated zone groundwater concentration is contingent upon loading from the source and fluctuates as a function of time.

Once the input parameters had been established for each site and contaminant, an interactive, trial-and-error approach was used to determine acceptable source concentrations. A soil concentration was entered and adjusted until the maximum downgradient concentration at the point of exposure did not exceed the groundwater goal.

ACL Demonstration - Major Chemical Manufacturer

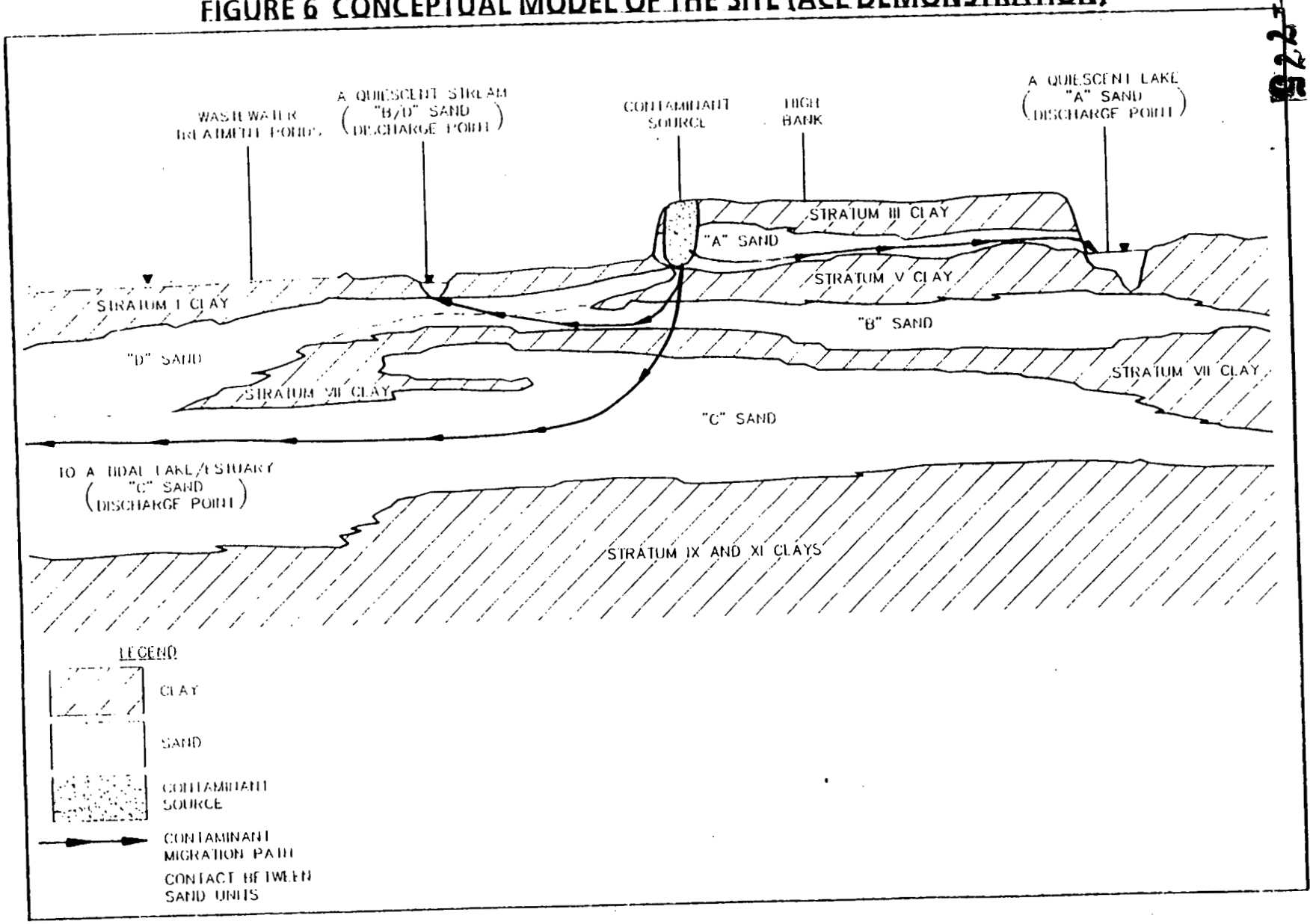
An Alternate Concentration Limit (ACL) demonstration based on discharge of contaminated groundwater to surface waters in the vicinity of a major chemical manufacturer's facility was completed. Incidental ingestion of surface water and ingestion of aquatic organisms that have accumulated discharged groundwater contaminants were considered the exposure routes of concern for human receptors. These points of exposure and exposure routes were considered to develop Maximum Allowable Exposure Concentrations (MAECs). ACLs were then determined via contaminant fate and transport analysis such that the MAECs are not exceeded.

Several unsuccessful attempts to develop a complex, numerical, groundwater flow and transport simulation model for the facility had been completed by other consulting firms. In view of the complexity of the site hydrologic conditions, HALLIBURTON NUS deemed it appropriate to employ simplified analytical solutions to simulate contaminant migration. Nevertheless, the previous studies provided input values for most of the required parameters for the ACL demonstration.

Figure 6 depicts a conceptual cross-section of the study area. Two of the three surface water bodies in the vicinity of the site were treated as quiescent bodies with no dilution potential. An accumulation/volatilization model was developed and incorporated into the spreadsheet to simulate the exposure point concentrations in these two surface water bodies. A tidal dilution model was developed for the third surface water body to estimate chemical concentration distributions. Based on groundwater discharge rate, chemical concentrations in the groundwater, and a tidal amplitude, the model was used to estimate the steady-state daily maximum or average chemical concentrations in the bay. Therefore, the dilution factor between groundwater and each model segment resulting from mixing and tidal movement was determined.

