✿EPA

BIOPLUME III

Natural Attenuation Decision Support System

User's Manual
Version 1.0

The Plume of
Contaminated
Ground Water

The Source of
Contamination

Groundwater Flow ➡

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by

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NOTICE

BIOPLUME III and the field data were developed through a collaboration between the U.S. EPA (Subsurface Protection and Remediation Division, National Risk Management Research Laboratory, Robert S. Kerr Environmental Research Center, Ada, Oklahoma (RSKERC) and the U.S. Air Force (U.S. Air Force Center for Environmental Excellence, Brooks Air Force Base, Texas). EPA staff contributed conceptual guidance in the development of the BIOPLUME III mathematical model, and contributed field data generated by EPA staff supported by ManTech Environmental Research Services, Corp., the in-house analytical support contractor at the RSKERC. the computer code for BIOPLUME III was developed by Groundwater Services, Inc. through a contract with the U.S. Air Force. The graphical user interface (GUI) was developed by Deerinwater Environmental Management Services, Inc. through a subcontract to ZEi Engineering Inc. Development of the GUI was supported through a contract with the U.S. Air Force.

All data generated by EPA staff or by ManTech Environmental Research Services Corp. were collected following procedures described in the field sampling Quality Assurance Plan for an in-house research project on natural attenuation, and the analytical Quality Assurance Plan for ManTech Environmental Research Services Corp.

BIOPLUME III and the User's Manual have been subjected to the Agency's peer and administrative review and have been approved for publication as an EPA document. However, BIOPLUME III is made available on an *as-is* basis without guarantee or warranty of any kind, express of implied. Neither the United States Government (U.S. EPA or U.S. Air Force), Groundwater Services Inc., Deerinwater Environmental Management Services Inc., or ZEi Engineering Inc., nor any of the authors or reviewers accept any liability resulting from the use of BIOPLUME III and interpretation of the predictions of the model are the sole responsibility of the user. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

FOREWORD

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water; and prevention and control of indoor air pollution. The goal of this research effort is to catalyze development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

An extensive investment in site characterization and mathematical modeling is often necessary to establish the contribution of natural attenuation at a particular site. This document contains a mathematical model (BIOPLUME III) intended to describe natural attenuation of organic contaminants dissolved in ground water. The User's Manual provides instruction on the use of BIOPLUME III, and contains field data from representative sites to illustrate its appropriate application. This screening tool will allow ground water remediation managers to identify sites where natural attenuation is most likely to be protective of human health and the environment. It will also allow regulators to carry out an independent assessment of treatability studies and remedial investigations that propose the use of natural attenuation.

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iii

ACKNOWLEDGMENTS

TABLE OF CONTENTS

APPENDICES

LIST OF TABLES

LIST OF FIGURES

1.0   INTRODUCTION

The BIOPLUME III program is a two-dimensional, finite difference model for simulating the natural attenuation of organic contaminants in ground water due to the processes of advection, dispersion, sorption, and biodegradation. The model simulates the biodegradation of organic contaminants using a number of aerobic and anaerobic electron acceptors: oxygen, nitrate, iron (III), sulfate, and carbon dioxide.

Over the past several years, the high cost and poor performance of many pump and treat remediation systems have led many researchers to consider natural attenuation as an alternative technology for ground water remediation (Newell et al., 1996). Researchers associated with the U.S. EPA's National Risk Management Research Laboratory in Ada, Oklahoma, have suggested that anaerobic pathways could be significant, or even the dominant degradation mechanism at many petroleum fuel sites (Wilson, 1994). As a result, The Air Force Center for Environmental Excellence (AFCEE), Technology Transfer Division, launched a three-point technology development effort in 1993, consisting of the following elements:

1) Field data collected at over 30 sites around the country (Wiedemeier et al., 1995a) analyzing aerobic and anaerobic processes;

2) A technical Protocol, outlining the approach, data collection techniques, and data analysis methods required for conducting an Air Force Intrinsic Remediation Study (Wiedemeier et al., 1995b); and

3) Two intrinsic remediation modeling tools: the BIOSCREEN model developed by   Dr. Charles J. Newell of Groundwater Services, Inc. (GSI), and the BIOPLUME III model developed by Dr. Hanadi Rifai at Rice University.

In addition, the Air Force also oversaw development of a modified version of a sophisticated ground water modeling platform known as Environmental Information System (EIS) developed by Dr. Stergios Dendrou and Dr. Basil Dendrou of ZEi/MicroEngineering, Inc., of Annandale, Virginia.

This Windows"-based graphical platform model has been integrated with BIOPLUME III. The integration effort of the platform and the BIOPLUME III model was managed by the prime contractors, GSI and Deerinwater Environmental Management (DEM), and their subcontractors, Rice University and ZEi/MicroEngineering, respectively. The "team" was formed after review of the EIS system by AFCEE and EPA researchers who determined the inherent benefits of each modeling system would result in a more advanced and user-friendly natural attenuation model. Such a model was identified as a key requirement for broadening the use and acceptance of natural attenuation during the 1994 EPA/Air Force Natural Attenuation Symposium in Denver, Colorado.

Collectively, these software tools, the technical protocol, and the knowledge gained from numerous natural attenuation studies by the Air Force Center for Environmental Excellence and

the EPA's Risk Reduction Laboratory will provide users with the necessary assets to perform a complete natural attenuation study.

1.1   BIOPLUME III - An Extension of BIOPLUME I and II

BIOPLUME III is a two-dimensional, finite difference model for simulating the biodegradation of hydrocarbons in ground water. The model simulates both aerobic and anaerobic biodegradation processes in addition to advection, dispersion, sorption and ion exchange. BIOPLUME III is based on the U. S. Geologic Survey (USGS) Method of Characteristics Model dated July 1989 (Konikow and Bredehoeft, 1989; see Appendix A).

The BIOPLUME III code was developed primarily to model the natural attenuation of organic contaminants in ground water due to the processes of advection, dispersion, sorption and biodegradation. BIOPLUME III simulates the biodegradation of organic contaminants using a number of aerobic and anaerobic electron acceptors: oxygen, nitrate, iron (III), sulfate, and carbon dioxide. The model solves the transport equation six times to determine the fate and transport of the hydrocarbons and the electron acceptors/reaction by-products. For the case where iron (III) is used as an electron acceptor, the model simulates the production and transport of iron (II) or ferrous iron.

Three different kinetic expressions can be used to simulate the aerobic and anaerobic biodegradation reactions. These include: first-order decay, instantaneous reaction and Monod kinetics. The principle of superposition is used to combine the hydrocarbon plume with the electron acceptor plume(s).

Borden and Bedient (1986) developed the BIOPLUME I model based on their work at the United Creosoting Company, Inc. Superfund site in Conroe, Texas. BIOPLUME I is based on the assumption that aerobic biodegradation of hydrocarbons is often limited by the availability of dissolved oxygen in ground water aquifers. Borden and Bedient (1986) simulated the aerobic biodegradation of hydrocarbons as an instantaneous reaction between the hydrocarbon and oxygen.

Rifai et al. (1988) developed the BIOPLUME II model by incorporating the concepts developed by Borden and Bedient (1986) into the USGS two-dimensional solute transport model (Konikow and Bredehoeft, 1978).   The BIOPLUME II model tracks two plumes: oxygen and the hydrocarbon. The two plumes are superimposed to determine the resulting concentrations of oxygen and hydrocarbon at each time step. Anaerobic biodegradation in BIOPLUME II was simulated as a first-order decay in hydrocarbon concentrations.

Other major differences between BIOPLUME II and BIOPLUME III include:

- BIOPLUME III runs in a Windows95 environment whereas BIOPLUME II was mainly developed in a DOS environment.

- BIOPLUME III has been integrated with a modified version of a sophisticated ground water modeling platform known as EIS developed by ZEi/MicroEngineering, Inc.

1.2 Graphical User Interface

Intrinsic Remediation studies are data intensive and require the applicant to make the case that natural attenuation is occurring at a site and that it will persist over time. To help the environmental professional with the data management, visualization, and decision-making tasks involved, the Air Force adopted the EIS Graphical User Interface Platform. EIS (*Environmental Information System*) is the latest integrated software platform under Windows 95 in which to register, sort, and evaluate the site-specific data of the physical processes influencing the ground water migration of organic contaminants.

EIS is developed around the following integrating technologies:

∑ Object-based simulation environment

∑ Control tools for the creation of a spatial and temporal data base (4 dimensions)

∑ A patented Macroengineering framework for managing different algorithmic solutions

∑ Graphics that are embedded in a kriging scheme automatically adjusting to the required spatial resolution

∑ Open software architecture allowing a cost-efficient customization (other algorithmic solutions, link to other GIS systems) and expansion of the platform (support of different peripheral and field monitoring devices)

∑ Integration and quantification of the simulation and data processing error to the risk of health hazard

For these reasons, the EIS platform is at the forefront of the arsenal of tools that AFCEE is making available to the engineering community in support of natural attenuation (intrinsic remediation) studies.

1.3 What is in this Manual?

This user's guide is a stand-alone document for the BIOPLUME III model and the Graphical User Interface Platform. Following this brief introduction, Section 2.0 provides instructions for installing the software and getting started. Section 3.0 is a step-by-step tutorial that demonstrates the main features of the platform. Section 4.0 is devoted to a detailed discussion on the theoretical development of the BIOPLUME III model and Section 5.0 is a thorough user's guide for the Graphical User Interface Platform.

1.4   Fundamentals of Intrinsic Remediation[1]

Naturally occurring biological processes can significantly enhance the rate of organic mass removal from contaminated aquifers. Biodegradation research performed by Rice University, government agencies, and other research groups has identified several main themes that are crucial for future studies of natural attenuation:

> 1.   *The relative importance of groundwater transport vs. microbial kinetics is a key consideration for developing workable biodegradation expressions in models. Results from the United Creosote site (Texas) and the Traverse City Fuel Spill site (Michigan) indicate that biodegradation is better represented as a macro-scale wastewater treatment-type process than as a micro-scale study of microbial reactions.*

> 2.   *The distribution and availability of electron acceptors control the rate of in-situ biodegradation for most petroleum release site plumes. Other factors (e.g., population of microbes, pH, temperature, etc.) rarely limit the amount of biodegradation occurring at these sites.*

As mentioned previously, Borden and Bedient (1986) developed the BIOPLUME model, which simulates aerobic biodegradation as an "instantaneous" microbial reaction that is limited by the amount of electron acceptor, oxygen, that is available. In other words, the microbial reaction is assumed to occur at a much faster rate than the time required for the aquifer to replenish the amount of oxygen in the plume. Although the time required for the biomass to aerobically degrade the dissolved hydrocarbons is on the order of days, the overall time to flush a plume with fresh groundwater is on the order of years or tens of years.

Rifai et al. (1988) extended this approach and developed the BIOPLUME II model, which simulates the transport of two plumes: an oxygen plume and a contaminant plume. The two plumes are allowed to react, and the ratio of oxygen to contaminant consumed by the reaction is determined from an appropriate stoichiometric model. The BIOPLUME II model is documented with a detailed user's manual (Rifai et al., 1987) and is currently being used by EPA regional offices, U.S. Air Force facilities, and by consulting firms. Borden et al. (1986) applied the BIOPLUME concepts to the Conroe Superfund site; Rifai et al. (1988) applied the BIOPLUME II model to a jet fuel spill at a Coast Guard facility in Michigan. Many other studies using the BIOPLUME II model have been presented in recent literature.

The BIOPLUME II model has increased the understanding of biodegradation and natural attenuation by simulating the effects of adsorption, dispersion, and aerobic biodegradation processes in one model. It incorporates a simplified mechanism (first-order decay) for handling other degradation processes, but does not address specific anaerobic decay reactions. Early conceptual models of natural attenuation were based on the assumption that the anaerobic

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[1] Some of the information presented in this section is taken with permission from the BIOSCREEN Manual developed by Groundwater Services, Inc. for the Air Force Center for Environmental Excellence (Newell et al., 1996).

degradation pathways were too slow to have any meaningful effect on the overall natural attenuation rate at most sites. Accordingly, most field programs focused only on the distribution of oxygen and contaminants, and did not measure the indicators of anaerobic activity such as depletion of anaerobic electron acceptors or accumulation of anaerobic metabolic by-products.

1.4.1   Aerobic and Anaerobic Electron Acceptors

Naturally occurring biological processes can significantly enhance the rate of organic mass removal from contaminated ground water aquifers. Biologically mediated degradation reactions are oxidation/reduction (redox) reactions, involving the transfer of electrons from the organic contaminant compound to an electron acceptor. Oxygen is the electron acceptor for aerobic metabolism whereas nitrate, ferric iron, sulfate and carbon dioxide serve as electron acceptors for alternative anaerobic pathways. Tables 1.1 through 1.3 list the redox reactions for benzene, toluene, ethyl benzene, and xylene (BTEX).

In the presence of organic substrate and dissolved oxygen, microorganisms capable of aerobic metabolism will predominate over anaerobic forms. However, dissolved oxygen is rapidly consumed in the interior of contaminant plumes, converting these areas into anoxic (low oxygen) zones. Under these conditions, anaerobic bacteria begin to utilize other electron acceptors to metabolize dissolved hydrocarbons. The principle factors influencing the utilization of the various electron acceptors include: 1) the relative biochemical energy provided by the reaction; 2) the availability of individual or specific electron acceptors at a particular site; and 3) the kinetics (rate) of the microbial reaction associated with the different electron acceptors.

The transfer of electrons during the redox reaction releases energy which is utilized for cell maintenance and growth. The biochemical energy associated with alternative degradation pathways can be represented by the redox potential of the alternative electron acceptors: the more positive the redox potential, the more energetically favorable is the reaction utilizing that electron acceptor. With everything else being equal, organisms with more efficient modes of metabolism grow faster and therefore dominate over less efficient forms.

Electron Acceptor	Type of Reaction	Metabolic By-Product	Redox Potential (pH = 7, in volts)	Reaction Preference
Oxygen	Aerobic	CO_2	+ 820	*Most Preferred*
Nitrate	Anaerobic	N_2, CO_2	+ 740	fl
Ferric Iron (solid)	Anaerobic	Ferrous Iron (dissolved)3	- 50	fl
Sulfate	Anaerobic	H_2S	- 220	fl
Carbon Dioxide	Anaerobic	Methane	- 240	*Least Preferred*

Based solely on thermodynamic considerations, the most energetically preferred reaction should proceed in the plume until all of the required electron acceptor is depleted. At that point, the next most-preferred reaction should begin and continue until that electron acceptor is gone,

Table 1.1. Redox Reactions for Benzene

Oxidation	$C_6H_6 + 12H_2O$	$\rightarrow$	$6CO_2 + 30H^+ + 30e^-$	
Reduction	$7.5O_2 + 30H^+ + 30e^-$	$\rightarrow$	$15H_2O$	Oxygen
	$6NO3^- + 36H^+ + 30e^-$	$\rightarrow$	$3N_2 + 18H_2O$	Nitrate
	$15Mn^{4+} + 30e^-$	$\rightarrow$	$15Mn^{2+}$	Manganese
	$30Fe^{3+} + 30e^-$	$\rightarrow$	$30Fe^{2+}$	Iron
	$3.75SO_4^2 + 37.5H^+ + 30e^-$	$\rightarrow$	$3.75H_2S + 15H_2O$	Sulfate
	$3.75CO_2 + 30H^+ + 30e^-$	$\rightarrow$	$3.75CH_4 + 7.5H_2O$	Methanog.
Overall	$C_6H_6 + 7.5O_2$	$\rightarrow$	$6CO_2 + 3H_2O$	Oxygen
	$C_6H_6 + 6H^+ + 6NO_3^-$	$\rightarrow$	$6CO_2 + 3N_2 + 6H_2O$	Nitrate
	$C_6H_6 + 15Mn^{4+} + 12H_2O$	$\rightarrow$	$6CO_2 + 30H^+ + 15Mn^{2+}$	Manganese
	$C_6H_6 + 30Fe^{3+} + 12H_2O$	$\rightarrow$	$6CO_2 + 30H^+ + 30Fe^{2+}$	Iron
	$C_6H_6 + 3.75SO_4^{2-} + 7.5H^+$	$\rightarrow$	$6CO_2 + 3.75H_2S + 3H_2O$	Sulfate
	$C_6H_6 + 4.5H_2O$	$\rightarrow$	$2.25CO_2 + 3.75CH_4$	Methanog.

Table 1.2. Redox Reactions for Toluene

Oxidation	$C_7H_8 + 14H_2O$	$\rightarrow$	$6CO_2 + 36H^+ + 36e^-$	

Reduction	$9O_2 + 36H^+ + 36e^-$	$\rightarrow$	$18H_2O$	Oxygen
	$7.2NO3^- + 43.2H^+ + 36e^-$	$\rightarrow$	$3.6N_2 + 21.6H_2O$	Nitrate
	$18Mn^{4+} + 36e^-$	$\rightarrow$	$18Mn^{2+}$	Manganese
	$36Fe^{3+} + 36e^-$	$\rightarrow$	$36Fe^{2+}$	Iron
	$4.5SO_4^2 + 45H^+ + 36e^-$	$\rightarrow$	$4.5H_2S + 18H_2O$	Sulfate
	$4.5CO_2 + 36H^+ + 36e^-$	$\rightarrow$	$4.5CH_4 + 9H_2O$	Methanog.

Overall	$C_7H_8 + 9O_2$	$\rightarrow$	$7CO_2 + 4H_2O$	Oxygen
	$C_7H_8 + 7.2H^+ + 7.2NO_3^-$	$\rightarrow$	$7CO_2 + 3.6N_2 + 7.6H_2O$	Nitrate
	$C_7H_8 + 18Mn^{4+} + 14H_2O$	$\rightarrow$	$7CO_2 + 36H^+ + 18Mn^{2+}$	Manganese
	$C_7H_8 + 36Fe^{3+} + 14H_2O$	$\rightarrow$	$7CO_2 + 36H^+ + 36Fe^{2+}$	Iron
	$C_7H_8 + 4.5SO_4^{2-} + 9H^+$	$\rightarrow$	$7CO_2 + 4.5H_2S + 4H_2O$	Sulfate
	$C_7H_8 + 5H_2O$	$\rightarrow$	$2.5 CO_2 + 4.5CH_4$	Methanog.