ACLs were eventually developed for each of the chemicals of concern using the model. The observed concentrations of some chemicals exceed the ACLs based on the exposure pathways of concern. The fact that some of the protective ACLs have been exceeded indicates that containment efforts (interceptor trenches) are necessary and were implemented in a timely manner. Continued interception of groundwater plume is planned until acceptable concentrations (ACLs) are attained at the unit boundary.

FIGURE 6 CONCEPTUAL MODEL OF THE SITE (ACL DEMONSTRATION)



SUMMARY

The model is based on straight forward mass-balances and advection/dispersion equations but can be used to simulate a variety of complex conditions. To date, HALLIBURTON NUS has employed the model to determine soil cleanup goals, Alternative Concentration Limits, and to support baseline risk assessment/human health and environmental evaluations for both CERCLA and RCRA applications. The model is extremely user friendly and can be used by personnel with diverse technical backgrounds.

Several advantages of a spreadsheet-based model over a traditional "pre/post-processor and main program approach" are apparent. Because the simulation is implemented by a spreadsheet, the model input and output data are contained in the same file. It is extremely easy for the user to change values of any specific input parameters, and the effects of various input values can be seen on the computer screen. The graphical and statistical capability provided by the spreadsheet makes presentation of the model results very efficient and flexible.

REFERENCES

Domenico, P.A., 1987, "An Analytical Model for Multidimensional Transport of a Decaying Contaminant Species," J. Hydrol., Vol. 91, pp. 49-58.

Huyakorn, P.S., M. J. Ungs, L. A. Mulkey, and E.A. Sudicky, 1987. "A Three-Dimensional Analytical Method for Predicting Leachate Migration." Groundwater, Volume 25, No. 5, September-October.

McClymont, G. L., and F.W. Schivartz 1987, "Development and Application of an Expert System in Contaminant Hydrogeology - The Expert ROKEY Computer System," prepared for National Hydrology Research Institute, Environment Canada, Alberta Environmental Research Trust.

Salhotra, A. M., P. Mineant, S. Sharp-Hansen, and T. Allison, 1990, "Multimedia Exposure Assessment Model (Multimed) for the Evaluating the Land Disposal of Wastes - Model Theory." EPA Contract No. 68-03-3513 and No. 68-03-6304, USEPA, Athens, GA.

Thomann, R. V and J. A. Mueller, 1987, "Principles of Surface Water Quality Modeling and Control," Harper & Row, Publishers, New York.

APPENDIX C.2

TYPICAL SENSITIVITY ANALYSES

4775

601 Wythe Street, Alexandria VA 22314

Water Environment Federation
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Important Factors in Cleanup Goal Development for Contaminated Soil and Groundwater - Sensitivity Analyses by Model Simulations

J.D. Chiou, R.J. Hubbard, A.E. Hubbard
AC92-044-005

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IMPORTANT FACTORS IN CLEANUP GOAL DEVELOPMENT FOR CONTAMINATED SOIL AND GROUNDWATER - SENSITIVITY ANALYSES BY MODEL SIMULATIONS

4775

by

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ABSTRACT

An overview of the numerical effects of variable input parameters, exposure assessment methods, and physical/chemical processes on cleanup goals and/or Alternate Concentration Limits (ACLs) for contaminated soil and groundwater is provided. The impact of uncertainties in key parameters and different conceptual models for contaminant attenuation assessment is studied using a spreadsheet-based multimedia contaminant fate and transport model. Important factors in six major categories are considered under hypothetical site conditions. A sensitivity analysis approach is used to demonstrate the individual and cumulative effects of various input parameters and conceptual approaches on cleanup goals or ACLs. Soil cleanup goals and groundwater ACLs range over six orders of magnitude for a hypothetical site.

KEY WORDS

Cleanup Goal, Alternate Concentration Limit, Contaminated Soil, Contaminated Groundwater, Spreadsheet-based Contaminant Fate and Transport Model, Sensitivity Analysis.

INTRODUCTION

Groundwater and soil cleanup goals for uncontrolled hazardous waste sites and ACLs for treatment, storage, and disposal facilities are usually determined based on relevant regulations and/or risk assessment methods coupled with analytical or numerical modeling techniques. When concentrations of hazardous constituents in groundwater exceed background or Maximum Contaminant Levels, Alternate Concentration Limits (ACLs) [40 CFR 264.93(a)] can be established at the point of compliance [40 CFR 264.94(b)] if they are protective of human health and the environment. Because of the complexity involved, general guidelines for conceptualizing or quantifying most of the important factors to be considered in the cleanup goal development process are seldom available. Therefore, cleanup goal or ACL development usually requires selection of a proposed value from a large range of possible values. This large range may be the result of uncertainties in the specific values of input parameters, different conceptual models of the site (e.g., migration pathways and exposure routes), or as a result of decisions to include or neglect certain physical or chemical attenuation processes. Because of this large range

(and its associated financial implications), determination of the final cleanup goal or ACL may involve lengthy negotiation between an industry and regulatory agencies.

The objective of this paper is to provide a systematic overview of the impact of these factors on cleanup goal and ACL development.

IMPORTANT FACTORS IN CLEANUP GOAL OR ACL DEVELOPMENT

The first step in soil cleanup goal and/or ACL development includes defining the source of contamination, the physical, chemical, and toxic characteristics of the contaminants, and the site physical features that affect contaminant fate and transport. Once this is completed, current and future impacts on the environment and human health may be estimated. The second step is to define the extent and degree of source reduction and/or containment required to attain acceptable concentrations (if necessary). This process includes consideration of many chemical processes and hydrogeologic conditions that affect the migration and attenuation of contaminants. In general, site-specific combinations of the following factors are considered during the cleanup goal or ACL development process:

- Source Loading
- Contaminant Characteristics
- Hydrogeological Conditions
- Points of Exposure/Exposure Routes

In addition, exposure assessment assumptions and the impacts of feasible corrective measures will also affect the cleanup goals or ACLs.

THE COMPUTER MODEL USED IN THE STUDY

A spreadsheet-based multimedia contaminant fate and transport model developed to support screening-level risk assessment and cleanup goal/ACL development was used to complete the sensitivity analysis (Chiou and Hubbard, 1992). The model includes various components for simulating contaminant washout from a source area, downgradient solute transport, and estimation of receptor concentrations under various types of exposure scenarios. The model was implemented using a spreadsheet to accommodate linking of the various simulation modules and to simplify the model input, interactive execution, and output presentation processes.

The contaminant source module of the model relies on analytical equations based on straightforward mass balances to describe various aspects of source loading and contaminant washout from both the unsaturated and saturated zones. Any combination of the following conditions or processes may be simulated:

- Surface infiltration and percolation
- Contaminant loading via leakage or infiltration
- Sorption in the unsaturated zone
- Upgradient groundwater flow

- Contaminant loading via upgradient flow
- Sorption in the saturated zone
- Zone-specific contaminant decay rates
- Zone-specific initial contaminant concentrations
- Constant or time-varying concentration in the unsaturated zone

4775

The downgradient solute transport module of the model uses a simplified version of a general solution to a three-dimensional advection/dispersion/sorption/decay equation and the superposition technique to simulate solute transport (Domenico, 1987). The transport module calculates the contaminant concentration at a receptor location or discharge area downgradient of the source area under different source-loading conditions. Downgradient contamination caused by the source (or other sources) prior to remediation can also be considered.

The discharge/exposure module of the model uses analytical methods to estimate contaminant concentrations under four different types of exposure scenarios, including direct use of groundwater or various surface water uses based on groundwater discharge into a flowing stream, a closed lake/pond, or a tidally-affected estuary. This module can be used to estimate the dilution caused by mixing of contaminated groundwater with surface water and can account for various surface water attenuation mechanisms. Based on the requirements of the risk assessment, the model output provides the maximum or lifetime average (70-year) contaminant concentrations at the exposure point.

The simplicity of the model and the wide range of conditions that can be simulated make it suitable for testing different conceptual approaches as well as for performing a sensitivity analysis using variable input parameters.

SCENARIOS AND ASSUMPTIONS FOR A HYPOTHETICAL INDUSTRIAL SITE

As shown in Figures 1 and 2, a hypothetical (but typical) site with a drum disposal area was used as the basis for the modeling and sensitivity analyses. The source area consists of an unknown number of leaking buried drums which contain an organic chemical (X). The source has been defined as a 60 by 60 foot area at the center of the industrial facility. The groundwater table is 15 feet deep and the top of underlying impermeable bedrock is 50 feet from the ground surface. A stream is located 300 feet east of the property line. Local groundwater flows toward (and discharges into) the stream. As a result of high concentrations of chemical X in soil samples taken from both the unsaturated and saturated zones, source control measures are determined to be necessary. The proposed action includes removal of the buried drums, in-situ treatment of soil in the unsaturated zone, and pumping and treatment of contaminated groundwater. To support analysis of corrective measures and closure plan preparation, an unsaturated zone cleanup goal and a groundwater ACL are to be developed.

As required by 40 CFR 264.94(b), the following information was compiled:

- Potential adverse effects on groundwater quality, considering:
  a. The proximity and withdrawal rates of groundwater users