Table 1.3. Redox Reactions for Ethylbenzene and Xylene

Oxidation	$C_8H_{10} + 16H_2O$	$\rightarrow$	$8CO_2 + 42H^+ + 42e^-$	
Reduction	$10.5O_2 + 42H^+ + 42e^-$	$\rightarrow$	$21H_2O$	Oxygen
	$8.4NO3^- + 50.4H^+ + 42e^-$	$\rightarrow$	$4.2N_2 + 25.2H_2O$	Nitrate
	$21Mn^{4+} + 42e^-$	$\rightarrow$	$21Mn^{2+}$	Manganese
	$42Fe^{3+} + 42e^-$	$\rightarrow$	$42Fe^{2+}$	Iron
	$5.25SO_4^2 + 52.5H^+ + 42e^-$	$\rightarrow$	$5.25H_2S + 21H_2O$	Sulfate
	$5.25CO_2 + 42H^+ + 42e^-$	$\rightarrow$	$5.25CH_4 + 10.5H_2O$	Methanog.
Overall	$C_8H_{10} + 10.5O_2$	$\rightarrow$	$8CO_2 + 5H_2O$	Oxygen
	$C_8H_{10} + 8.4H^+ + 8.4NO_3^-$	$\rightarrow$	$8CO_2 + 4.2N_2 + 9.2H_2O$	Nitrate
	$C_8H_{10} + 21Mn^{4+} + 16H_2O$	$\rightarrow$	$8CO_2 + 42H^+ + 21Mn^{2+}$	Manganese
	$C_8H_{10} + 42Fe^{3+} + 16H_2O$	$\rightarrow$	$8CO_2 + 42H^+ + 42Fe^{2+}$	Iron
	$C_8H_{10} + 5.25SO_4^{2-} + 10.5H^+$	$\rightarrow$	$8CO_2 + 5.25H_2S + 5H_2O$	Sulfate
	$C_8H_{10} + 5.5H_2O$	$\rightarrow$	$2.75CO_2 + 5.25CH_4$	Methanog.

leading to a pattern where preferred electron acceptors are consumed one at a time, in sequence. Based on these principles, one would expect to observe monitoring well data with "no-detect" results for the more energetic electron acceptors, such as oxygen and nitrate, in locations where evidence of less energetic reactions is observed (e.g., monitoring well data indicating the presence of ferrous iron).

In practice, however, it is unusual to collect samples from natural attenuation monitoring wells that are completely depleted in one or more electron acceptors. Two processes are probably responsible for this observation:

1. *Alternative biochemical mechanisms having very similar energy potentials (such as aerobic oxidation and nitrate reduction) may occur concurrently when the preferred electron acceptor is reduced in concentration, rather than fully depleted. Facultative aerobes, for example, can shift from aerobic metabolism to nitrate reduction when oxygen is still present but in low concentrations (i.e. 1 mg/L oxygen; Snoeyink and Jenkins, 1980). Similarly, noting the nearly equivalent redox potentials for sulfate and carbon dioxide (-220 volts and -240 volts, respectively) one might expect that sulfate reduction and methanogenic reactions may also occur together.*

2. *Standard monitoring wells, having 5 to 10 foot screened intervals, will mix waters from different vertical zones. If different biodegradation reactions are occurring at different depths, then one would expect to find geochemical evidence of alternative degradation mechanisms occurring in the same well. If the dissolved hydrocarbon plume is thinner than the screened interval of a monitoring well, then the geochemical evidence of electron acceptor depletion or metabolite accumulation will be diluted by mixing with clean water from zones where no degradation is occurring.*

Therefore, most natural attenuation field sampling programs yield data that indicate a general pattern of electron acceptor depletion, but not complete depletion, and an overlapping of electron acceptor/metabolite isopleths into zones not predicted by thermodynamic principles. For example, a zone of methane accumulation may be larger than the apparent anoxic zone. Nevertheless, these general patterns of geochemical changes within the plume area provide strong evidence that multiple mechanisms of biodegradation are occurring at many sites.

The data collected by Weidemeier et al. (1995a) and Newell et al. (1996) provides interesting observations on intrinsic bioremediation. For example, while the energy of each reaction is based on thermodynamics, the distribution of electron acceptors is dependent on site specific hydrogeochemical processes and can vary significantly between sites as seen in Table 1.4.

At Hill AFB, the sulfate reactions are extremely important because of the large amount of available sulfate for reduction. Note that different sites in close proximity can have quite different electron acceptor concentrations, as shown by the two sites at Elmendorf AFB. For data on more sites, see Table 1.5. Calculated biodegradation capacities at different U.S. Air Force Natural Attenuation research sites have ranged from 7 to 70 mg/L (Table 1.5). The median value for 28 AFCEE sites is 28.5 mg/L.

Table 1.4. Electron Acceptor/By-Product Data From Air Force Sites

Measured Background Electron Acceptor/By-Product Concentration (mg/L)					
Base Facility	Background Oxygen	Background Nitrate	Maximum Ferrous Iron	Background Sulfate	Maximum Methane
POL Site, Hill AFB, Utah*	6.0	36.2	55.6	96.6	2.0
Hangar 10 Site, Elmendorf AFB, Alaska*	0.8	64.7	8.9	25.1	9.0
Site ST-41, Elmendorf AFB,Alaska*	12.7	60.3	40.5	57.0	1.5
Bldg. 735, Grissom AFB, Indiana	9.1	1.0	2.2	59.8	1.0
SWMU 66 Site, Keesler AFB, Mississippi	1.7	0.7	36.2	22.4	7.4
POL B Site, Tyndall AFB, Florida	1.4	0.1	1.3	5.9	4.6

*Data from Wiedemeier et al. (1995a); all other data from Newell et al. (1996)

1.4.2   Kinetics of the Biodegradation Reactions

Aerobic biodegradation can be simulated as an "instantaneous" reaction that is limited by the amount of electron acceptor (oxygen) that is available. The microbial reaction is assumed to occur at a much faster rate than the time required for the aquifer to replenish the amount of oxygen in the plume. Although the time required for the biomass to aerobically degrade the dissolved hydrocarbons is on the order of days, the overall rate that groundwater is replenished in most plumes is on the order of years or tens of years.

For example, microcosm data presented by Davis et al. (1994) show that microbes that have an excess of electron acceptors can degrade concentrations of dissolved benzene (~1 mg/L) very rapidly. In the presence of a surplus of oxygen, aerobic bacteria can degrade dissolved benzene in about 8 days, which can be considered "instantaneous" compared to years required for flowing ground water to replenish the plume area with oxygen.

Recent results from the Air Force Natural Attenuation Initiative indicate that the anaerobic reactions, which were originally thought to be too slow to be of significance in ground water, can also be simulated as instantaneous reactions (Newell et al., 1995). For example, Davis et al. (1994) also ran microcosms with sulfate reducers and methanogens that indicated that benzene could be degraded within a couple of weeks time frame (after acclimation). When compared to the time required to replenish electron acceptors, the anaerobic reactions can also be considered to be instantaneous at many sites.

This conclusion is supported by observing the pattern of anaerobic electron acceptors and by-products along the plume at natural attenuation research sites:

Table 1.5. Biodegradation Capacity/Expressed Assimilative Capacity at AFCEE Intrinsic Remediation Sites
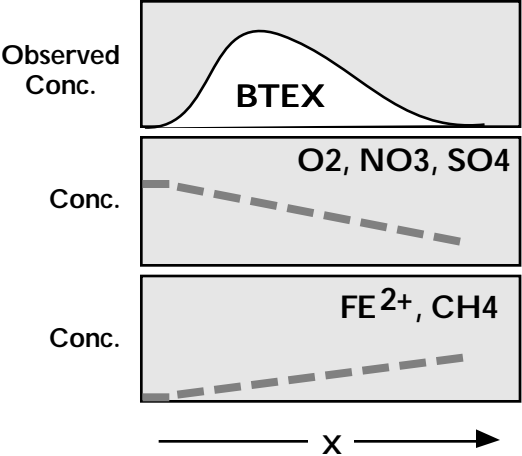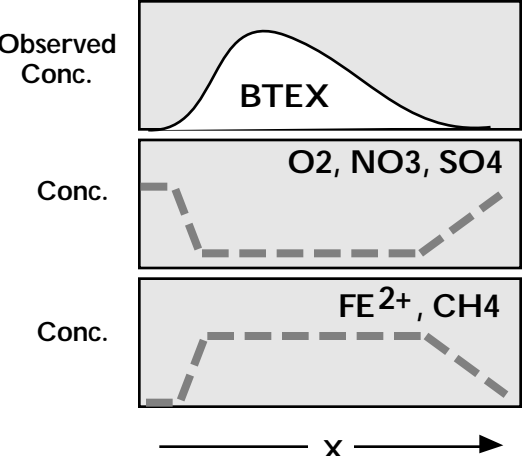
Site Number	Base	State	Site Name	Maximum Total BTEX Concentration (mg/L)	Observed Change in Concentration (mg/L)					Biodegradation Capacity/Expressed Assimilative Capacity (mg/L)					Total Biodegradation Capacity (mg/L)	Type of Data/ Source of Data
					O2	Nitrate	Iron	Sulfate	Methane	Aerobic Respiration	Denitrification	Iron Reduction	Sulfate Reduction	Methanogenesis		
1	Hill AFB	Utah		21.5	6.0	36.2	55.6	96.6	2.0	1.9	7.4	2.6	21.0	2.6	35.4	EAC/PES
2	Battle Creek ANGB	Michigan		3.6	5.7	5.6	12.0	12.9	8.4	1.8	1.1	0.6	2.8	10.8	17.1	EAC/PES
3	Madison ANGB	Wisconsin		28.0	7.2	45.3	15.3	24.2	11.7	2.3	9.2	0.7	5.3	15.0	32.5	EAC/PES
4	Elmendorf AFB	Alaska	Hangar 10	22.2	0.8	64.7	8.9	25.1	9.0	0.3	13.2	0.4	5.5	11.6	30.9	EAC/PES
5	Elmendorf AFB	Alaska	ST-41	30.6	12.7	60.3	40.5	57.0	1.5	4.0	12.3	1.9	12.4	1.9	32.5	EAC/PES
6	King Salmon AFB	Alaska	FT-001	10.1	9.0	12.5	2.5	6.8	0.2	2.9	2.6	0.1	1.5	0.2	7.2	EAC/PES
7	King Salmon AFB	Alaska	Naknek	5.3	11.7	0	44.0	0	5.6	3.7	0	2.0	0	7.2	12.9	EAC/PES
8	Plattsburgh AFB	New York		6.0	10.0	3.7	10.7	18.9	0.3	3.2	0.7	0.5	4.1	0.4	8.9	EAC/PES
9	Eglin AFB	Florida		3.7	1.2	0	8.9	4.9	11.8	0.4	0	0.4	1.1	15.2	17.0	EAC/PES
10	Patrick AFB	Florida		7.3	3.8	0	2.0	0	13.6	1.2	0	0.1	0	17.4	18.7	EAC/PES
11	MacDill AFB	Florida	Site 56	29.6	2.4	5.6	5.0	101.2	13.6	0.8	1.1	0.2	22.0	17.4	41.5	EAC/PES
12	MacDill AFB	Florida	Site 57	0.7	2.1	0.5	20.9	62.4	15.4	0.7	0.1	1.0	13.6	19.7	35.0	EAC/PES
13	MacDill AFB	Florida	Site OT-24	2.8	1.3	0	13.1	3.7	9.8	0.4	0	0.6	0.8	12.6	14.4	EAC/PES
14	Offutt AFB	Nebraska	FPT-A3	3.2	0.6	0	19.0	32.0	22.4	0.2	0	0.9	7.0	28.8	36.8	EAC/PES
15	Offutt AFB	Nebraska		103.0	8.4	69.7	0	82.9	0	2.7	14.2	0	18.0	0	34.9	EAC/PES
16	Westover AFRES	Massachusetts	FT-03	1.7	10.0	8.6	599.5	33.5	0.2	3.2	1.8	27.5	7.3	0.2	40.0	EAC/PES
17	Westover AFRES	Massachusetts	FT-08	32.6	9.9	17.2	279.0	11.7	4.3	3.1	3.5	12.8	2.6	5.5	27.5	EAC/PES
18	Myrtle Beach	South Carolina		18.3	0.4	0	34.9	20.7	17.2	0.1	0	1.6	4.5	22.0	28.2	EAC/PES
19	Langley AFB	Virginia		0.1	6.4	23.5	10.9	81.3	8.0	2.0	4.8	0.5	17.7	10.2	35.3	EAC/PES
20	Griffis AFB	New York		12.8	4.4	52.5	24.7	82.2	7.1	1.4	10.7	1.1	17.9	9.1	40.2	EAC/PES
21	Rickenbacker ANGB	Ohio		1.0	1.5	35.9	17.9	93.2	7.7	0.5	7.3	0.8	20.3	9.8	38.7	EAC/PES
22	Wurtsmith AFB	Michigan	SS-42	3.1	8.5	25.4	19.9	10.6	1.4	2.7	5.2	0.9	2.3	1.8	12.9	EAC/PES
23	Travis AFB	Califonia		-	3.8	15.8	8.5	109.2	0.2	1.2	3.2	0.4	23.7	0.3	28.9	EAC/PES
24	Pope AFB	North Carolina		8.2	7.5	6.9	56.2	9.7	48.4	2.4	1.4	2.6	2.1	62.0	70.5	EAC/PES
25	Seymour Johnson AFB	North Carolina		13.8	18.3	4.3	31.6	38.6	2.7	5.8	0.9	1.5	8.4	3.5	20.0	EAC/PES
26	Grissom AFB	Indiana	Bldg. 735	0.3	9.1	1.0	2.2	59.8	1.0	2.9	0.2	0.1	13.0	1.2	17.4	BC/GSI
27	Tyndall AFB	Florida	POL B	1.0	1.4	0.1	1.3	5.9	4.6	0.5	0	0.1	1.3	5.9	7.7	BC/GSI
28	Keesler AFB	Mississippi	SWMU 66	14.1	1.7	0.7	36.2	22.4	7.4	0.5	0.1	1.7	4.9	9.5	16.7	BC/GSI
			Average	14.2	5.9	17.7	49.3	39.5	8.4	1.9	3.6	2.3	8.6	10.8	27.1	
			Median	7.3	5.8	6.3	16.6	24.6	7.2	1.9	1.3	0.8	5.4	9.3	28.5	
			Maximum	103.0	18.3	69.7	599.5	109.2	48.4	5.8	14.2	27.5	23.7	62.0	70.5	
			Minimum	0.1	0.4	0	0	0	0	0.1	0	0	0	0	7.2	

-　　　= Data not available.
EAC = Expressed Assimilative Capacity;　　　　BC = Biodegradation Capacity
PES = Parsons Engineering Science (Wiedemeier et. al., 1995a); GSI = Groundwater Services, Inc. (Newell et. al., 1996)

If microbial kinetics were limiting the rate of biodegradation:	If microbial kinetics were relatively fast (instantaneous):
• Anaerobic electron acceptors (nitrate and sulfate) would be constantly **decreasing** in concentration as one moved downgradient from the source zone, and	• Anaerobic electron acceptors (nitrate and sulfate) would be mostly or totally **consumed in the source zone,** and
• Anaerobic by-products (ferrous iron and methane) would be constantly **increasing** in concentration as one moved downgradient from the source zone.	• Anaerobic by-products (ferrous iron and methane) would be **found in the highest concentrations in the source zone.**

The second pattern is observed at natural attenuation field sites (see Figure 1.1), supporting the hypothesis that anaerobic reactions can be considered to be relatively instantaneous at most petroleum release sites. The only cases where this might not be true is sites with very low hydraulic residence times (very high groundwater velocities and short source zone lengths).

Biodegradation Capacity. To apply an electron-acceptor limited kinetic model, such as the instantaneous reaction model, the amount of biodegradation that the groundwater that moves through the source zone can support must be calculated. The conceptual model is that:

1. Ground water upgradient of the source contains electron acceptors;

2. As the upgradient ground water moves through the source zone, hydrocarbons in NAPLs and contaminated soil release dissolved hydrocarbons (in the case of petroleum sites, BTEX);

3. The biological reactions continue until the available electron acceptors are consumed (Two exceptions to this conceptual model are the iron reactions, where the electron acceptor ferric iron dissolves from the aquifer matrix; and the methane reactions, where the electron acceptor CO_2 is also produced as an end-product of the reactions. A simplifying assumption can be made that the by-products ferrous iron and methane can be used as
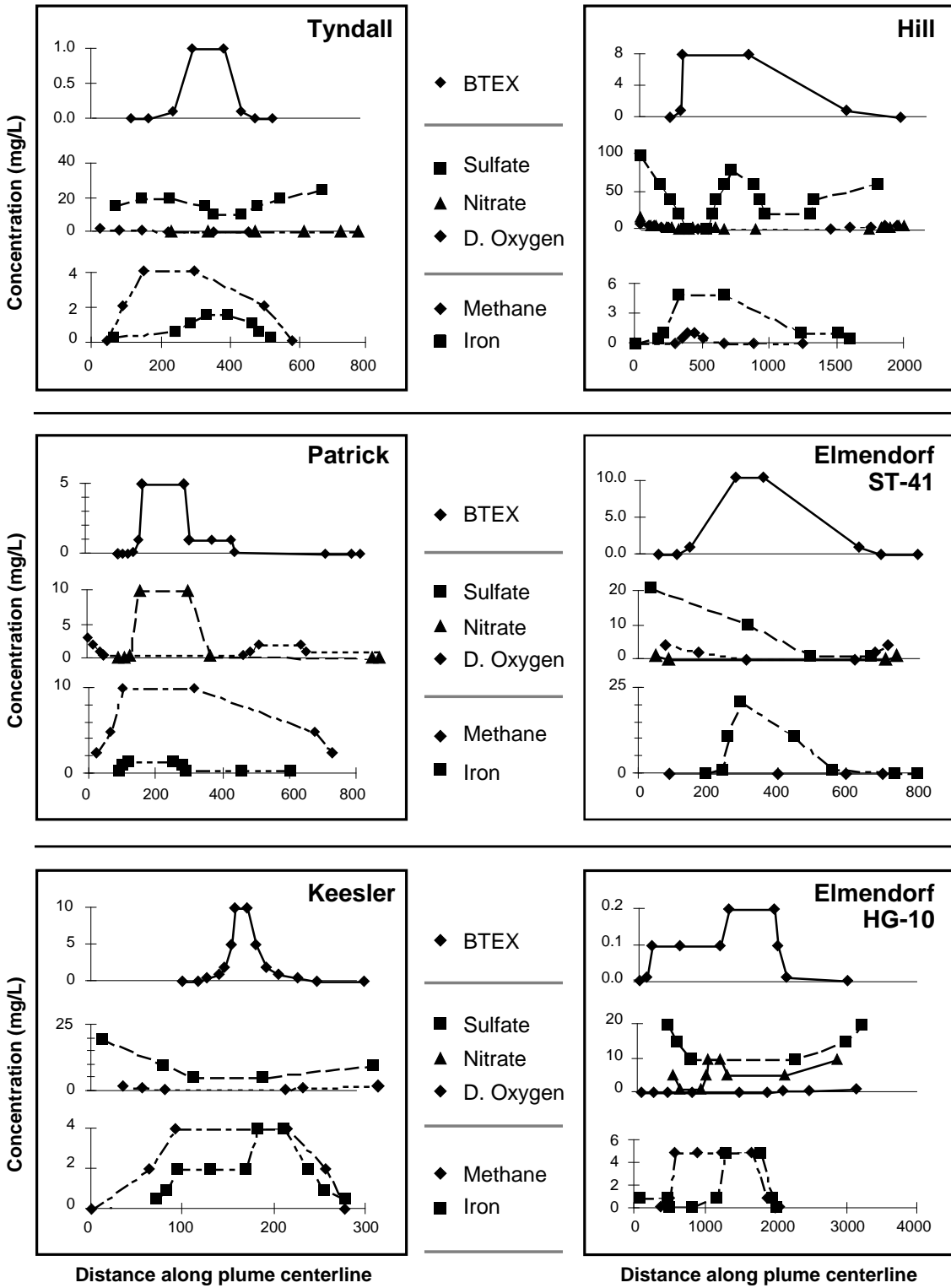
Figure 1.1 Distribution of BTEX, Electron Acceptors, and Metabolic By-Products vs. Distance Along Centerline of Plume.