98

4775

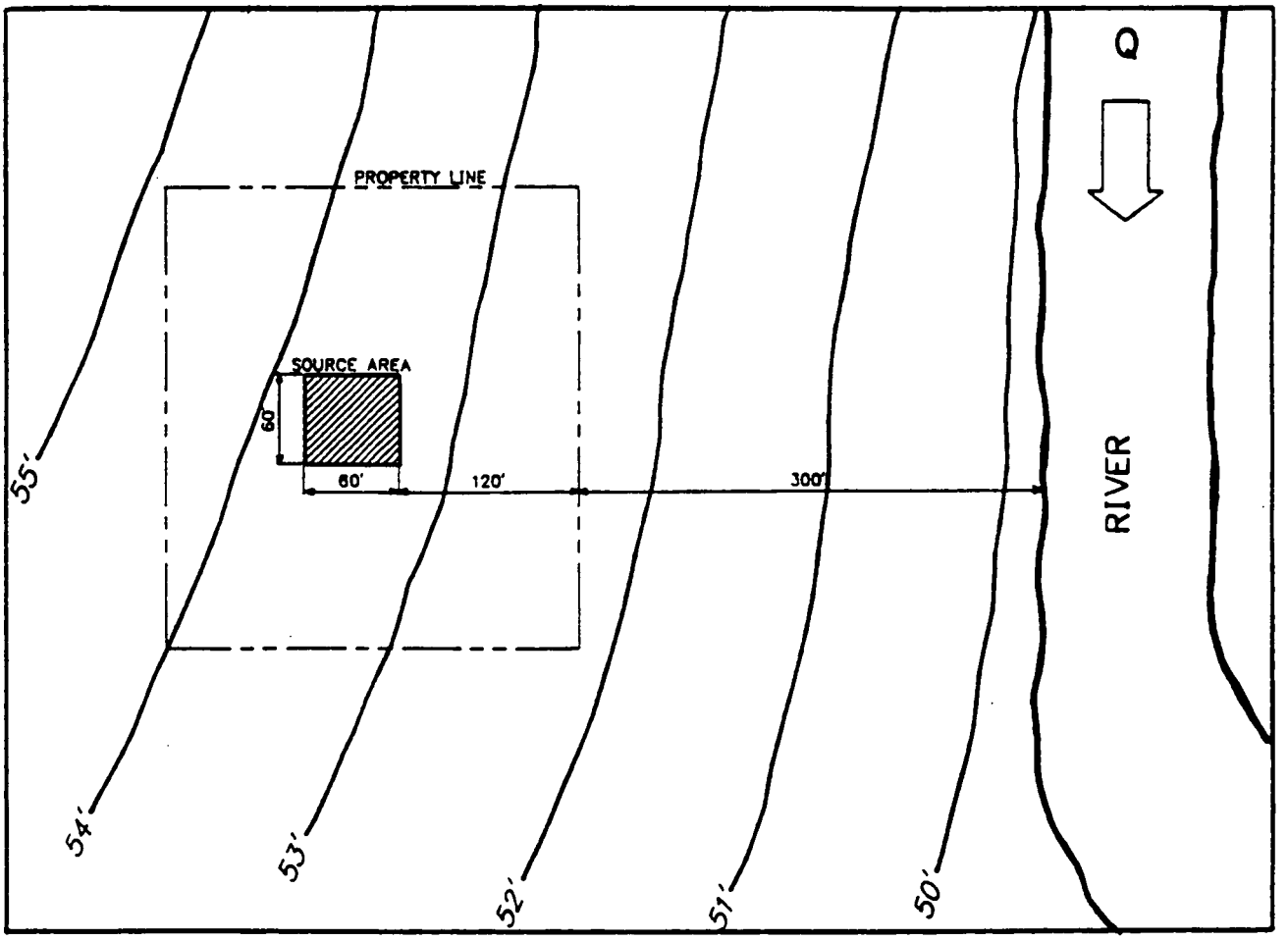

FIGURE 1 - SITE MAP AND GROUNDWATER CONTOURS

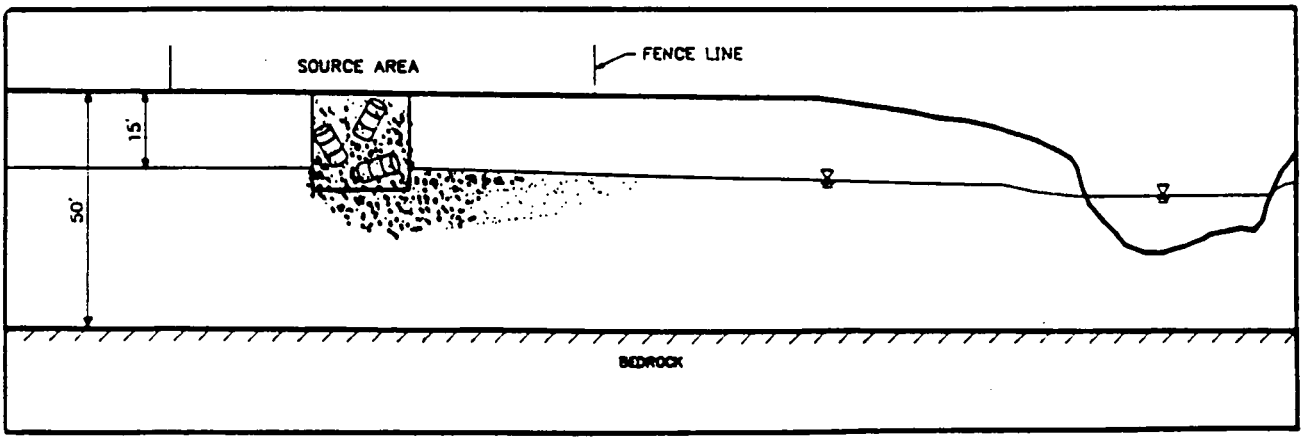

FIGURE 2 - REPRESENTATIVE CROSS-SECTION OF THE SITE

99

b. The current and future uses of groundwater in the area
c. The existing quality of groundwater, including other sources of contamination and their cumulative impact on the groundwater quality

- Potential adverse effects on the quality of hydraulically connected surface water bodies, considering:
  a. The patterns of rainfall in the region
  b. The proximity of the regulated unit to surface waters
  c. The current and future uses of surface waters in the area and any water quality standards
  d. The existing quality of surface water, including other sources of contamination and the cumulative impacts on surface water quality
- General considerations common to groundwater and surface water environment:
  a. The volume and physical and chemical characteristics of the waste in the regulated unit
  b. The hydrogeological characteristics of the facility and surrounding land
  c. The quantity and quality of groundwater, and the direction of groundwater flow
  d. The potential for health risks caused by human exposure to waste constituents
  e. The potential damage to wildlife, crops, vegetation, and physical structures caused by exposure to waste constituents
  f. The persistence and permanence of potential adverse effects