Sampling Date and Source of Data: Tyndall 3/95, Keesler 4/95, (Newell et al., 1996), Patrick 3/94 (note: one NO₃ outlier removed, sulfate not plotted), Hill 7/93, Elemdorf Site ST41 6/94, Elemdorf Stie HG 10 6/94, (Wiedemeier et al., 1995a).

13

proxies for the potential amount of biodegradation that could occur from the iron-reduction and methanogenesis reactions.);

4. The total amount of available electron acceptors available for biological reactions can be estimated by: a) calculating the difference between the upgradient wells and source zone wells for oxygen, nitrate, and sulfate; and b) measuring the production of by-products ferrous iron and methane in the source zone;

5. Using stoichiometry, a utilization factor can be developed to convert the mass of oxygen, nitrate, and sulfate consumed to the mass of dissolved hydrocarbon that are used in the biodegradation reactions. Similarly, utilization factors can be developed to convert the mass of metabolic by-products that are consumed to the mass of dissolved hydrocarbon that are used in the biodegradation reactions. Tables 1.6 a through c illustrate the method for calculating utilization factors for benzene, toluene, ethyl benzene, and xylene and Table 1.7 lists the overall utilization factors for BTEX;

6. For a given background concentration of an individual electron acceptor, the potential contaminant mass removal or "biodegradation capacity" depends on the "utilization factor" for that electron acceptor. Biodegradation capacity is also referred to as "Expressed Assimilative Capacity" or EAC. Dividing the background concentration of an electron acceptor by its utilization factor provides an estimate (in concentration units) of the assimilative capacity of the aquifer by that mode of biodegradation.

When the available electron acceptor/by-product concentrations (Step 4) are divided by the appropriate utilization factor (Step 5), an estimate of the "biodegradation capacity" of the groundwater flowing through the source zone and plume can be developed.

Table 1.6a. Utilization Factor Calculation for Benzene

Aerobic $\qquad$ $C_6H_6 + 7.5O_2 \qquad \rightarrow \qquad 6CO_2 + 3H_2O$

              1 mole benzene reacts with 7.5 moles oxygen
or $(6 \times 12 + 6)$ gms benzene react with (7.5×32) gms of oxygen
$\rightarrow$ 78 gms benzene react with 240 gms of oxygen

    Utilization Factor $=$ 240/78 $=$ 3.08

Nitrate $\qquad$ $C_6H_6 + 6H^+ + 6NO_3^- \qquad \rightarrow \qquad 6CO_2 + 3N_2 + 6H_2O$

    1 mole benzene reacts with 6 moles nitrate
    Utilization Factor $=$ 372.06/78 $=$ 4.77

Manganese $\qquad$ $C_6H_6 + 15Mn^{4+} + 12H_2O \qquad \rightarrow \qquad 6CO_2 + 30H^+ + 15Mn^{2+}$

    1 mole benzene reacts with 15 moles manganese
    Utilization Factor $=$ 824.1/78 $=$ 10.57

Iron $\qquad$ $C_6H_6 + 30Fe^{3+} + 12H_2O \qquad \rightarrow \qquad 6CO_2 + 30H^+ + 30Fe^{2+}$

    1 mole benzene reacts with 30 moles ferric iron
    Utilization Factor $=$ 1675.5/78 $=$ 21.48

Sulfate $\qquad$ $C_6H_6 + 3.75SO_4^{2-} + 7.5H^+ \qquad \rightarrow \qquad 6CO_2 + 3.75H_2S + 3H_2O$

    1 mole benzene reacts with 3.75 moles sulfate
    Utilization Factor $=$ 360.26/78 $=$ 4.62

Carbon Dioxide $\qquad$ $C_6H_6 + 4.5H_2O \qquad \rightarrow \qquad 2.25CO_2 + 3.75CH_4$

    1 mole benzene reacts with 3.75 moles CO_2 (see Table 1.2)
    Utilization Factor $=$ 165/78 $=$ 2.12

Table 1.6b. Utilization Factor Calculation for Toluene

Aerobic	$C_7H_8 + 9O_2$	$\rightarrow$	$7CO_2 + 4H_2O$

1 mole toluene reacts with 9 moles oxygen
or $(7\times12 + 8)$ gms benzene react with (9×32) gms of oxygen
$\rightarrow$ 92 gms benzene react with 288 gms of oxygen

Utilization Factor   =   288/92   =   3.13

Nitrate	$C_7H_8 + 7.2H^+ + 7.2NO_3^-$	$\rightarrow$	$7CO_2 + 3.6N_2 + 7.6H_2O$

1 mole toluene reacts with 7.2 moles nitrate
Utilization Factor   =   446.5/92   =   4.85

Manganese	$C_7H_8 + 18Mn^{4+} + 14H_2O$	$\rightarrow$	$7CO_2 + 36H^+ + 18Mn^{2+}$

1 mole toluene reacts with 18 moles manganese
Utilization Factor   =   988.9/92   =   10.75

Iron	$C_7H_8 + 36Fe^{3+} + 14H_2O$	$\rightarrow$	$7CO_2 + 36H^+ + 36Fe^{2+}$

1 mole toluene reacts with 36 moles ferric iron
Utilization Factor   =   2011/92   =   21.85

Sulfate	$C_7H_8 + 4.5SO_4^{2-} + 9H^+$	$\rightarrow$	$7CO_2 + 4.5H_2S + 4H_2O$

1 mole toluene reacts with 4.5 moles sulfate
Utilization Factor   =   432.3/92   =   4.70

Carbon Dioxide	$C_7H_8 + 5H_2O$	$\rightarrow$	$2.5CO_2 + 4.5CH_4$

1 mole toluene reacts with 4.5 moles CO_2 (see Table 3.3)
Utilization Factor   =   198/92   =   2.15

Table 1.6c. Utilization Factor Calculation for Ethylbenzene and Xylene

Aerobic $\qquad$ $C_8H_{10} + 10.5O_2 \qquad \rightarrow \qquad 8CO_2 + 5H_2O$

or
$\rightarrow$

1 mole ethylbenzene/xylene reacts with 10. 5 moles oxygen
$(8\times12 + 10)$ gms benzene react with (10.5×32) gms of O_2
106 gms benzene react with 336 gms of oxygen

Utilization Factor $\quad = \quad 336/106 \quad = \quad 3.17$

Nitrate $\qquad C_8H_{10} + 8.4H^+ + 8.4NO_3^- \qquad \rightarrow \qquad 8CO_2 + 4.2N_2 + 9.2H_2O$

1 mole ethylbenzene/xylene reacts with 8.4 moles nitrate
Utilization Factor $\quad = \quad 520.9/106 \quad = \quad 4.91$

Manganese $\qquad C_8H_{10} + 21Mn^{4+} + 16H_2O \qquad \rightarrow \qquad 8CO_2 + 42H^+ + 21Mn^{2+}$

1 mole ethylbenzene /xylene reacts with 21 moles Mn
Utilization Factor $\quad = \quad 1154/106 \quad = \quad 10.89$

Iron $\qquad C_8H_{10} + 42Fe^{3+} + 16H_2O \qquad \rightarrow \qquad 8CO_2 + 42H^+ + 42Fe^{2+}$

1 mole ethylbenzene /xylene reacts with 42 moles ferric iron
Utilization Factor $\quad = \quad 2346/106 \quad = \quad 22.13$

Sulfate $\qquad C_8H_{10} + 5.25SO_4^{2-} + 10.5H^+ \rightarrow \qquad 8CO_2 + 5.25H_2S + 5H_2O$

1 mole ethylbenzene /xylene reacts with 5.25 moles sulfate
Utilization Factor $\quad = \quad 504.4/106 \quad = \quad 4.76$

Carbon Dioxide $\qquad C_8H_{10} + 5.5H_2O \qquad \rightarrow \qquad 2.75CO_2 + 5.25CH_4$

1 mole ethylbenzene /xylene reacts with 5.25 moles CO_2
(see Table 3.4)
Utilization Factor $\quad = \quad 231/106 \quad = \quad 2.18$

Table 1.7. Utilization Factors for BTEX

	B	T	E	X	Average1	Average2
Aerobic	3.08	3.13	3.17	3.17	3.14	3.15
Nitrate	4.77	4.85	4.91	4.91	4.86	4.88
Manganese	10.57	10.75	10.89	10.89	10.78	10.82
Iron	21.48	21.85	22.13	22.13	21.90	22.00
Sulfate	4.62	4.70	4.76	4.76	4.71	4.73
Carbon Dioxide	2.12	2.15	2.18	2.18	2.17	2.17

Notes:

Average1   =   Arithmetic Average

Average2   =   Mass Weighted Average

2.0 GETTING STARTED

2.1 Installing the Graphical User Interface

This section tells you how to install the Graphical User Interface Platform using the automatic "Install" program and what you need to know before you start running the program. To begin with, your computer should be set up and running MS Windows 3.x or MS Windows 95. The BIOPLUME III Graphical User Interface Platform consists of several executables (.EXE), and Dynamic Link Libraries (.DLL). In addition, the software package includes the Bioplume3.EXE file. All Graphical Platform software runs readily on both Windows 3.x and Windows 95. The Bioplume3.exe executable runs on Windows 95. It also runs on Windows 3.x if the Win32s library is installed. The Win32s library is available from Microsoft (can be downloaded from their Web Site). Even so, some network Windows 3.11 versions exhibit problems in running Bioplume3.exe (fatal Windows exception, returning to DOS). Clearly, the preferred medium for running BIOPLUME III is Windows 95.

To proceed with the installation, the user should also know how to use the Basic Windows/DOS commands for creating and changing directories, copying files and disks, and listing directory information.

For more information about these commands consult the documentation provided with your equipment. In this section you can briefly overview the following topics:

- Microsoft Windows Fundamentals (optional for those who want to refresh their memory on the basic commands of MS-Windows),

- What you need to get started,

- How to install the Graphical User Interface Platform for BIOPLUME III,

- Description of the Graphical User Interface Platform Menus,

If you are familiar with the MS-Windows operations, you can go directly to Section 2.1.2 and proceed with the installation of the program.

2.1.1 Microsoft Windows Fundamentals

The BIOPLUME III Graphical User Interface Platform runs under Microsoft Windows-3.x and Windows 95, and makes extensive use of many Microsoft Windows features. This means that you can adjust settings in your system without having to adjust the Platform.

In order to be able to activate all Windows features, you must install Windows separately. For instructions on how to install Windows and run applications see the Microsoft Windows User's Guide.

Before you begin using the Platform you need to be familiar with a few basic Windows features. This will be done concisely with the instructions of this section. Those familiar with Windows can move directly to the next section which provides important information on how to install the software.

At this stage we will focus on the following topics:

- What are the components of a Windows Application,

- How to use the mouse,

- How to use the menus,

- What is a dialog box.

WHAT ARE THE COMPONENTS OF A WINDOWS APPLICATION ?

Many different applications can be accessed from a basic Windows environment. Each open application is displayed in a new window on your screen. Windows applications are made up of several common components. These components, as shown in Figure 2.1 are:

MENU BAR:

Appears beneath the Windows title bar and contains the names of all principal menus used in the "BIOPLUME III" program.

PULL-DOWN MENU:

A list of menu items that is "pulled-down" from the menu bar by clicking on a main menu item. Windows menus are also called pull-down menus.

MAXIMIZE BOX:

A small box with an up-bar icon in the window's upper right corner. Allows the user with a mouse to enlarge a window to its maximum size.

MINIMIZE BOX:

A small box with a down-bar icon in the window's upper right corner. Allows the user with a mouse to shrink a window to an icon.

CLIENT AREA:

The "work area" of the screen over which the application has complete control.

SMARTICONS:

SmartIcons are mouse shortcuts for "BIOPLUME III" features, functions, and commands. "BIOPLUME III" displays a palette of smartIcons on the right-hand-side of the screen in a child window that can be moved around the screen to fit the needs of the user by clicking on the "Select" display area.
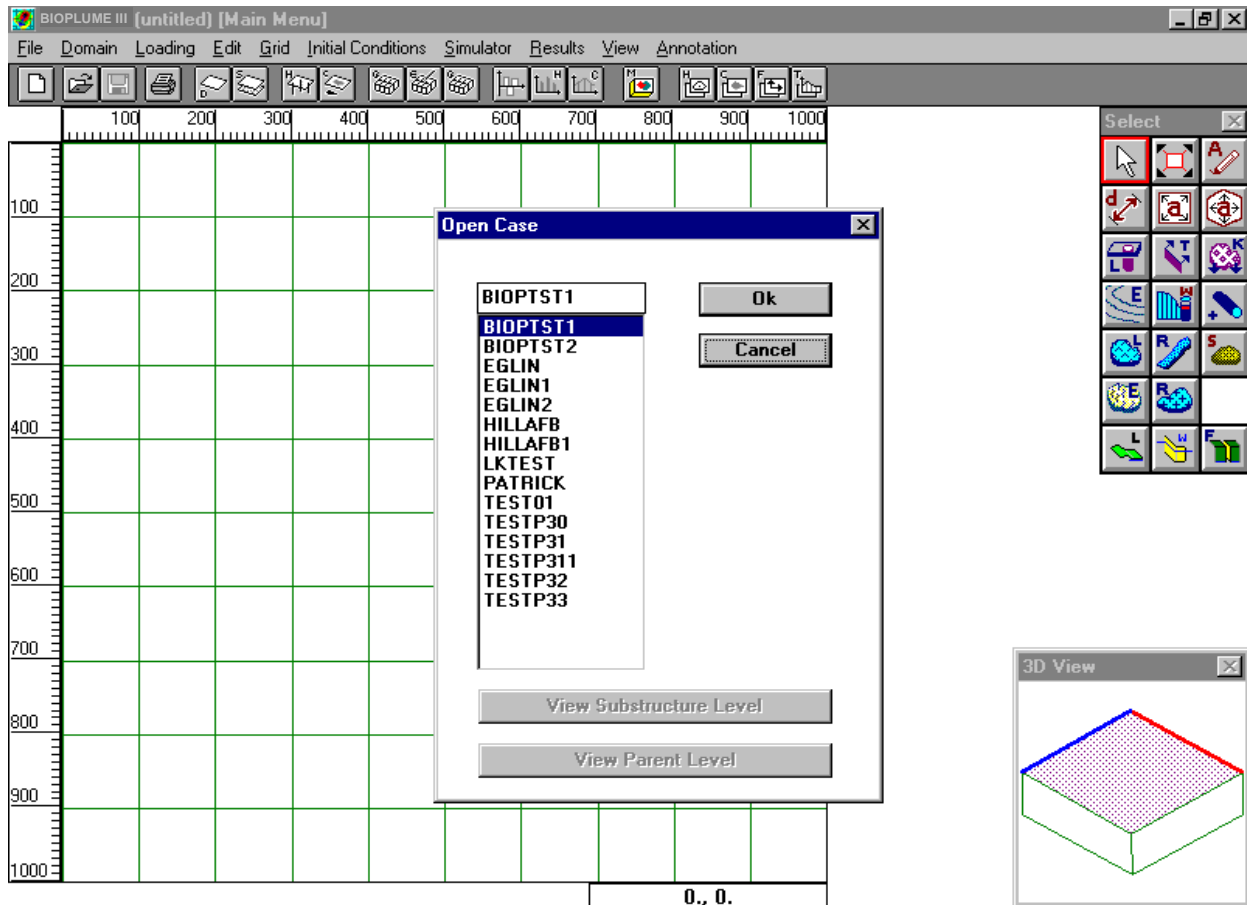
Figure 2.1. Components of an MS-WINDOWS Application.

USING A MOUSE

A mouse is a hand-held pointing device. As you move the mouse across your desk, a pointer moves on the screen. You can pick up the mouse and reposition it without moving the pointer on the screen. All BIOPLUME III Platform actions require the main mouse button. These actions are the following:

POINT: *Move the tip of the mouse pointer on top of an object on the screen.*

CLICK : *To quickly press and release a mouse button.*

CLICK and DRAG: *To press and hold a mouse button while dragging the mouse to highlight an area.*

DOUBLE CLICK*: To quickly press and release a mouse button twice in succession.*

RELEASE: *To quit holding down a mouse button.*

SELECT : *To point on a menu or to highlight text or graphics so they will be affected by the next action you take within the Platform.*

The pointer assumes different shapes to denote different functions as you proceed with different tasks of the Platform.

USING PULL-DOWN MENUS

Menus are lists of commands. When you select a menu in the Graphical Platform it drops down on your screen showing all the items you can activate from that menu.

To select a MENU:

1. Point on the name of the menu you want.

2. Hold down the main mouse button. (The menu drops down on your screen.)

To activate an ITEM :

1. Select the menu that contains the item you want

2. Select the item you want. (The selected item is highlighted.)

When you click the main mouse button, the Platform carries out the action specified by the highlighted item.

WHAT IS A DIALOG BOX ?

In many cases the Platform needs additional information from you before it can carry out a specific command. In that case, the Platform displays a dialog box for you to fill in the information. Once a dialog box appears, you must fill it in before continuing on. Sometimes you will type in text. Other times you will simply select an option within the dialog box. Each dialog box has different kinds of "Controls" that the user can select. They are as follows:

Type of Control	How it Appears on the Screen	What is your Action
Scroll Bar	Two arrows, two white boxes and a white area	Click on the arrows or the gray area, or drag the small white box to move the viewing area.
List Box	A set of items that you can select from.	Drag the pointer down the list to highlight the option you want and click to activate it.
Check Box	One option	Click once to turn the option on, click again to turn it off.
Text Box	Text or empty space	Review the text and if necessary type in appropriate text.
Option Button	A set of options	Click the option you want.
Command Button	A command name	Click once to carry out the command shown inside the button.

These are typical controls needed to effectively use the Platform as illustrated in Figure 2.2. In particular you enter the required input parameters using the corresponding "Text Editing" box. Then you use the "Command Button" "OK" to accept these input values and move on to other modeling activities.
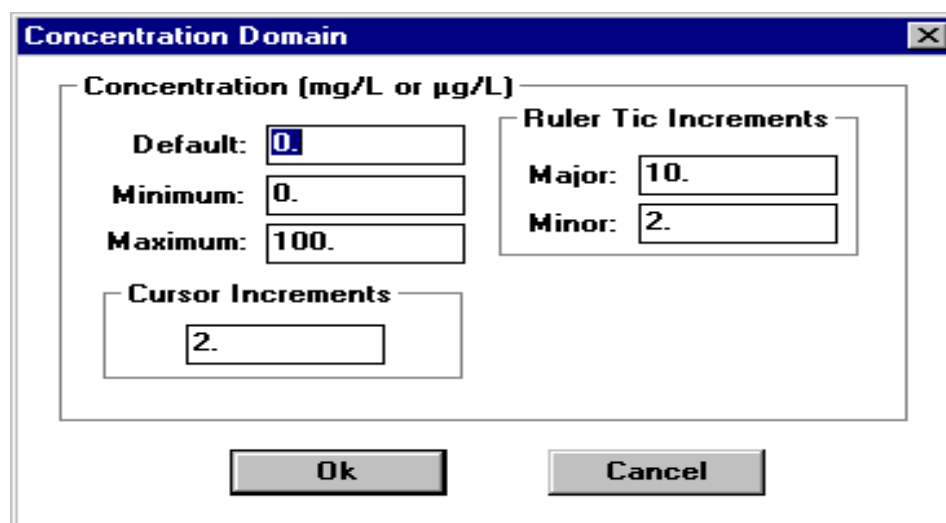
Figure 2.2. Typical Controls in a Dialog Box.

2.1.2   What You Need to Get Started

First, make sure you have the correct equipment. While setting up MS-Windows 3.x or Windows 95, you will be prompted to identify your pointing device, keyboard, printer(s), graphics adapter, and monitor. Windows will copy the necessary driver files to your hard disk. We recommend that you use equipment with the following specifications to run the BIOPLUME III Graphical User Interface Platform:

IBM- Compatible Personal Computer, with Intel 486, or (preferably) Pentium processor.

Your system should include an 800 MB or larger (1GigaB) hard (fixed) disk.

At least 8 MB of RAM memory- possibly 16 MB, especially if you are using memory-resident programs on a network, or Windows 95.

A Microsoft Windows -compatible graphics adapter and a compatible color graphics monitor.

Microsoft Disk Operating system (DOS) version 3.0 and above.

A Windows-compatible pointing device (mouse).

A Windows-compatible printer.

In general, if your equipment can run and print from MS-Windows, you can run and print from the BIOPLUME III Graphical User Interface Platform.

2.1.3   How to Install the Graphical User Interface Platform

The easiest way to install the Graphical User Interface Platform is to rely on the "Install" program. Once you start, the Install program prompts you on the screen for all the operations that need to take place.

To Install the Platform proceed as follows:

1. Turn on your PC,

2. Insert the Platform Install disk (disk 1) into drive A or B,

3. To activate the MS-Windows-3.x environment, at the prompt > type WIN and press the Enter key.   For Windows 95, or if you are already in Windows proceed with step

4. From the Program Manager or File Manager (Start, Run in Windows 95) select file - RUN, type A:\INSTALL or B:\INSTALL, and press the Enter key. The install program begins.

5. Follow the instructions on your screen.

Note: MS-Windows-3.x or Windows 95 must be previously set up on your system before installing the BIOPLUME III Graphical User Interface Platform. You may find answers to any questions by consulting the section "WHAT YOU NEED TO GET STARTED."

As you insert disks, the Install program copies the necessary files from the Platform disks onto your hard disk. You can change the default drive and directory names of the install program to any drive and names of your liking, when prompted.

The install procedure will create a sub-directory C:\EISBIOP on drive C: or any other drive of your choice and will decompress all the executable files needed to run the program. Then, it will copy in this new directory all the files required to run the different tutorials. Once the installation procedure is completed, you will be automatically placed in the new sub-directory. Note that to run properly the Platform you need at least 3MB of memory available on your hard disk. Consult your "Microsoft Windows User's Guide" for complete information about Microsoft Windows-3.x or Windows 95.

To check if everything is running properly test run the program: a Group Application " Platform" has been created automatically by the "Install" program; double click on the icon representing the BIOPLUME III program.

This will activate the Platform to run under MS-Windows-3.x or Windows 95. Now you are ready to consult Sections 2.2 and 2.3 to quickly navigate through the program and check that everything is properly installed.

2.2   Description of the Platform Controls

2.2.1   Operating the Graphical User Interface Platform Commands and Controls

Learning and using the BIOPLUME III Graphical User Interface Platform is easy and natural. The system arranges windows in a hierarchy of parent, child, and sibling, starting with the desktop (background) window. Each window is an *Instance* of a window class and each class has a window *procedure*. All the user needs to know is the controls that allow him or her to activate these window classes and associated procedures.

The Platform offers a very powerful set of controls that allow the user to build a Case Study "on the fly." This set includes:

- **A Menu of Program operations and,**

- **a Tool Box.**

The *Menu* provides access to all operations of the Graphical environment: from file management, to graphical editing, to the activation of a particular simulation and visualization of the results; the menu control gives instantaneous access to all the tasks necessary for the simulation of a groundwater contamination episode.

The *Toolbox* provides the user all the necessary tools to build a model. The basic modeling features (objects, lakes, wells, logpoints, etc.) are contained in the toolbox for easy access. All the user has to do is point, click, and drag. *Et voila !* The selected modeling feature is created on the spot.

Figure 2.3 illustrates the general configuration of these various controls as they are displayed on the screen.
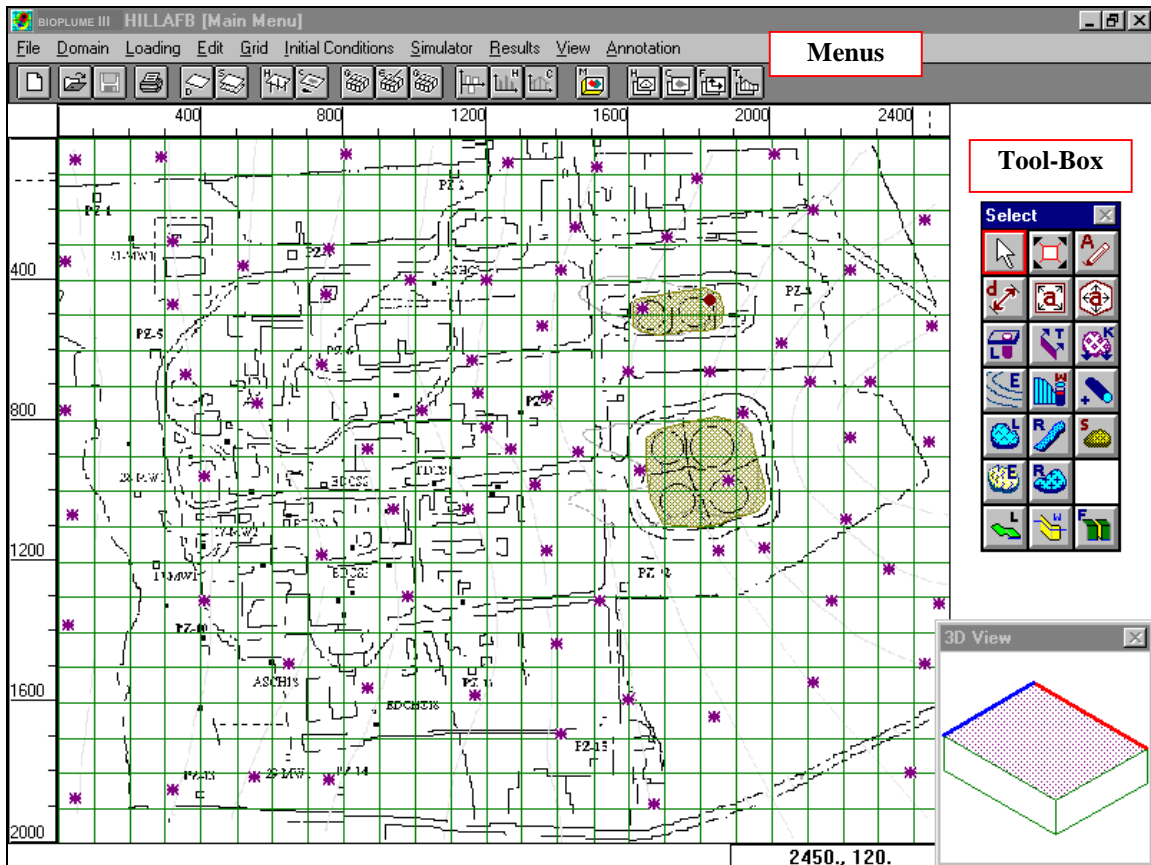
Figure 2.3. Graphical User Interface Platform Menu and Toolbox.

2.2.2 Description of the Graphical User Interface Platform Menus

All Platform options fall under ten basic Menus. Each of the main menus is associated with secondary pull-down menus which give access to the various options, allowing the user to generate pertinent input data, and activate different tasks of the program. There is a logical sequence to activating these menus. A particular case study necessitates several iterations, starting from a simple model and

adding more refinements until we reach the desired accuracy. The Menus in the program are designed to assist the user in the difficult tasks of model calibration and validation of the results.

Each Menu is in fact an editor with its own particular functions. These Menus are as follows (refer also to Figure 2.3):

Menu Name	Menu Function
File	Performs all file management operations, open, save, restore, delete, close, view file content.
Domain *(Editor of Global Parameters)*	Control parameters defining the geometry of the groundwater problem and the time domain. Appropriate selection of the cursor resolution.
Loading *(Editor of Heads and Concentrations)*	Defining all existing loading (Hydraulic heads, and concentrations) as a function of time.
Edit *(Editor of Modeling Features, Wells, Sources, Lakes…)*	All editing capabilities for the modeling features given in the toolbox for the groundwater contaminant migration problem.
Grid *(Editor of Boundary Conditions and all Distributed parameters inside the Modeling Grid Area)*	Definition and generation of the grid geometry used for different resolution processes. Editing of cell properties, constant/variable flow, inactive cells.
Initial Conditions *(Editor of Simulation Period and Initial Conditions)*	Selecting initial conditions for the simulation.
Simulator	Selecting appropriate Simulation module to run.
Results *(Graphical Editor of Simulation Results)*	Visualization of all data related to the results of various analysis options.
View *(Editor of Viewing Configurations)*	Select/Remove features appearing on the screen of the Platform.
Annotation	Activating/deactivating Annotations in all graphical screens.

The BIOPLUME III Graphical User Interface Platform is a WYSIWYG ("What You See Is What You Get") application. The Platform shows you on screen exactly how a document will appear when it prints. It also adheres to Microsoft Windows conventions for using menus, menu commands, dialog boxes, command buttons, option buttons, list boxes, check boxes, and a mouse. The mouse

pointer becomes an essential tool in the Platform and is the most efficient vehicle to build a simulation model. In that respect, the prompt assumes different shapes according to each editing mode, as shown in the next section.

2.2.3   Navigating Through a Simulation

Typically, the user starts by opening a new file (case) and proceeds to the menu **"Domain"** to characterize the geometric boundaries of the problem. Modeling tools available to the user include:

- mouse pointer for selecting modeling features for editing

- creation of wells

- creation of pollution source, and recharge areas

- impose boundary and initial conditions

Using the S*martIcons* of the *toolbox* the user then selects the basic features of the model and proceeds to the menu   **"Edit"** to input their properties. The feature edit option is also accessible by *double-clicking* on the feature (e.g. well) in the geographic domain. Similar tools are also available for editing the numerical grid and for specifying boundary conditions (constant head, concentrations, general head boundary).

The next step is to determine the loading conditions in the simulation through the options of menu **"Loading.**" Loading features, such as hydraulic heads and concentrations, pumping schedules, and other boundary conditions, require the specification of time series. This operation is automated in the Platform, where entries are limited to the times of change in loading attribute. All simulation time-stepping is done automatically, with values interpolated at the simulation required time steps.

After defining the initial conditions, the program is now ready for activating the simulation (Menu **"Simulator"**), and for viewing the results (Menu **"Results"**). If the results are not satisfactory, several options are offered; the user can change the simulation domain, alter the loading parameters, readjust the simulation grid, or redefine the initial conditions. The beauty of the program is that these changes and alterations are built on-the-fly, <u>without</u> the need to reenter any of the fundamental data. The program cleverly assists the user on each step, and keeps track of all the new parameters that enter the simulation.

It is very simple to navigate through the Platform using the mouse pointer which helps you activate the different menu options and select the appropriate commands and modeling features.   What distinguishes this program from other software is the fact that it provides the user with a completely integrated computer environment for all modeling tasks: input data preparation, execution, and analysis with interactive graphics, geostatistical (kriging) routines for input error control and optimal use of existing geological information; and expert assistance in all phases of the simulation. The Platform supervises the generation of all data needed to run the flow and migration problem as shown below. The user operates in an "Object-Based" environment which offers remarkable flexibility in

making the appropriate adjustments needed in the simulation of the groundwater contaminant migration problem.

2.3   Checking Platform Installation

You can activate the Platform from either a DOS prompt or from the Program Manager window if Microsoft Windows is already running (always the case for Windows 95).

To start the "Platform" from DOS:

- Display a DOS prompt for the drive that contains Windows. For example, C:\

- Type: WIN BIOPLUME. (This assumes the existence of the appropriate set path command in the autoexec.bat file)

- Press Enter.

To start the "Platform" from within Windows :

BIOPLUME III

- Display the Program Manager window.

- If necessary, open the group window that contains the **"BIOPLUME"** icon.

- Double click on the **"BIOPLUME"** icon.

For the implementation of this software architecture, the Platform sets up several sub-directories (folders in Windows 95) to manage the flow of different software operations. Table 2.1 describes the sub-directories that are automatically constructed during the installation procedure of the program. File CONFIG.INI in sub-directory '..\CONFIG' initializes the version of the Platform activating the appropriate modules. All the executables of the program reside in sub-directory '..\RELEASE' which houses the engine of the program. Sub-directory '..\DATA' contains all the files pertinent to a particular application. Sub-directory '..\IMAGE' stores all the bitmaps (raster images) that are necessary to build a remediation study. Finally, sub-directories '..\IMPORT' and '..\EXPORT'' contain all pertinent peripheral data that need to be imported or exported from the platform for a case study. But the heart of the platform resides in the user interface with its process scale operator. It controls all simulation activities through the "Configuration" file, "Menus" and menu options.

Table 2.1. Sub-directories of the BIOPLUME III Graphical User Interface Platform

Sub-directories	Description
Config	Contains the file with list of active Configuration options
Release	Contains all executables and Dynamic Link Libraries (DLL) of different modules of the platform
Data	Contains all sub-directories related to different applications. The name of these sub-directories corresponds to the name of the different current applications.
Image	Contains all the raster background images (*.BMP files).
Import	Contains all pertinent Import Files
Export	Contains all pertinent Export Files
Report	Contains all pertinent Report files and result bitmaps

These sub-directories are all created automatically by the installation program. This program also installs and checks the content of each sub-directory. However, you still need to ascertain that these 'Execution', 'BMP' (Graphics) and 'AVI' (Animation) files work properly on your system by running the following cases:

1. Check that the BIOPLUME III executables work properly

2. Check the Graphics executables that handle the background image

3. Check the Animation executables.

Note that the entire procedure requires only a few minutes of your time. All the input files and data needed to run these cases are already installed by the installation program and the only thing that you are asked to do is to activate the appropriate modules of the program following the instructions given below.

2.3.1   Checking the Platform Executables

Test that all files are properly installed by following the steps below:

Step 1: Use the mouse to go to menu "File" and select option "Open". Among the different input files that exist in your directory select case **"TESTP31"**. Double click on TESTP31.

Automatically all appropriate files are loaded into the Platform and the name of the opened case is displayed at the top of the screen as shown in Figure 2.4.

Step 2: At this stage all input parameters needed to run this simple case are available to the system, and all that is required from you is to initialize your particular run. This is done by moving to Menu "Initial Conditions" and selecting sequentially (in the same order) options "Simulation Period", "Starting Heads" and "Starting Concentrations". These options activate appropriate dialog boxes in which you define the simulation period, the initial heads and concentrations for your particular run. Figure 2.5 shows the dialog box allowing you to enter the simulation period. You do not need to enter any value, just click on the "OK" button. You do the same for the menu options 'starting heads' and 'starting concentrations'.