The soil cleanup goal and groundwater ACL are to be developed based on the preceding information. Although the ACL demonstration must justify all claims regarding the potential effects of groundwater/surface water contamination on human health and environment, detailed guidelines for establishing the soil cleanup goal and the ACL are not available. A decision was made to examine the range of possible cleanup goals and ACLs for various conceptual approaches to the problem using a computer model to simulate the different scenarios. To achieve this, the requisite information was categorized in six distinct groups. Different conceptual models/approaches were then identified and simulated, as follows:

- **Group 1 : Source Loading**
  a. Constant source vs. limited source
  b. With and without additional source loading
  c. Historical source vs. recent/instantaneous source
  d. With and without an upgradient source
- **Group 2 : Contaminant Characteristics**
  a. With and without decay
  b. With and without adsorption
- **Group 3 : Hydrogeological Conditions**
  a. Limited mixing depth vs. entire saturated thickness
  b. With and without hydrodynamic dispersion
  c. With and without downgradient groundwater recharge
  d. With and without upgradient flow
- **Group 4 : Points of Exposure/Exposure Routes**
  a. Various distances to the point of exposure
  b. Unsaturated zone vs. saturated zone

4775

g. Groundwater vs. surface water (discharge point)

- **Group 5 : Risk Assessment Assumptions**
  a. Lifetime average dose vs. maximum dose
  b. Various exposure scenarios
  c. Current vs. future land and water use
- **Group 6 : Impacts of Feasible Corrective Measures**
  a. With and without short-term containment
  b. With and without a surface cap
  c. Duration of remedial action

In addition to simulations for the preceding scenarios, the most conservative and reasonable cases developed through combinations of each set of controlling factors were also simulated and considered for final cleanup goal and ACL selection.

THE BASELINE SCENARIO

For the sensitivity analysis, a baseline scenario was first established to serve as a point of reference for the various approaches. The following conditions were assumed for the baseline scenario:

- **Group 1 :** After removal of the buried drums it was assumed that no additional loading occurs (limited residual contamination in the soil). The impact of upgradient sources and existing contamination in the downgradient area were neglected in the baseline scenario.
- **Group 2 :** The effect of adsorption of chemical X was considered. Chemical decay was not simulated because of the uncertainty in the decay rate of chemical X.
- **Group 3 :** The entire saturated thickness was used as the mixing depth for the contaminant and groundwater. Upgradient groundwater flow and both longitudinal and lateral dispersion were also considered. Dilution as a result of infiltration in the downgradient area was not simulated in the baseline scenario.
- **Group 4 :** The point of exposure was assumed to be a drinking water well along the stream. Therefore, no dilution by the stream was considered.
- **Group 5 :** Direct comparison between the maximum concentration at the exposure point with a risk-based criterion for chemical X was used to determine the acceptability of the cleanup goal.
- **Group 6 :** The baseline scenario did not include the possible impact of additional corrective measures (beyond drum removal) in the source area.

The conditions assumed for the baseline scenario are considered to be typical. Table I presents the printout from the spreadsheet model for the baseline scenario showing the model input parameters and simulated results. Figure 3 is a graphical presentation of the simulated contaminant concentrations at the source area and at the exposure point. With a maximum allowable exposure concentration of 5 μg/L, a cleanup goal of 126 μg/kg for the soil in the unsaturated zone of the source area was calculated using the model. The groundwater ACL was determined to be 43.5 μg/L using the downgradient edge of the source area as the Point of Compliance.

101

TABLE I - MODEL INPUTS AND OUTPUTS FOR THE [redacted] 4775 BASELINE SCENARIO

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HALLIBURTON NUS ENVIRONMENTAL CORPORATION
SCREENING-LEVEL MULTIMEDIA CONTAMINANT FATE AND TRANSPORT MODEL
EXPOSURE SCENARIO #1: TIME VARYING SOURCE AND DIRECT USE OF GROUNDWATER

SITE:	X CHEMICAL SOMEWHERE	CONTAMINANT:	X
		KOC (L/KG):	65.00
		HALF LIFE (YRS):	
		UNSATURATED:	.00
INVESTGATOR:	J. D. CHIOU	SATURATED:	.00
DATE:	7-5-92	D.G. PLUME:	.00

ALLOWABLE EXPOSURE CONC. (UG/L): 5.0
UNSATURATED ZONE SOIL CLEAN UP GOAL (MG/KG): .126

SOURCE AREA:		UNSATURATED ZONE		SATURATED ZONE		DOWN GRADIENT AREA / EXPOSURE POINT			
LENGTH (FT):	60	FOC (KG/KG):	.002	FOC (KG/KG):	.0020	Q3 (L/DAY):	1826.06	FOC (KG/KG):	.002
WIDTH (FT):	60	KD (L/KG):	.13	KD (L/KG):	.130	GW V.(FT/YR):	37.36	KD (L/KG):	.13
		SATURATION:	.3	SATURATION:	1.00	DISTANCE (FT):	420.00	RETARDATION:	1.737
POROSITY:	.3	THICKNESS (FT):	15.00	THICKNESS (FT):	35.00	EFF. POROSITY:	.30		
DENSITY (G/CM3):	1.7	DECAY (1/DAY):	0	DECAY (1/DAY):	0	DECAY (1/YR):	0	ACCEPT THE GOAL!	
AGE (YEARS):	0	CWO (PPB):	9.65e2	CWAO (PPB):	0	DISPERSIVITY:			
INFILT. (FT/YR):	.5	C (PPB):	0	CU (PPB):	0	Ax (FT):	42.00		
GW VEL. (FT/YR):	34.5	Q1 (L/DAY):	139.66	Q2 (L/DAY):	1686.40	Ay (FT):	14.00		

TIME INTERVAL(YRS): 2		UNSATURATED ZONE CONC. (UG/L)	SATURATED ZONE CONC. (UG/L)	EXPOSURE POINT CONC. (UG/L)	70-YEAR AVERAGE (UG/L)
ELAPSED TIME - YRS	DAYS				
0	0	965.38	.00	.0000	
2	730	779.05	33.59	.0000	
4	1460	628.67	43.50	.0000	
6	2190	507.33	43.10	.0003	
8	2920	409.40	38.69	.0192	
10	3650	330.38	33.13	.1492	
12	4380	266.61	27.66	.5089	
14	5110	215.15	22.78	1.1280	
16	5840	173.62	18.60	1.9320	
18	6570	140.11	15.12	2.7920	
20	7300	113.06	12.25	3.5870	
22	8030	91.24	9.92	4.2310	
24	8760	73.63	8.01	4.6800	
26	9490	59.42	6.47	4.9280	
28	10220	47.95	5.23	4.9900	
30	10950	38.69	4.22	4.8970	
32	11680	31.22	3.41	4.6860	
34	12410	25.20	2.75	4.3920	
36	13140	20.33	2.22	4.0440	
38	13870	16.41	1.79	3.6700	
40	14600	13.24	1.44	3.2890	
42	15330	10.69	1.17	2.9170	
44	16060	8.62	.94	2.5630	
46	16790	6.96	.76	2.2340	
48	17520	5.62	.61	1.9330	
50	18250	4.53	.49	1.6630	
52	18980	3.66	.40	1.4230	
54	19710	2.95	.32	1.2110	
56	20440	2.38	.26	1.0270	
58	21170	1.92	.21	.8674	
60	21900	1.55	.17	.7300	
62	22630	1.25	.14	.6125	
64	23360	1.01	.11	.5124	
66	24090	.82	.09	.4276	
68	24820	.66	.07	.3561	
70	25550	.53	.06	.2958	2.0193
72	26280	.43	.05	.2453	2.0262
74	27010	.35	.04	.2030	2.0318
76	27740	.28	.03	.1678	2.0365
78	28470	.23	.02	.1385	2.0403
80	29200	.18	.02	.1141	2.0429
82	29930	.15	.02	.0939	2.0414
84	30660	.12	.01	.0772	2.0294
86	31390	.10	.01	.0634	1.9998
88	32120	.08	.01	.0520	1.9476
90	32850	.06	.01	.0426	1.8712
92	33580	.05	.01	.0349	1.7726
94	34310	.04	.00	.0285	1.6558
96	35040	.03	.00	.0233	1.5265
98	35770	.03	.00	.0191	1.3901
100	36500	.02	.00	.0156	1.2519
MAXIMUM:		965.38	43.50	4.990	2.0429