Step 3: You are now ready to execute the simulation. Move to Menu **"Simulator**," select (click on) **Bioplume III** and click on the **"Save Data and Run Simulation"** button. It should take only a few minutes to run the BIOPLUME III algorithms, (sequentially, close window Wbiop3.exe which creates the input stream; then close window Biopl3.exe when the cursor starts blinking, after BIOPLUME III has finished executing; finally, close window Pbiop3.exe after the graphics files have been executed, as explained in the next Step. "Exit Code zero" signifies a successful run).
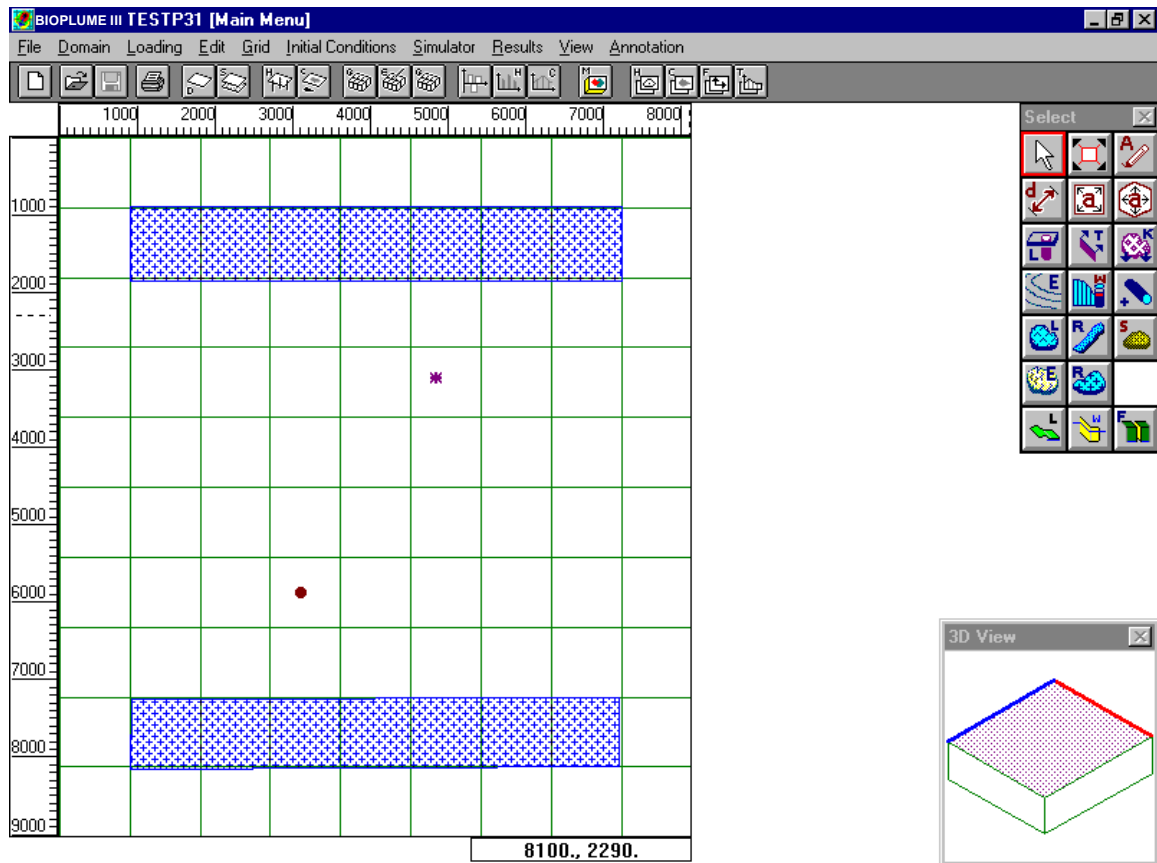
Figure 2.4. Screen View of Case Study "TESTP31".
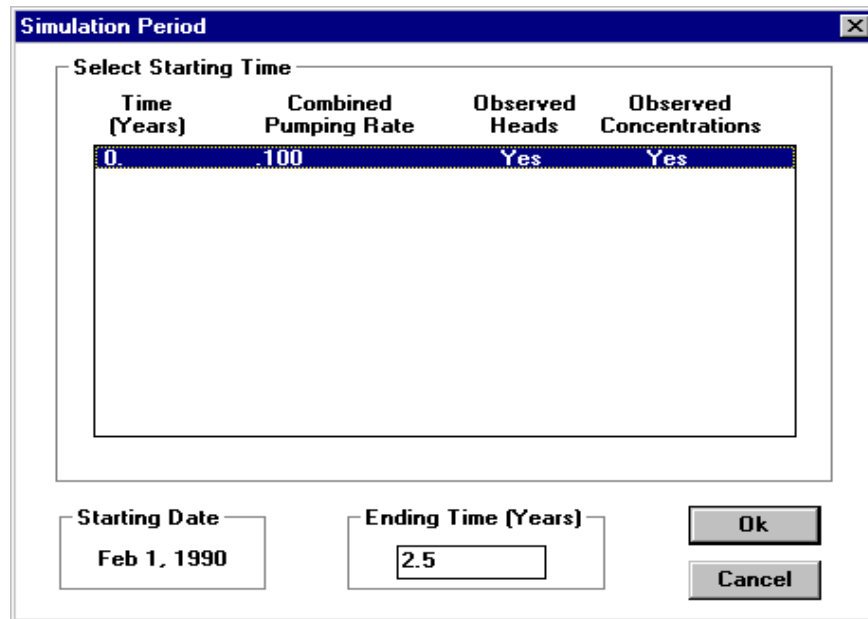
Figure 2.5. Defining the Simulation Period.

Step 4:   Three different modules are now activated sequentially by the program. All you have to do is to click on the "Yes" button when the first module (Data file module) is finished, click on the "No" button when the second module (BIOPLUME III module) is finished and finally click on the "Yes" button when the third module (Graphics file module) is finished (Note that "Exit Code zero" signifies a successful run). At this point if there are no messages displayed on the screen, you have an indication that the execution and graphics files worked properly. You can now visually inspect the output results in Menu "Results" under option "Hydraulic Heads". Figure 2.6 shows the contours of the computed hydraulic heads at time 2.5 years that you should obtain on the screen.

Note the cone of depression due to the pumping well. Also on the contour levels of the hydraulic heads, you should read a maximum head of 100 ft. and a minimum head of 99.51 ft. A final visual check requires activation of the concentration results.

Step 5: In Menu "Results" activate option "Concentrations/Hydrocarbons" to obtain the computed distributions of the Hydrocarbon concentrations at time 2.5 years as shown in Figure 2.7. As it can be seen this is a uniform field across the aquifer. Hydrocarbons decreased from 100 ppb to 96 ppb after 2.5 years due to the biodegrading action of Iron reduction. If these are the values that you read on your screen (Contour levels) then you have successfully completed the installation of the test case execution files.
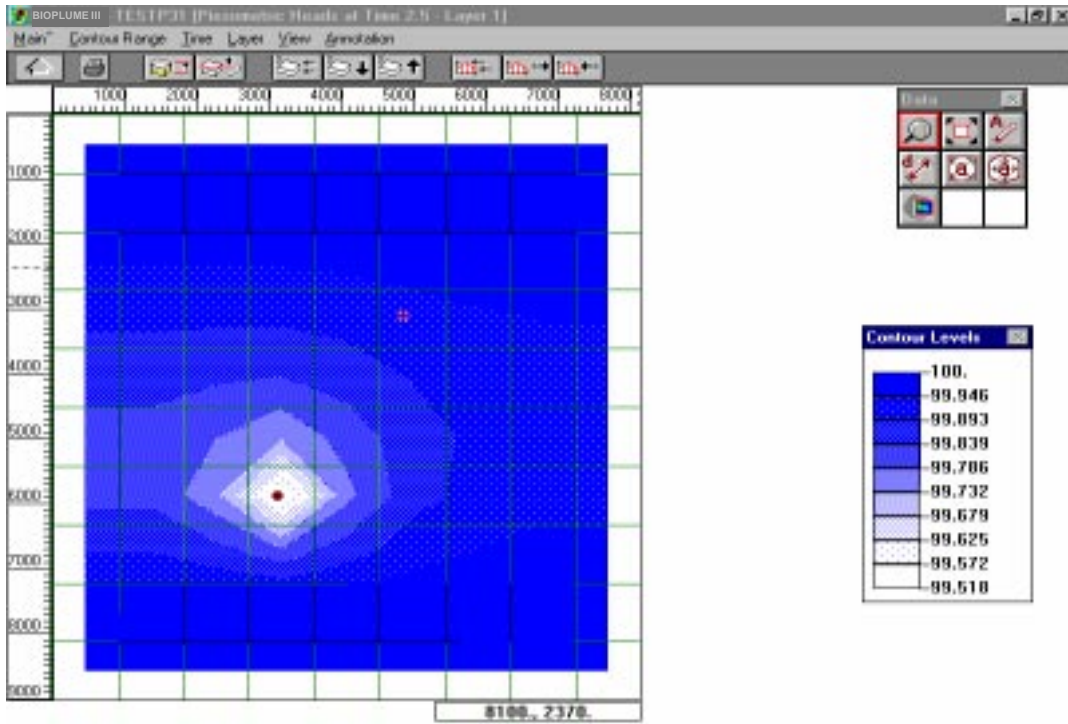
Figure 2.6. Computed Hydraulic Heads at Time 2.5 Years.
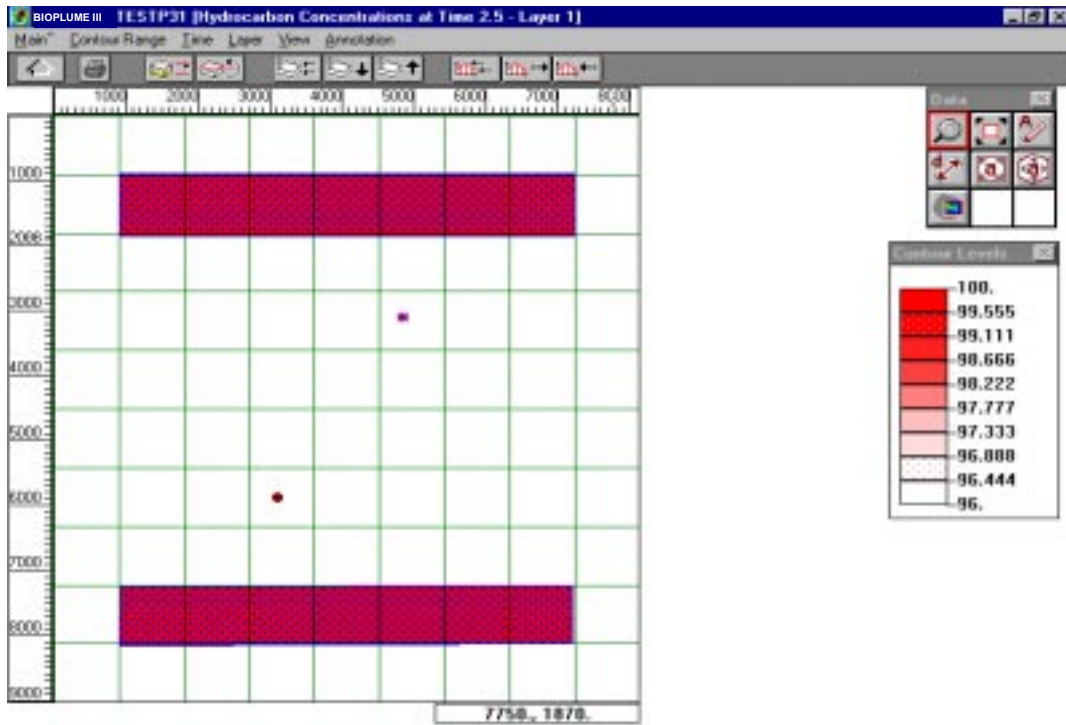
Figure 2.7   Computed Concentrations of Hydrocarbons at Time 2.5 Years.

2.3.2 Checking the Graphics and the Background Image

To check the graphics drivers you need to open a new file case ("**HILLAFB1**") and proceed with the following steps:

Step 1: Use the mouse to go to menu "File" and select option "Open". Select case **"HILLAFB1"**. Double click on HILLAFB1. Again automatically all appropriate files are loaded into the Platform. This case study simulates the Hydrocarbon migration at the Hill AFB UST 870 site.

Site Characteristics

The UST 870 site at Hill AFB covers an area 2600 x 2000 ft. It is seated on a plateau-like bench formed by river deposits of the ancient Weber river. There are three aquifers present in the area. However, the hydrocarbon contamination is believed to be limited to the shallow (unconfined) aquifer, which is the subject of this simulation. Groundwater flow in this aquifer is in the SW direction. Total dissolved BTEX within a contour level of 70 ppb is considered as the source of contamination, as shown in Figure 2.8. More details of this case study can be found in the referenced tutorial documents.
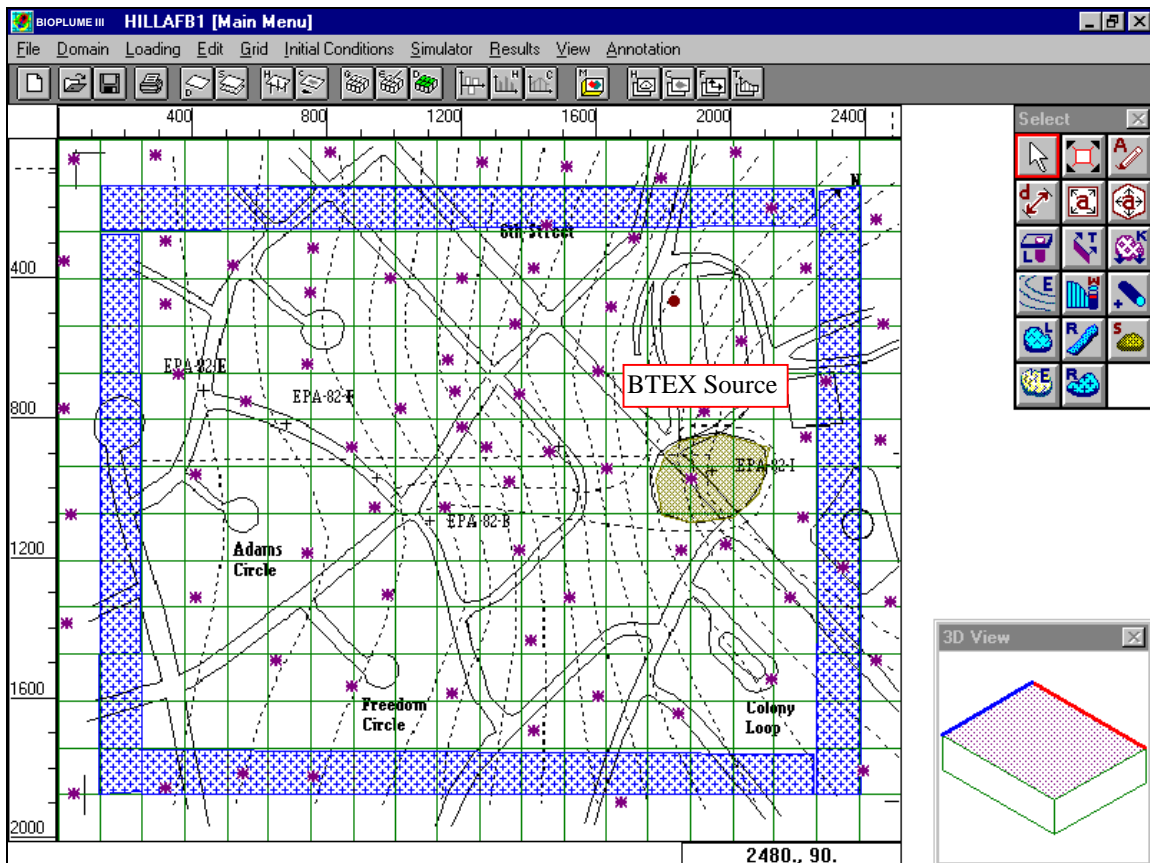
Figure 2.8   Screen View of Case Study "HILLAFB1".

Now on your screen you have an image similar to Figure 2.8. Note that the background of the working area is covered by the raster image (Bitmap) available for this case. The bitmap can be found as file HILLAFIM.BMP in sub-directory "..\Image". The graphics drivers automatically load the image when you open the case. If for some reason you do not get the background image, check whether the HILLAFIM.BMP file is corrupted using any available graphics program like "Paintbrush" or "Paint".

Step 2:   In this step you will only view the results of the simulation and check if the color palette is loaded properly. Move to Menu "Results" and sequentially activate the following options: "Concentrations\ Hydrocarbon" and "Concentrations\ Oxygen". On the screen you will obtain the illustrations shown in Figure 2.9. On the left you have the hydrocarbon contaminant plume as it is displayed on the screen at the end of a 1 year simulation and on the right you have the oxygen depletion at the end of same time period. (Note that we removed the graphical representation of the recharge zone at the boundaries by deactivating option "View\ Features"
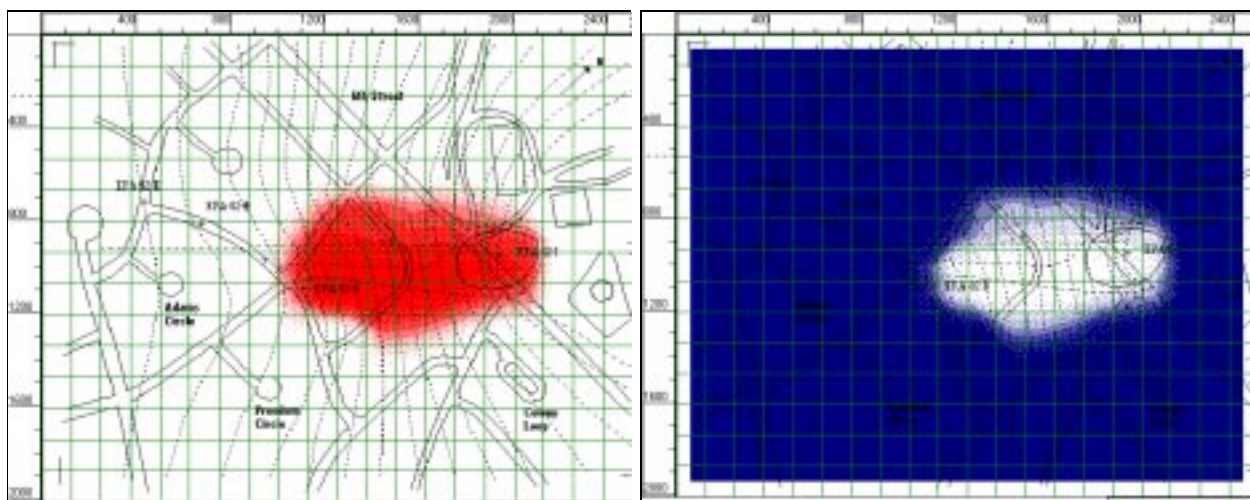
Figure 2.9 Plume Migration for BTEX and Oxygen After a 1 Year Simulation.

As it can be seen, the computed hydrocarbon and electron acceptor concentrations are superimposed on the raster image of the site. This greatly facilitates the location of points of compliance and long term monitoring wells.

2.3.3   Checking the Animation Executables and Files

Finally, to complete the installation check-list you need to verify if the video animation (AVI) files work properly. The video animation option runs on Windows 95 only. Note that the standard format for Windows digitized video is the Audio-Video Interleaved (AVI) format. An AVI file can be played in Windows with no additional hardware (of course it will be smoother and faster with a video accelerator). The Platform supports Microsoft Video for Windows 95 AVI-format (*.AVI) video files. To verify the video drivers you do not need to open another study, just continue with the HILLAFB1 case, using the following step.