102

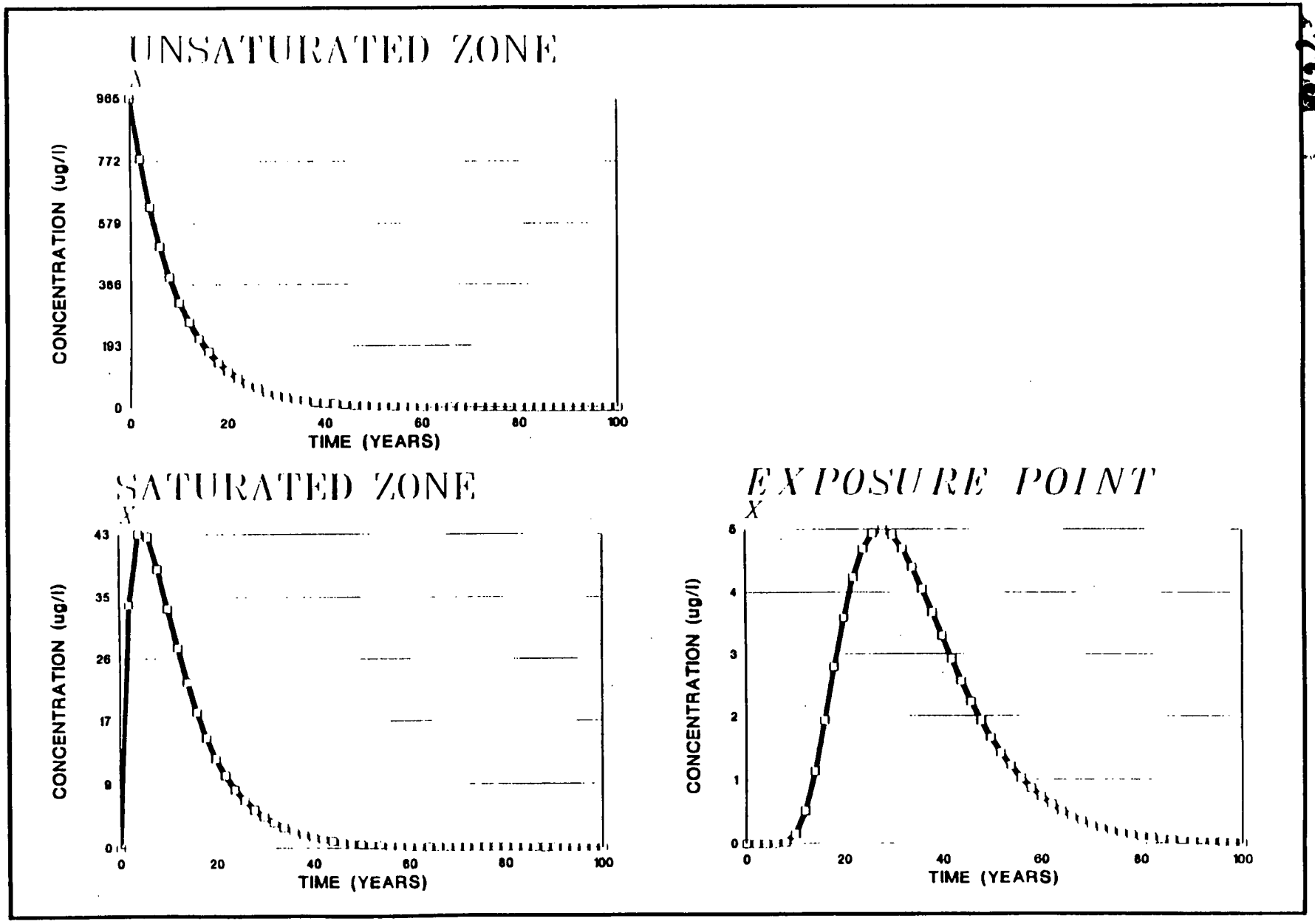

FIGURE 3 - SIMULATED CONTAMINANT CONCENTRATIONS VS. TIME FOR THE BASELINE SCENARIO

SENSITIVITY ANALYSIS AND IMPLICATIONS

After the baseline condition was established, the sensitivity of the cleanup goal and ACL to the different controlling factors was investigated. Table II shows the soil cleanup

TABLE II - RANGE OF THE SOIL CLEANUP GOALS BY CHANGING ONE CONTROLLING FACTOR

CONTROLLING FACTOR GROUP	CASE	DEVIATIONS FROM THE BASELINE SCENARIO	SOIL CLEANUP GOAL (ug/kg)	% CHANGE
	BASELINE	NONE	126	0
GROUP 1	1-1	AS A CONSTANT SOURCE	39	-69
	1-2	WITH ADDITIONAL LOADING	123	-2
	1-3	AS A HISTORICAL SOURCE	35	-72
	1-4	WITH UPGRADIENT SOURCE	109	-13
GROUP 2	2-1	WITH DECAY	2037	1,517
	2-2	NO ADSORPTION	10	-92
GROUP 3	3-1	LIMITED MIXING DEPTH	65	-48
	3-2	NO DISPERSION	14	-89
	3-3	WITH DOWNGRADIENT RECHARGE	262	108
	3-4	NO UPGRADIENT FLOW	90	-29
GROUP 4	4-1	PROPERTY LINE AS THE POE	25	-80
	4-2	USE SOIL CRITERIA	230000	182,440
	4-3	SURFACE WATER EXPOSURE	6288	4,890
GROUP 5	5-1	LIFE-TIME AVERAGE	307	144
	5-2	FISH CONSUMPTION	2500	1,884
	5-3	CONSIDER FUTURE WATER USE	66	-48
GROUP 6	6-1	WITH SHORT-TERM CONTAINMENT	280	122
	6-2	SURFACE CAP	1960	1,456
	6-3	DURATION OF THE CLEANUP	92	-27

goals for different scenarios created by changing only one controlling factor from the baseline condition. The following assumptions were made for the sensitivity analysis:

- Case 1-1 : To simulate a continuous leak, the unsaturated zone concentration in the source area was set as a constant (i.e., the cleanup goal).
- Case 1-2 : To consider possible additional spills in the facility, the contaminant concentration of the surface infiltration into the source area was set at 5 µg/L.
- Case 1-3 : The source was assumed to have been releasing contamination at a constant rate and concentration for the past 10 years (resulting in a 35 µg/L concentration in the saturated zone beneath the source).
- Case 1-4 : To include the possible upgradient contaminant source, the concentration of the upgradient groundwater was set at 5 µg/L.
- Case 2-1 : The half life of chemical X in the contaminant (biodegradation or other chemical reactions), was set at 5 years.
- Case 2-2 : To reduce the effect of adsorption, the fractional organic carbon content of the saturated and unsaturated zones were set at 0.0001 (20 times lower than the baseline condition).

- Case 3-1 : The saturated thickness available for contaminant migration was set at 17.5 feet (the top half of the saturated zone).
- Case 3-2 : The longitudinal and lateral dispersivity were set at 0.001 and 0.0003, respectively.
- Case 3-3 : Dilution by surface infiltration in the downgradient area was simulated by adjusting the decay rate in the transport simulation.
- Case 3-4 : The upgradient groundwater flow was set at 0.
- Case 4-1 : The point of exposure was moved to the property line.
- Case 4-2 : Assuming local groundwater was not a drinking water source, allowable soil concentration based on human exposure during construction and maintenance activities (dermal contact and inhalation of dust) was used as the cleanup criterion directly.
- Case 4-3 : Surface water in the stream (which was assumed to have a dilution factor of 50) was used as the exposure media (i.e., source of drinking water).
- Case 5-1 : Lifetime (70 years) averaged contaminant concentrations at the point of exposure were compared to the water quality criteria.
- Case 5-2 : Water criteria based on bioaccumulation of the contaminant and human consumption of fish from the stream was used as acceptable surface water concentration.
- Case 5-3 : A drinking water well is to be installed 150 feet from the property line.
- Case 6-1 : A hydraulic containment (pumping) system was designed to intercept the downgradient migration of contaminated groundwater for 10 years.
- Case 6-2 : A surface cap on the source area was designed to reduce the surface infiltration rate to 0.01 feet/year.
- Case 6-3 : It was assumed that the remedial action will take 1.5 years thus allowing the contaminant to be released from the source during the cleanup.