Step 1: Move to Menu "Results" and activate option "AVI Animation". This will invoke the animation module. As it can be seen a new menu bar appears at the top of the screen. Move to Menu "File" and click on the option "Open AVI". A dialog box appears on the screen with the list of all available video clips (.AVI) files Select the file **"HILLAFB.AVI"** to obtain the screen shown in Figure 2.10. To playback the video clip showing the simulated migration of hydrocarbons, just click on the "Forward" play button that appears at the bottom left corner of the AVI window.
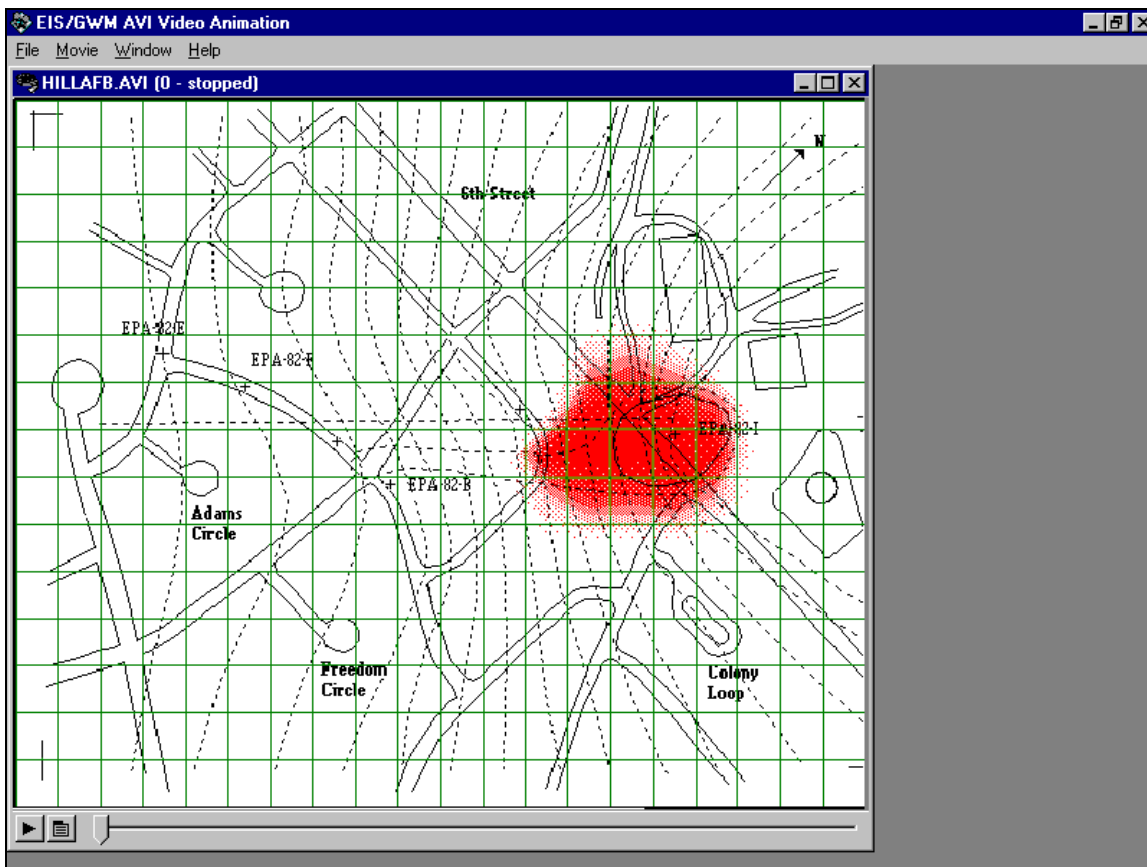
Figure 2.10 Playback Screen of AVI Files.

Et voila! The screen comes to life and the video clip stops after a few seconds. The detailed procedure on how to create this AVI file is given in the User's Guide manual. All you need to know at this point is that the "HILLAFB.AVI" file was generated from only 4 Bitmaps (snapshots) depicting the simulated plume at times 0.25, 0.50, 0.75 and 1 year. These bitmaps were selected and created using the grasping tool activated from the available Platform tool box.

At this stage, if no error messages are encountered, the installation is successful and you may proceed with the implementation of your own case studies. You can also consult the other sections of this Manual, in particular: the **Platform User's Guide**, and the **Tutorial**.

2.4　Checking the Installed Case Studies

Each case study is identified by its name and all pertinent input and output files reside in a sub-directory (folder) that bears the same name as the case study and is located in sub-directory (folder) C:\EISBIOP\DATA\. There are two categories of case studies that are installed with the program, namely:

1. Simple academic cases that show the fundamental features and operations of the program. The detailed description of their operations is given in the tutorial manual; and,

2. Real case studies from different Air Force Bases across the U.S.

Table 2.2 lists all the installed real case studies while Table 2.3 shows the complete list of all the installed test cases.

Table 2.2　List of Installed Real Case Studies.
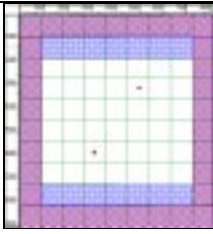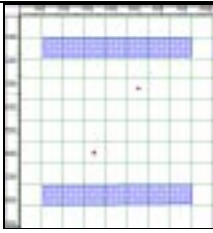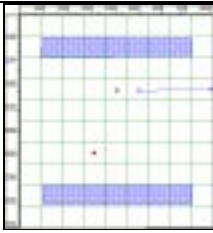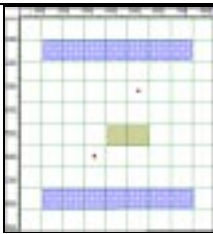
Configuration	Name	Description	Features	Size
	HILLAFB	Hill Air Force Base	Recharge + Source	25x20

Table 2.3   List of Installed Test Cases.

Configuration	Name	Description	Features	Size
	TESTP30	Base case	Recharge zone + Well + Iron Reduction	9x10
	TESTP31	Base case with optimal input setup	Recharge zone + Well + Iron Reduction	9x10
	TESTP32	Testing Drains	Recharge zone + Well + Iron Reduction +Drain	9x10
	TESTP33	Testing Sources	Recharge zone + Well + Iron Reduction + Source	9x10
	TESTP34	Testing Lakes	Recharge zone + Well + Iron Reduction +Lake	9x10
	TESTP35	Testing Rivers	Recharge zone + Well + Iron Reduction +River	9x10

2.5   Concluding Remarks

This concludes the installation guide. The main objective of this Section is to guide the user through all the installation procedures.   A brief description of the basic features of the program allows the user to quickly navigate through the platform. However, to get a better insight about the proper use of the program we suggest to also consult the following Sections:

- Platform User's Guide

- Tutorial

- BIOPLUME III Theoretical Development, and

- Implementing the Air Force Protocol for Intrinsic Remediation.

3.0   TUTORIAL

This section gives a series of tutorial examples which allow the user to learn by example how to operate the Graphical User Interface Platform using the Platform menus and tools.   Before presenting the tutorial examples, we start by summarizing the fundamental steps required to perform a complete simulation.

If the Platform software is not already running, start the Platform by double clicking on the **"BIOPLUME III"** icon on your Windows Desktop:

The main page of the Bioplume III application looks as in the picture below. After closing (O.K.) the "About Box," the user will have access to the main Menu which lists the following entries: 'File,' 'Domain,' 'Loading,' 'Edit,' 'Grid,' 'Initial Conditions,' 'Simulator,' 'Results,' 'View,' and 'Annotation.'
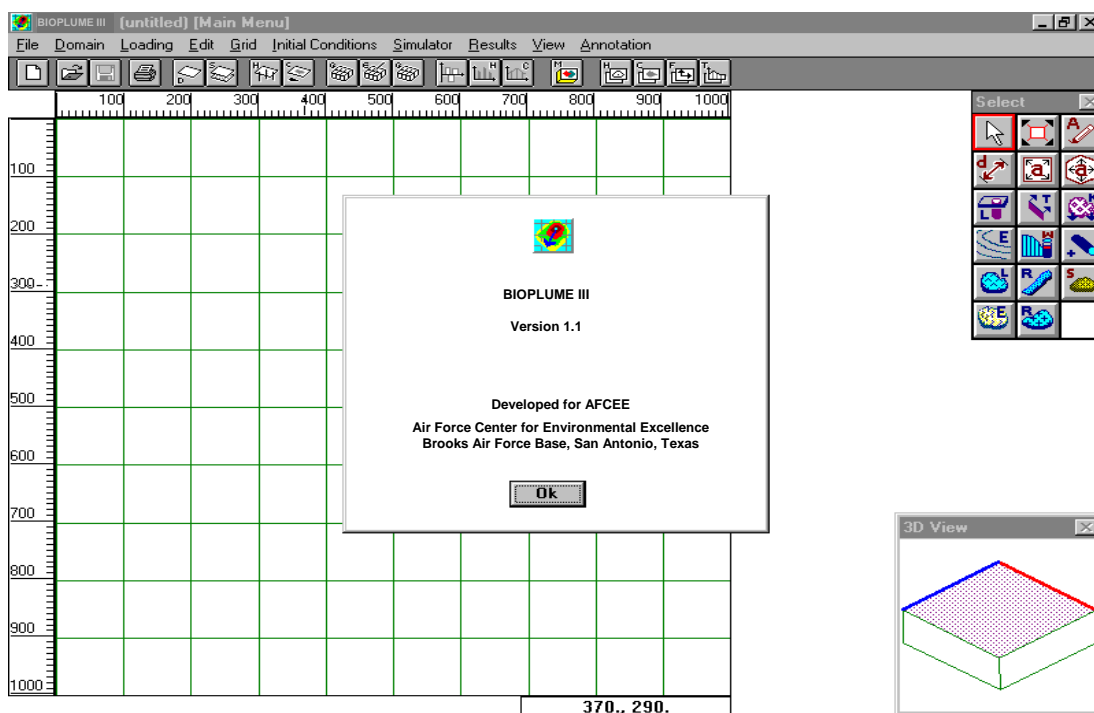
The logical sequence of these entries is as follows:

- Access or create a new case (menu **'File'**),

- Create the graphical (geographic) environment of the application (case study), (menus **'Domain,'** and **'Edit,'**),

- Specify any/all time series data of state variables -hydraulic heads and concentrations (menu **'Loading'**),

- Specify the numerical grid for simulation and perform parameter interpolation -kriging (menu **'Grid'**),

- Select initial conditions for simulation among previously entered 'Loading' data (menu **'Initial Conditions'**); then,

- Perform Bioplume III simulation (menu **'Simulator'**) after selecting run-time options; and finally,

- Graphically view the results of the simulation (menu **'Results'**).

Menus **'View'** and **'Annotation'** are service menus allowing to control the layout of the computer screen. Also, menu 'Edit' is operated in conjunction with the **'Tool Box'** displayed at the top right corner of the screen. With the pointing device (mouse) the user selects features (e.g. wells, pollution source, recharge areas), and places them on the screen within the modeled Domain and specifies their properties.

Using the *SmartIcons* of the *toolbox* the user selects the basic features of the model and proceeds to the menu **'Edit'** to input their properties. The feature edit option is also accessible by *double-clicking* on the feature (e.g. well) in the geographic domain. Similar tools are also available for editing the numerical grid and for specifying boundary conditions (constant head, concentrations, general head boundary).

The next step is to enter any time series data for hydraulic heads and concentrations using menu **'Loading.'** All above data are real (not interpolated) data at log-points, and over appropriate time intervals.

As in any software application (e.g. Word Processing), the user is encouraged to frequently "save" his/her work, especially after entering new data, modeling features or 'Loading' data. This is done by activating the 'Save' option in menu 'File.' (The 'Save As' option also allows the user to create a new case name from a previous case, useful when creating a suite of "scenarios"). However, the save operation in the Platform also automatically triggers a data synthesis operation, i.e. mapping of log-point data to the numerical grid via Kriging. Therefore, the save operation is the last operation to do prior to performing a simulation. The program is now ready to initiate a simulation.

The first step in preparing for an actual simulation is the selection of initial conditions (menu **'Initial Conditions.'** The Platform is now ready for activating the simulation (menu **'Simulator'**) - without performing a "save" operation again!

Then, for viewing the results graphically activate menu **'Results'.** If the results are not satisfactory, several options are offered; the user can change the simulation domain, alter the loading parameters, readjust the simulation grid, or redefine the initial conditions. The beauty of the program is that

these changes and alterations are built on-the-fly, <u>without</u> the need to reenter any of the fundamental data. The program cleverly assists the user on each step, and keeps track of all the new parameters that enter the simulation.

The best way to learn is by example: you are now ready to apply these general operating principles to the tutorial examples of this section.

3.1   Tutorial Overview

The tutorial examples are grouped in sessions. The user is provided with instructions on how to develop and run a new simulation.   An "academic" example of a study area is provided as an example. The attributes of the study area are highly simplified so that operational concepts can be developed and tested without undue complexity.

The goal in this tutorial is to systematically develop site characteristics and test the model incrementally. To that end, instructions are given in the form of six sessions:

- Session 1: Basic model development;
- Session 2: Ground water flow modeling;
- Session 3: Non-attenuated hydrocarbon mass transport;
- Session 4: Addition of electron acceptors and biological interaction;
- Session 5: Introduction of special features (wells, drains, lakes, etc.)
- Session 6: Animation and graphical presentation (Windows 95 version)

The Graphical User Interface Platform uses a hierarchical menu system using parent menus which, in turn, activate a series of child or sub-menus. For many applications, input is required in several sibling menus. To simplify the tutorial the following convention is used:

- Each menu or submenu is written in bold and italic typeface and preceded by a ➔ symbol which can be interpreted as the command "go to".
- Each submenu will be sequentially indented under the parent menu. For example to go to the parent menu "Domain" then the submenu "Surface Domain" would be written:
  ➔ *Domain*
  ➔ *Surface Domain*
- Entry fields listed on a submenu are written in bold and italic type face and are also indented according to hierarchy.
- Data to be input will be placed in brackets. For example the instruction to enter 30% porosity is given as [.30]. In the program you'd only enter 0.30 not the brackets!
- Commands to be executed with the mouse or keyboard are enclosed in <> symbols. For example, after data is entered you may need to use the mouse to click on the OK button. Here this step is written as <OK>.
- Where the enter button is to be pressed the following is used ↵.
- Grid coordinates are entered as (x-number, y-number)

- All instructional comments within a command string are written in italic text. For example, to describe the "Domain" level:

> ➔ **Domain** *- Used for defining the range of minimum and maximum values to be used in the model and appearing on graphs that follow*

Before beginning, copy the base images of the test site to the default EIS image directory. The base images are provided on the accompanying floppy disk as Test01.bmp, Test02.bmp, Test03.bmp, and Test04.bmp. Using DOS or the windows File Manager copy those files to C:\EISBIOP\IMAGE\ assuming C:\ is the root directory you installed the Platform on (check first, these files may have already been copied from your self-installation package).

3.2 Session 1: Basic Model Development

Turn on your computer and click on the Bioplume icon to start running the program. The program will appear on your screen along with a default uniform 10 by 10 model grid with an x and y range of 0 to 1,000 feet.

Main
> ➔ *File*
>> ➔ *Save As* [Test01] **<OK>** *- Saves the session as "Test01" file name*

> ➔ **Domain** *- Used for defining the range of minimum and maximum values to be used in the model and appearing on graphs that follow. In some cases this directory also establishes default aquifer parameters.*
>> ➔ *Surface Domain*
>>> *Surface Bounds*
>>>> **Left** [0] *- Sets minimum x grid value range for work area to 0*
>>>> **Right** [2000] *- Sets maximum x grid distance for work area to 2000 feet*
>>>> **Top** [0] *- Sets minimum y grid value range for work area to 0*
>>>> **Bottom** [2000] **-** *Sets maximum y grid value to 2000*
>>> *Ruler Tic Increments*
>>>> **Horizontal Major** [100] *- Sets horizontal major ruler tic increment to 100 for work area ruler*
>>>> **Horizontal Minor** [10] *- Sets horizontal minor ruler tic increment to 10 for work area ruler*
>>>> **Vertical Major** [100] *- Sets vertical major ruler tick increment to 100 for work area ruler*
>>>> **Horizontal Minor** [10] *- Sets vertical minor ruler tick increment to 10 for work area ruler* **<OK>**

The 10 by 10 grid appears to have shrunk by half and now resides in the upper left corner of the work space. Do not panic! This is normal and we'll fix it now.

Main

  ➔ *Grid - Menu used for defining the model grid and major site aspects represented on that grid. In addition to defining grid geometry, boundary conditions for hydraulic heads and the concentrations of the contaminant and electron acceptors can be established across the grid in this menu.*

    ➔ *Generate Grid*

      Computational Bounds

        Left [0] *- Sets minimum x-direction grid value to 0 feet*
        Right [2000] *- Sets maximum x-direction grid values to 2,000 feet*
        Top [0] *Sets minimum y-direction grid value to 0 feet*
        Bottom [2000] *- Sets minimum y-direction grid value to 0 feet*

      Grid Size

        Number of Columns [20] *- Sets the number of columns in the grid to 20 and automatically establishes that each cell will be 100 feet in the x-direction*;
        Number of Rows [20] **<Generate Grid>** *- Sets the number of rows in the grid to 20 and automatically establishes that each cell will be 100 feet in the y-direction.*

Note that under ➔ *Grid* ➔ *Generate Grid*, the "*Grid Increment*" entry items *Column Increment* and *Row Increment* both changed to 100 feet when the number of rows and columns was set under *Grid Size* to 20. It would have also been possible to directly set the *Column Increment* and *Row Increment* to 100 then the values under *Grid Size* would have automatically been set to 20. It's time to save your work:

Main

  ➔ *File* **<Save>**

You will now notice that the model grid extends all the way across the work area. A useful aspect of the Platform is that the grid geometry (number of rows or columns or length of the grid) can be changed at any time during a simulation without affecting any previously entered model data (wells, log-points, strata elevations and other features).

Next we want to incorporate the base image for the test site onto the working grid. The Platform accepts windows meta (*.bmp) files. These files can be generated from many different graphics programs including Paintbrush, CorelDraw!, AutoCad Rel. 12, and others. To import the Test01.bmp image for this session:

Main

  ➔ *Domain*

    ➔ *Base Image* **<test01.bmp><OK>**

The site background image should now be pasted on the work area; however, you will notice that the image does not conform to the ruler. The test site has dimensions of 2,000 by 2,000 feet and

needs to be "registered" to the same dimensions as the grid. To adapt the image, click on the Register button on the tool box which looks like this:

Note that the normal pointer icon changes to a star-burst pattern. Move the pointer to the upper, left-hand corner of the site image and click and hold down on the mouse button. While holding down on the button drag over to the lower, right-hand corner of the site image. You'll note that as you drag, a black box will form. When you position the cursor on the lower, right corner of the image release the mouse button. The entire picture of the site should be covered with a dark gray shading and a "*Register*" menu will appear. Enter values as follow:

> ➔ *Register*
>> **First Point**
>>> X: [0] - *0 foot x-position for the first register point we entered in the upper left hand corner*
>>> Y: [0] - *0 foot y-position for the first register point we entered in the upper left hand corner*
>> **Second Point**
>>> X: [2000] - *2000 foot x-position for the second register point we entered in the lower right hand corner*
>>> Y: [2000] **<OK> <Main>** - *2000 foot y-position for the second register point we entered in the lower right hand corner.*

The base map should now fit nicely on the defined model grid. If the image appears correct then save the session:

Main
> ➔ *File* **<Save>**

If it <u>does not</u> look right you'll need to redo this last step by exiting without saving and reopen the Test01 model file:

Main
> ➔ *File*
>> ➔ *Open* **<NO> <Test01> <OK>**

3.3   Session 2: Basic Flow Modeling

3.3.1   Domain and Boundary Conditions

Now we want to continue defining model range and basic aquifer values in preparation for flow modeling under static (steady-state) conditions.

Main
> ➔**Domain**

➔*Elevation Domain - Defines default range for the top and bottom of the aquifer. Note, that this does not set the actual top and bottom of the aquifer for the model; it merely defines the range over which we will work. Set the top and bottom of aquifer at some nice even increment slightly above and below the highest actual piezometric surface for your system. For this example, the piezometric surface will range from an elevations of 2 to 8 feet; however, the base of the aquifer ranges in elevation from about -3 to -7 feet in elevation. So, we'll set the top elevation to 10 and the bottom to -10.*

Elevation

Maximum [10] - *Sets maximum elevation range for the aquifer to 10 feet*

Minimum [-10] - *Sets minimum elevation range for the aquifer to 0 feet*

Ruler Tic Increments

Major [10] - *Sets major tic increments for every 10 feet on any graphs rulers where aquifer elevations are shown. Here, as defined we'll only have one major tic of ten feet.*

Minor [1] - *Sets minor increments on any following rulers or graphs to 1 foot. As defined here, our system will show ten minor tics.*

Cursor Resolution [1] <**OK**> - *Allows graphical entry of elevation data on subsequent log points to be adjusted in increments of one foot.*

Let's check to see that our latest set of commands works correctly by adding a *log point*. A **"Log Point"** is a graphical method of assigning aquifer top and bottom data to the grid. You can think of it as an actual data point derived from a soil boring or test hole, but log points can also be used to assign grid values between actual test holes and "force" the grid to an interpretational value. The log point icon is found on the button bar which is usually in the upper right hand corner of the work space. It looks like:

Using the mouse, click on the log point icon. The mouse pointer will change to a kind of star-like design. Move that pointer to any cell on the graph and click on the left mouse button once. The star burst design will be transferred to the grid and, you will notice, that the mouse pointer has returned to it's original arrow design. Using the mouse, place the cursor on the new log point and double click the left mouse button(click that mouse button quickly twice). The "*Log Point 1*" menu will appear. Then click on "*Cross Section*". A graph should appear that shows the default aquifer top and bottom (0 to 10) with a minor tick-increment every 1 foot (If you don't get this repeat the steps above). Note the blue and red dots beside the elevation graph. By clicking and dragging either the red or blue dot one can graphically adjust aquifer elevation top and bottom. Log points can also be used to modify hydraulic conductivity, specific yield, effective porosity, and longitudinal dispersivity as we'll discuss later.

Note that at least one log point must be entered to run the BIOPLUME III model. To delete Log Point #1 you would simply click on it with the mouse then press the **<Delete>** button on the

key board. Maintain this Log Point for the time being. We will come back to log points later. For now though let's save the model and continue establishing Loading Domain parameters.

Main
      ➔ *File* **<Save>**
      ➔ *Domain*
           ➔ *Loading Domain*
                ➔ *Time*
                      Maximum Time [10] - *Sets maximum model run to ten years and for all time domain graphs that follow*
                      Ruler Tic Increments
                          Major [10] - *Sets major tic increments on all time domain graphs to every 10 years*
                          Minor [1] **<OK>** - *Sets minor tic increments on all time domain graphs to one every year.*

Now, as established above, any time domain graphs shown in the model will range from 0 to 10 years with minor tic increments set for one for each year. The pumping rate domain is the next submenu under domain. This submenu item only has relevance if you are planning on incorporating a pumping or injection well into your model and it can be skipped if not needed. We will examine pumping effects in Session 5 but the topic will be skipped for now.

Main
      ➔ *Domain*
           ➔ *Loading Domain*
                ➔ *Pumping Rates -* *Skip this function for now. Keep all default settings.*

Next, we continue with quickly establishing the balance (remainder) of the ***Loading Domain*** values:

Main
      ➔ *Domain*
           ➔ *Loading Domain*
                ➔ ***Concentrations -*** *Skip this function for now and accept all default values*
Main
      ➔ *Domain*
           ➔ *Loading Domain*
                ➔ ***Infiltration*** *- Sets infiltration or recharge range parameters. This is not used in the current simulation just click on* **<OK>**
Main
      ➔ *Domain*
           ➔ *Loading Domain*
                ➔ *Hydraulic Heads*
                      Default [10] - *Sets default upper limit hydraulic head to 10. This value should be an even increment slightly higher than the highest*

piezometric head to be incorporated in the model. For the current simulation the maximum piezometric head is 8 so we set this value to 10 ft.

Maximum [10] - *Sets maximum default piezometric head to 10 ft*
Ruler Tic Increments

> **Major** [10] - *Establishes that there will be only one major tick increment of 10 feet for this simulation*
> **Minor** [1] - *Divides the major tic increment into 10 equal parts of one foot each.*

Cursor Increment [1] <OK> - *Permits graphical adjustment of piezometric head graphs in one foot increments.*

For the current session, we are not modeling chemical transport or biological reactions. Therefore, for the time being, ignore the ***Chemical Species*** submenu of ***Domain*** but continue defining strata properties:

Main
> ➔***Domain***
>> ➔***Define Strata***
>>> ***Horiz. Hydraulic Conductivity (ft/sec)*** [3e-4] - *Defines the default hydraulic conductivity across the entire grid. If hydraulic conductivity is not modified via log points then this is the value used for the whole grid.*
>>> ***Anisotropy*** [1] - *Establishes that the aquifer is isotropic with respect to vertical and horizontal hydraulic conductivity*
>>> *Angle of Conductivity with x-axis (in degrees) [90] - For cases where the principal axes of conductivity are at an angle with the x-y coordinate system of the site.*
>>> ***Storage Coefficient*** [.20] - *Sets storativity if model is to be run under transient conditions. For this simulation, steady state is assumed, but it is acceptable to put a realistic value here (the selection of steady-state or transient conditions is specified later at the run-time options irrespective of the S value entered here).*
>>> ***Effective Porosity*** [0.20] - *Sets the porosity for the model. For unconfined aquifers Storage Coefficient = Effective Porosity. For confined systems Effective Porosity >> Storage Coefficient.*
>>> ➔***Transport Properties*** - *Sets mass transport properties and is not used in the current session. Just click <OK> <OK> to return to the work space.*

Boundary conditions are required so that the numerical model can approximate flow across the grid. Each general cell in the grid is fundamentally defined in terms of Darcy's Law wherein water flow across a cell boundary is directly proportional to head flux and hydraulic conductivity. The goal is to allow head elevations for most cells in the grid to be variable based on the prevailing hydraulic conditions and imposed stress (such as pumping). This is accomplished by simultaneously solving a series of mathematical equations describing each cell. To provide mathematical stability; however, a certain number of known values must be defined yielding a system of equations

consisting of *n*-equations for *n*-unknowns. Known values are supplied through the use of boundary conditions.

BIOPLUME III supports three types of boundary conditions, inactive, constant head, and constant flow (flux). Constant flow cells produce the effects of pumping wells and may or may not be used in a simulation.   Constant head and inactive cells; however, are required for BIOPLUME III simulations. Inactive cells are technically excluded from the active portion of the model domain. All the cells around the perimeter of the grid must be defined as inactive for the model MOC and BIOPLUME III. These perimeter cells are automatically set to inactive in the Platform; you can also define those cells manually as described below.

The constant head condition fixes the water table elevation at a constant value in certain cells throughout the simulation. For example, often the second row from top or bottom of the grid, or the second column from left and right, are defined as constant heads. Other cells, however, can also be defined as constant head cells.

It is important to note that BIOPLUME III, as was the case with the predecessor program MOC, calculates head values across the body of the grid based on the values of the constant head cells defined within the grid.   The Platform allows you to essentially draw the complete hydraulic head surface map across the grid (initial conditions).   By Kriging, interpolated head values are established across the entire grid.   The Platform then assigns the Kriged value to the defined constant head cell automatically. So at this stage we establish boundary condition types and not the actual head values.

To establish boundary condition types for the current session:

Main
> *Grid*
> *Edit Grid* <OK>

Using the mouse click on the inactive cell icon in the tool box which looks like this:

Note that the normal pointer icon changes to an x-shape. By clicking and dragging you can paint the outermost perimeter of the grid (one row and one column at a time) with inactive cells. Next, we need to establish constant head conditions. Click on the constant head cell icon that looks like this:

Now the pointer icon will be shaped in a triangular pattern. Paint around the next-to-the-outside cells. Note that there is a normal cell icon in the tool box that looks like this:
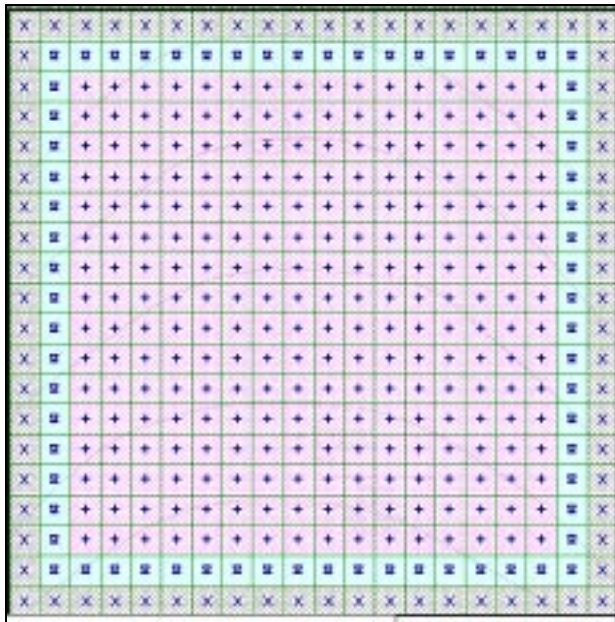
Figure 3.1 Boundary Conditions in Test
Simulation.

If you make a mistake simply click on the proper tool box icon and correct it. When you're finished the grid pattern should appear like that shown on Figure 3.1. If it doesn't keep working with it till it does then click on **<Main>** to return to the main menu. Save the file:

Main

 ➔ File **<Save>**

3.3.2   **Hydraulic Head Conditions**

Now that the boundary conditions have been established head values need to be assigned to constant head cells. The Platform ascribes actual site head elevations to the defined constant head cells automatically. The best method to enter the piezometric surface for the model is to actually trace the water level isopleths (head contour lines) shown on the site map image. Go to:

Main
  ➔ *Loading*
    ➔ *Observed Heads*

On the tool box click on the Head Line tool that looks like this:

Notice that the mouse pointer is changed to a "+" sign indicating the Head Line tool is active. This tool will allow you to draw a line on the grid and give it the proper elevation attribute. Start at one end of the 7.0 isopleth and click once then continue to click along the trace of the contour. When you reach the end, double click to complete the line. Every point you clicked to define the line will be represented by a small triangle. Next, put the mouse pointer anywhere on the line and double click to activate the "*Head Contour 1*" menu, then:

Main
   ➔ *Head Contour 1*
       Piezometric Heads
          Head *[7] - Enters the head value of seven for the contour line just drawn*
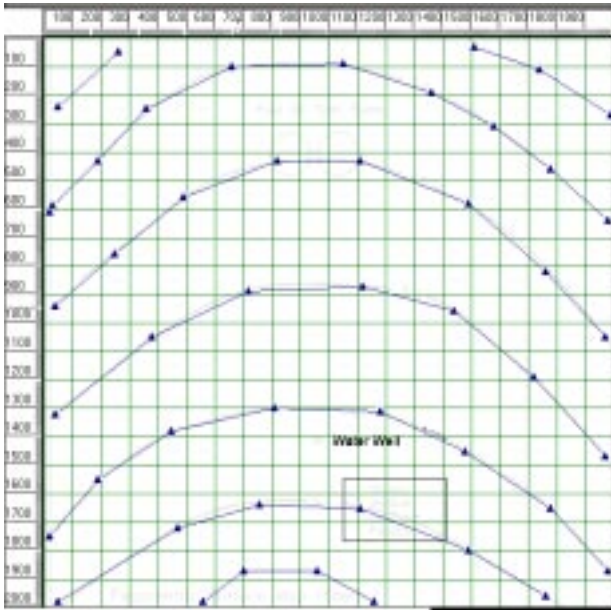
Figure 3.2 Entering Piezometric Head Data
Using the Line Tool.

Repeat the process by drawing on top of each contour (3 through 7 ft.) shown on the base map. Remember, after drawing a line you need to append the elevation attribute to the line otherwise a default value of "0" will be entered for that isopleth. If desired, you can enter values for the 2 and 8 foot elevations by interpolating the approximate location of those contours. Note that regions of constant (uniform) elevation can be introduced by using the Area Head tool that looks like this:

When finished tracing the contours your screen should appear something like that shown in Figure 3.2. Next, click on **<Main>** to return to the Main Menu. A File (Case) Save automatically Krigs all entered data using the default Kriging procedure. Custom (selected) Kriging can also be performed as follows:

Main
   ➔ *Grid*
      ➔ *Select Kriging*
          ➔ *Observed Heads* **<Quick Kriging> <OK>** - Selects the Kriging method
            used to interpolate entered head values across the grid.

The next time the file is saved the observed head values just entered will be automatically interpolated across the grid using the selected Kriging technique. Save now:

Main
   ➔ *File* **<Save>**

Now, let's check the hydraulic head system we just defined:

Main

      ➔ *Grid*

            ➔ *Observed Heads <2-D Contours>*

A color shaded map will appear on the screen showing the hydraulic heads across the site in 2-dimensions as shown in Figure 3.3. Note that the value of any cell can be viewed by clicking on that cell or group of cells (click and drag over a window). Contours can also be viewed in a three dimensional perspective by:
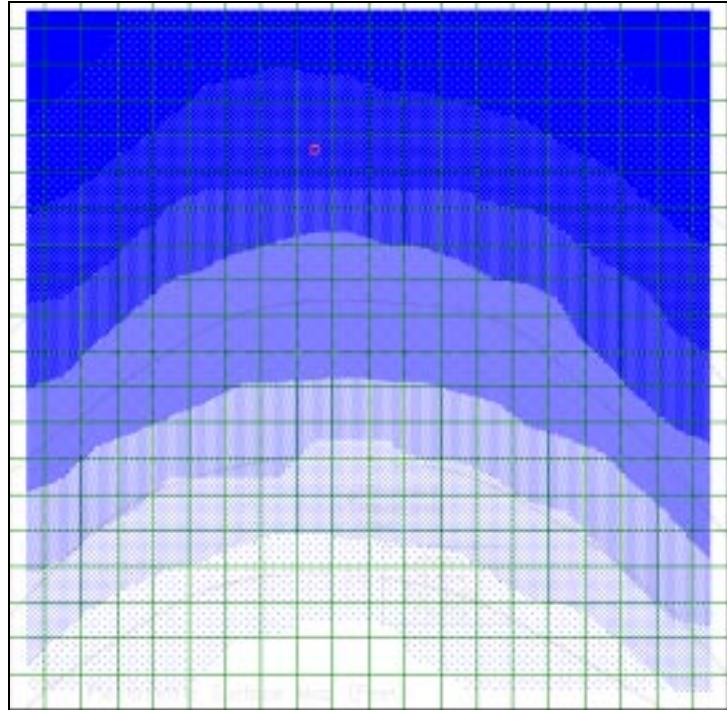
Main

      ➔ *Grid*

            ➔ *Observed Heads <3-D Contours>*

or by:

Main

      ➔ *Grid*

            ➔ *Observed Heads <3-D Distribution>*

Figure 3.3 Kriged Piezometric Head Contour Map.

Return to the main menu by clicking on the **<Main>** button. Next, let's check to see if certain distributed aquifer properties have been entered correctly:

Main

      ➔ *Grid*

            ➔ *Distributed Properties*

                  ➔ *Horiz. Hydraulic Conductivity <2-D Contours> - Click on any cell to read a value of 3e-4* **<Main>**

Continue going through each element of the *Main* ➔*Grid* ➔*Distributive Properties* submenu to check for each of the following values:

- Storage Coefficient = 0.20

- Effective Porosity = 0.20
- Longitudinal Dispersivity = 0.0
- Horizontal Hydraulic Conductivity = 0.0003

If there are any deviations from the values listed above return to ➔*Domain* and track the problem down. For the current model, these distributed properties are constant across the site. By introducing log points, variations in these parameters can be introduced to the grid. To view these options click on the existing log point:

> ➔ *Log Point 1*
> > ➔*Cross Section*
> > > ➔ *Stratum Properties*
> > > > ➔*Edit at Selected Elevation*

Note that horizontal hydraulic conductivity, storage coefficient, effective porosity, and longitudinal dispersivity can all be activated by clicking on the **<Activate>** box. When only one log point is entered these distributed properties are automatically defined as being constant across the grid. When more than one log point is used the log point values are interpolated across the grid by Kriging when the model is saved. Return to the *Main Menu* by clicking *<OK><OK>.*

3.3.3   Aquifer Thickness

For this simulation we want the base of the aquifer to be approximately 10 feet below the water table surface yielding ten feet of saturated thickness. To do this we'll need to enter a series of log points and define the base of the aquifer. Log points can represent actual well or core hole points; however, it is often convenient to add a sufficient number of additional "log points" to better define the condition of interest.

First, delete the existing log point. Using the mouse pointer, click on the log point symbol then press the *<Delete>* key*.* Click on the log point tool. Again, this button looks like this:

Click anywhere near the end of the 7.0 ft. contour line. Double click on the log point symbol you just inserted.

> ➔ *Log Point 1*
> > ➔*Cross Section*

Click on the upper dot next to the footage scale and drag it down to 7.0 ft. Click on the lower dot next to the footage scale and drag it up to the -3.0 ft level. The aquifer is now defined as being 10 foot thick at that point. Add five to ten additional log points along the 7.0 foot contour line. Continue by adding about the same number of log points to each of the other contour lines. For each log point drag the upper dot to the elevation of it's associated contour line and set the bottom

dot 10 feet below the top. When you're finished the log point distribution should look something like Figure 3.4.
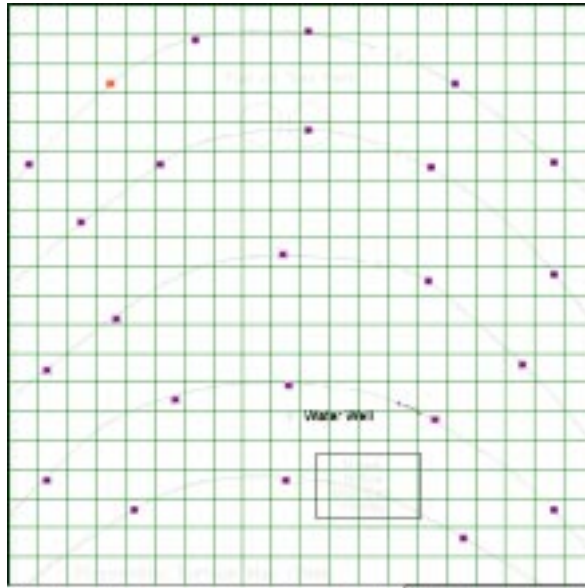
Figure 3.4 Example of Log Point Distribution to Define
Top and Bottom of Aquifer.

Next, the thickness values we just entered need to be geostatistically distributed across the grid. Let's use Select Kriging as follows:

Main
> ➔ *Grid*
>> ➔ *Select Kriging*
>>> ➔ *Cross-Sectional Parameters*
>>>> **Parameter**
>>>>> **[Elevation]** - *Selects elevation as the current Kriging parameter*
>>>> **Kriging Options**
>>>> **<Quick Kriging>**
>>> **<OK>**

Main
> ➔ *File* **<Save>**

Now check aquifer thickness by observing graphical output:

Main
> ➔ *Grid*
>> ➔ *Layer Thicknesses*
>>> ➔ *2D Contours*

After viewing aquifer thickness return to **Main**. Experiment a little by slightly changing one or more log point elevations, but ultimately return to about a 10 foot thickness across the grid.