Cleanup goal/ACL simulations for scenarios with more than one variable controlling factor were also determined. Results and assumptions for four illustrative examples are shown in Table III. The first three cases show that the soil cleanup goal based on surface water exposures can exceed the soil exposure criteria (230 mg/kg based on dermal contact and inhalation) under certain conditions. The last case shows that under very conservative scenario the cleanup goal can be lower than a typical detection limit for a volatile organic chemical. Soil cleanup goals for this hypothetical site ranged from the detection limit (approximately 0.01 mg/kg) to as high as 3,450 mg/kg (see Table III).

CONCLUSIONS

The hypothetical chemical used in the simulations is considered typical of the moderately water-soluble volatile organic chemicals typically found in soils and groundwater at active industrial facilities or abandoned hazardous waste sites. The results of the sensitivity analysis demonstrate that variations in all of the important input parameters and exposure assessment assumption may have a significant impact on cleanup goals for such chemicals.

As shown in Table II, variations in aquifer physical properties, temporal source characteristics, and adsorption potential have a substantial impact of the final soil (and

TABLE III - SOIL CLEANUP GOALS FOR ILLUSTRATIVE CASES WITH MULTIPLE CONTROLLING FACTORS CHANGED

CASE	SAME ASSUMPTION AS IN CASE	DEVIATIONS FROM THE BASELINE SCENARIO	SOIL CLEANUP GOAL (ug/kg)	% CHANGE
BASELINE		NONE	126	0
A	2-1 3-3 5-1 5-2	WITH DECAY WITH DOWNGRADIENT RECHARGE LIFE-TIME AVERAGE FISH CONSUMPTION	456753	362,402
B	2-1 3-3 5-1 5-2 6-1 (4 YEARS)	WITH DECAY WITH DOWNGRADIENT RECHARGE LIFE-TIME AVERAGE FISH CONSUMPTION PUMP AND TREAT FOR 4 YEARS	886737	703,660
C	2-1 3-3 5-1 5-2 6-1	WITH DECAY WITH DOWNGRADIENT RECHARGE LIFE-TIME AVERAGE FISH CONSUMPTION PUMP AND TREAT FOR 10 YEARS	3452234	2,739,768
D	2-2 3-1 3-2 4-1	NO ADSORPTION LIMITED MIXING DEPTH NO DISPERSION PROPERTY LINE AS POE	.46	-100

groundwater) cleanup goals. However, three of the factors to which the simulation is most sensitive are those which are established as a result of the conceptual approach to the problem and chemical specific information.

For example, consideration of a receiving surface water body (rather than a drinking water well) as the point of exposure resulted in a 4,900 percent increase in the allowable soil cleanup goal as a result of attendant dilution. Future land and water use and aquifer classification should be carefully considered by modelers/risk assessors if an ACL demonstration/soil cleanup goal development process is to be based on such an approach.

Although the hypothetical chemical used for the sensitivity analysis is not particularly bioaccumulative, this is typical for water soluble volatile organic chemicals. Development of a soil cleanup goal based on fish consumption (rather than water ingestion) resulted in a 1,900 percent increase in the allowable cleanup goal. Fish consumption may be the primary realistic exposure route under conditions where neither surface water nor groundwater are used as a potable water source. Cleanup goals based on this route will typically greatly exceed those based on surface water or groundwater ingestion. Game and commercial fishing activities and regional consumption patterns should be carefully considered under such a scenario. Furthermore, some consideration of potential adverse effects on aquatic organisms is also generally warranted.

Inclusion of a containment measure (capping) also resulted in a substantial increase in the allowable soil cleanup goal as a result of the decrease in source loading. Inclusion of such a component in the conceptual model should be based on the feasibility of such containment, a cost evaluation, and future land use constraints. Encapsulation is

essentially closure in place and some institutional controls on future disturbances (e.g., deed recordations) could be necessary. Furthermore, the long term maintenance and monitoring costs associated with the cap should be considered.

Finally, inclusion of a first order decay mechanism resulted in a 1,500 percent increase in the allowable soil cleanup goal. For the most part, decay mechanisms and rates are not well documented and conservative (worst-case) values should be used, if at all, during the cleanup goal development process. Under certain circumstances, it may be appropriate to perform laboratory decay rate studies (e.g., using radiolabeled isotopes) to verify the significance of chemical attenuation mechanisms.

The specific values of the cleanup goals and the increases or decreases between the different scenarios considered in this study are not representative of all sites. However, the wide range (six orders of magnitude) of soil cleanup goals developed for the hypothetical site is typical and indicates that an important component of the cleanup goal development process is selection of appropriate values for each group of controlling factors. All assumptions should be clearly defined and documented to the greatest extent possible to allow for acceptance by the regulatory agency.

REFERENCES

Chiou, J. D. and R. J. Hubbard, 1992, "Development and Application of a Spreadsheet-Based Multimedia Contaminant Fate and Transport Model," in Proceedings of Solving Ground Water Problems with Models, Dallas, Texas, pp. 623-637.

Domenico, P.A., 1987, "An Analytical Model for Multidimensional Transport of a Decaying Contaminant Species," J. Hydrol., Vol. 91, pp. 49-58.