3.3.4   Steady-State Simulation

We are now finally ready for the first model run. From the **Main Menu** click on **Simulator**. Notice that Bioplume III is "grayed out" indicating that the program is not yet available (operational). A number of steps must be visited prior to the simulation, and the Platform assists you by not allowing you to skip a step. Before any simulation can be run the following set of initial conditions must be defined:

Main
    →Initial Conditions
        → Simulation Period
            Ending Time [10] - *Sets simulation period to 10 years*
            <OK>
Main
    → Initial Conditions
        → Starting Heads
            Use Observed Values - *Should be checked*
            <OK>
Main
    → Initial Conditions
        → Starting Concentrations - *Use Observed Values should be checked*
 <OK>

Next, we move on to the simulator:

    → Simulator
        → Bioplume III
            Data Set Heading <Static Piezometric Surface >
            Runtime Options
                → Time Parameters
                    Maximum No. of Time Steps [10] - *Divides model run observation periods into ten one year increments which will can be viewed sequentially after the simulation is concluded.*
                    Time Increment Multiplier [0] - *Not used*
                    Initial Time Step in Seconds [0] - *Not used for steady state runs but should be set to 3,600 for transient conditions*
                    <OK>
                    Steady State Run ☯ - *Should be checked indicating steady state conditions*
                → Execution Parameters
                    No. of Iteration Parameters [7]

> ***Convergence Criteria*** [.001]
> ***Maximum No. of Iterations*** [100]
> ***Maximum Cell Distance per Move of Particles*** [0.50]
> ***Maximum No. of Particles*** [3000]
> ***No. Particles per Node*** [16] **<OK>**
>> ➔ ***Program Options***
>>> ***Time Step Interval for Complete Printout*** [1] *- All other input items in this submenu should be equal to zero.* **<OK>**
>> ➔ ***Transport Subgrid*** *- Not used. Default values only* **<OK>**
>> ➔ ***Biodegradation*** *- Not used in this simulation. Oxygen, nitrate, ferric iron, sulfate, and carbon dioxide all should be checked* **<Inactive> <OK>**
> ➔ ***Save Data and Run Simulation***

The translator to generate the BIOPLUME III input stream from the graphics files has now been executed. If successful the following message will appear "Program Terminated with exit code 0". Click **<Yes>.**

A second window will open stating that the Input File name is BIOP3in.dat; the ASCII Output File name is: BIOP3out.dat; and that the Graphical Output File name is BIOP3g.dat. <u>BIOPLUME III is now running</u>. Notice a black cursor square in the Input/Output window. While BIOPLUME III is running this square is solid. When the simulation is complete the cursor square will begin to blink. When the simulation is completed close the BIOPL3.exe window:

BIOPL3.exe
> ➔ ***File***
> **<Exit>** *- Exits the window*
> **<No>** *- Does not save the Input/Output window*

The window "PBIOP3" will pop up on the screen and begin scrolling a series of variable values. Upon completion the following message will appear "Program Terminated with exit code 0. Exit Window?". Enter **<Yes>.**

Model results can be graphically viewed immediately upon completion of the simulation. Recall, that in this first test only a steady state hydraulic head surface was modeled. To see the results:

Main
> ➔ ***Results***
>> ➔ ***Hydraulic Heads*** **<2-D Contours>**

The simulated static water level should look a lot like the piezometric surface shown on the site base map. Because we specified steady-state conditions the piezometric surface does not vary with respect to time; however, one can view different time steps by using these icons (the opening snap shot is always the last time step):

For those familiar with the program output file, the ASCII output file generated by BIOPLUME III can also be accessed and viewed within the Platform as follows:

➜ *File* **<Report>** *- After viewing* **<OK>**

Finally, graphics are good but graphics together with numerical values are even better: with the cursor in the "spy glass" mode (data tool in the tool box, top right corner), **<click and drag>** over a window of grid cells; **<release>**, and a spread sheet table with the corresponding hydraulic head values appears, graphics and numbers all at once as shown in Figure 3.5.
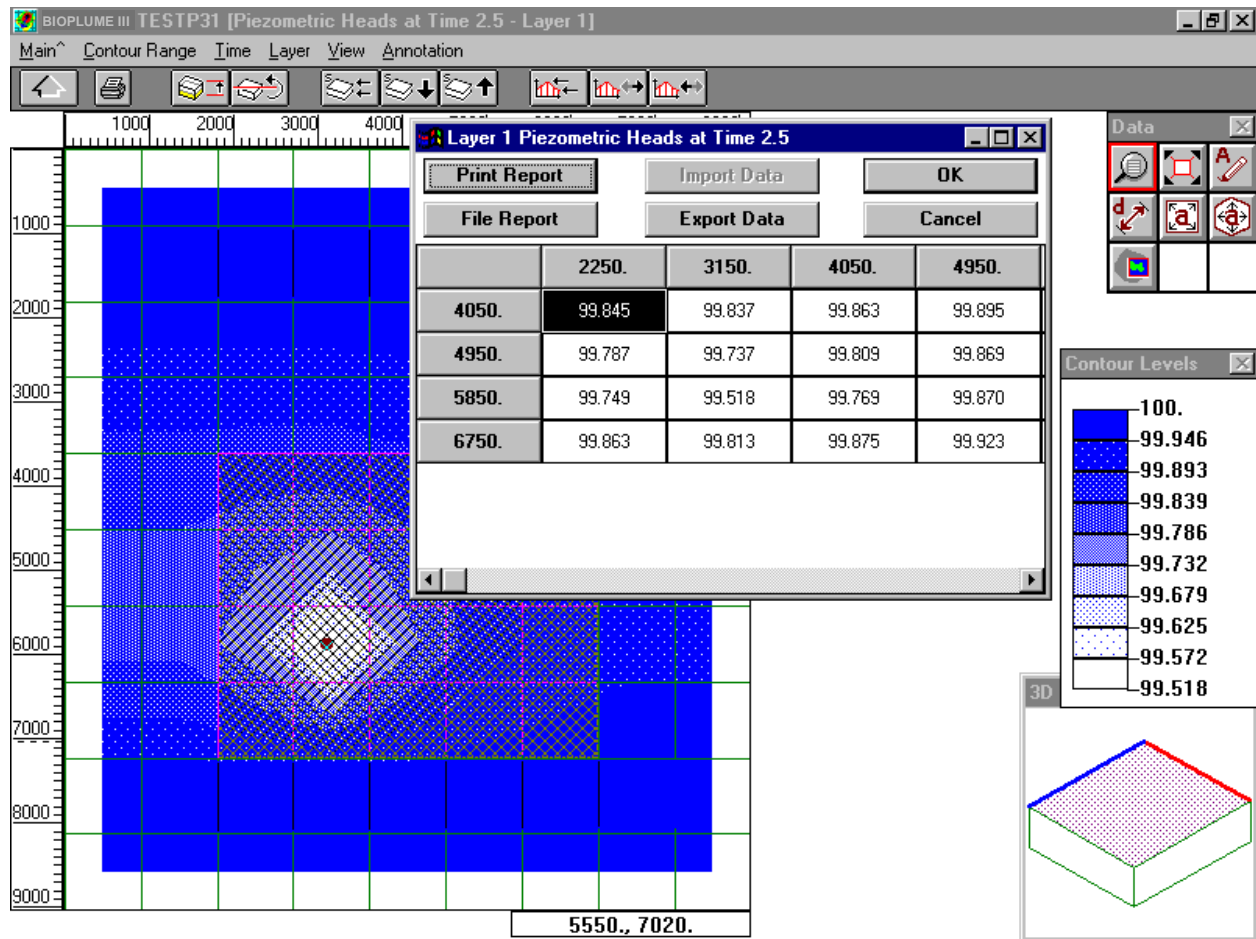
Figure 3.5 Spread-Sheet Representation of Simulated Hydraulic Heads.

After viewing, go back to **<Main>**.

3.4   Session 3: Non-Attenuated Hydrocarbon Mass Transport

3.4.1   Observed Contaminant Plume Addition

In this session we will build on the existing model by introducing a hydrocarbon source to the system. First, the source will be modeled as a single pulse of hydrocarbon. Later, a constant source of contamination will be examined.   At this time the solute will be modeled with retardation effects but without biological attenuation. If you do not already have case *Test01* active then open the file now (or go to the previous section and create it):

Main
>   ➔ *File*
>   ➔ *Open* **<Test01> <OK>**

First, save this simulation to a new file name:

Main
>   ➔ *File*
>   ➔*Save As* **<Test02> <OK>** - *Saves current session as Test02.*

Next, change the base image to show the current distribution of hydrocarbon contamination at the site:

>   ➔ *Domain*
>   ➔ *Base Image*
>   ➔ *Select*
>   ➔ *From File* **<Test02.bmp>**

A new site map should appear on the work space showing the distribution of the hydrocarbon plume as shown in Figure 3.6. As in **Session 1,** register the image to adjust it to the model coordinate system.

First, we need to revisit the *Domain* menu to establish the range and default values for hydrocarbon.

Figure 3.6 Contaminant Distribution Image.
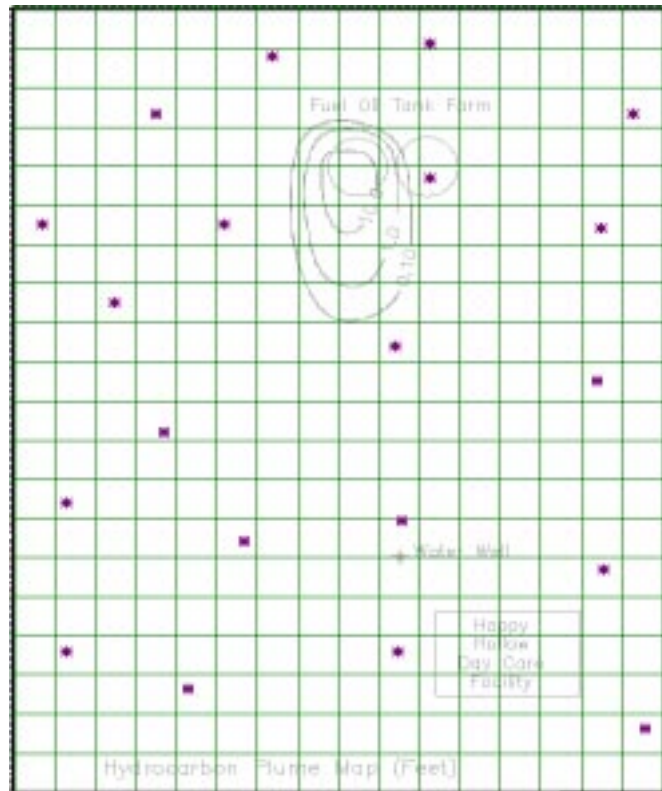
Main

→ ***Domain***

   → ***Loading Domain***

      → ***Concentrations***

         Default [0] - *Sets default concentrations for all contaminants and electron acceptors to 0 mg/L or ug/L. Note that the units can be either mg/L or ug/L but that those units must be consistent for the organic contaminant as well as for all electron acceptors. For this example we use units of mg/L.*

         Minimum [0] - *Sets minimum concentration to 0 mg/L*

         Maximum [100] - *Sets maximum concentration to 100 mg/L*

         Ruler Tic Increments

            Major [10] - *Sets major tic increments on concentration graphs in 10 mg/L units*

            Minor [2] - *Sets minor tic in increments of 10 mg/L each between each major tic increment*

         Cursor Increment [2] - ***<OK>*** *Permits graphical changes in concentrations in 2 mg/L increments*

59

➔ *Domain*
    ➔ *Chemical Species*
        ➔ *Contaminant*
            ➔ *Reaction*

                <Linear Isotherm> - *Establishes that contaminant will interact with soil according to linear sorption.*

                ➔ *Sorption Parameters*

                    Distribution Coefficient [0.093] <OK> - *Sets approximate retardation factor (Rf) of 2 by solving the equation Rf = (1+(bulk density * distribution coefficient)/porosity).*

                ➔ *Bulk Density*

                    Bulk Density [2.14] **<OK> <OK> <OK>** - *Here we assume the aquifer is comprised of quartz sand (2.68 g/cm^3) with 20% porosity. Therefore, the bulk density is 2.68 x (1-0.20) = 2.14 g/cm^3.*

➔ *Domain*
    ➔ *Define Strata*
        ➔ *Transport Properties*

            Dispersivity [10]

            Dispersivity Ratio [0.10] - *Ratio of transverse to longitudinal dispersivity is 1:10 or 0.10*

            Vertical Dispersivity Ratio [1] - *Not used*

            Molecular Diffusion [0] - *Not used*

            Bulk Density (g/cm^3) - [2.14] **<OK> <OK>**

    ➔ *File* **<Save>**

(For more information on these parameters see Section 4, Theoretical Development, and Appendix B, Air Force Intrinsic Remediation Protocol Implementation).

Now, we will graphically introduce hydrocarbon concentrations to the grid with a slight modification of the procedure used in developing the piezometric surface in **Session 2**. Recall, that earlier we traced over the piezometric surface using the line tool. Here we use that technique again; but for concentrations it is also necessary to specifically define the area outside the plume as having zero concentration.

To begin this process:

    ➔ *Loading*
        ➔ *Observed Concentrations*
        ➔ *Hydrocarbon*

Select the Concentration Area Tool from the tool box. It looks like this:

Begin by clicking just <u>outside</u> of the 0.10 contour line. Continue tracing around that isopleth by clicking a point about every ¼ - inch. Then extend the field around the perimeter of the grid. When you have traced nearly all the way back to your point of origin double click to exit the Concentration Area Tool. The traced area should appear shaded with small triangles representing line points. Next, double click anywhere on the shaded area to activate the ***Concentration Contour 1*** dialog box:

➔***Concentration Zone 1***
    Concentrations
        Concentration [0] - *Enters 0 mg/L concentration for the area defined just outside of the plume.*

Next, use the Concentration Line Tool to specify the concentrations of the plume. Recall that the Concentration Line Tool looks like this:
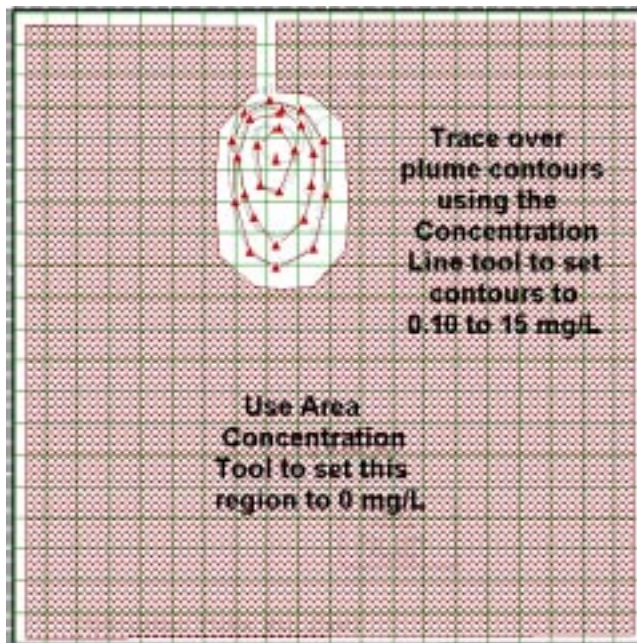
After clicking on the Concentration Line Tool, trace over the top of the 0.1 mg/L contour line and double click when finished. Next, double click on the line you've just drawn and enter a concentration of 0.10. Repeat this process with the 1 and 10 mg/L contour lines. Finally, click on the concentration line tool one more time and add a single point in the center of the plume giving it a value of 15 mg/L. The finished product should look something like Figure 3.7.

Figure 3.7 Example of Establishing Hydrocarbon Distribution Over the Grid.

Finally, you'll need to distribute the input hydrocarbon concentrations just entered to the grid:

➔ *Grid*
　　➔ *Select Kriging*
　　　➔ *Observed Concentrations*
　　　　➔ *Hydrocarbon* **<Quick Kriging> <OK>** - *Selects Kriging Method.*
➔ *File* **<Save>** - *Saves session, automatically Krigs data and extrapolates concentration values to grid.*

Next, we want to view and check the concentrations just entered:

➔ *Grid*
　　➔ *Observed Concentrations*
　　　➔ *Hydrocarbon*
　　　　➔ *2-D Concentrations*

A 2-dimensional shaded contour map should appear on the work space showing hydrocarbon concentrations that looks like Figure 3.8. You can click on any cell to view the concentration at that point. Note that in some areas several contour lines passed through a single cell; however, the Platform has assigned a single concentration value to that cell from the latest contour line. If the concentrations are not what you want, you can always modify or delete the old contours.
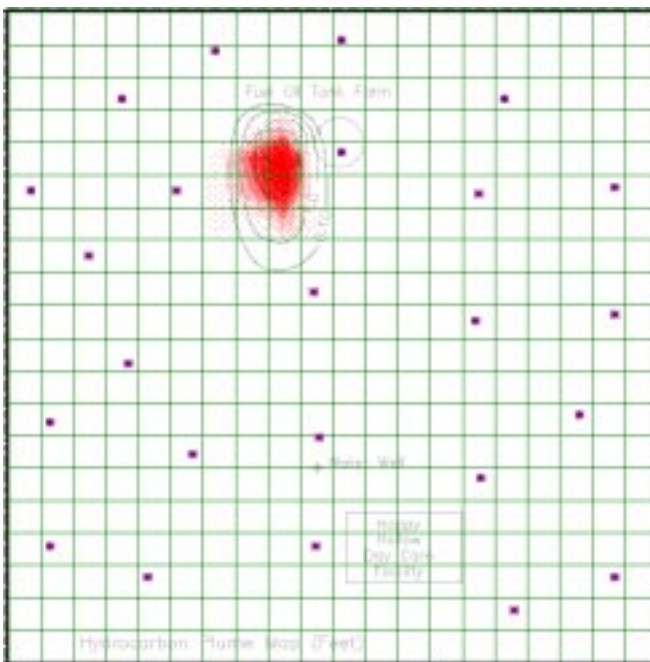
Figure 3.8 Example Kriged Hydrocarbon Distribution**.**

It is a good idea to check on the condition of the piezometric head distribution under *Main* ➔ *Grid* ➔ *Observed Head* ➔ *2D Contours*. If the head distribution looks correct then return to the Main Menu. Otherwise go through the Kriging process again for the piezometric surface under *Main* ➔ *Grid* ➔ *Select Kriging* ➔ *Observed Heads*. When finished return to the *Main Menu*.

3.4.2   Transport Execution and Results

You are now ready to run the mass transport simulation. As above, step through the ***Initial Conditions*** menus:

Main
    ➔***Initial Conditions***
        ➔ ***Simulation Period***
            ***Ending Time* [10] -** *Sets simulation period to 10 years*
            <OK>
Main
    ➔ ***Initial Conditions***
        ➔ ***Starting Heads***
            Use Observed Values - *Should be checked*
             <OK>
Main
    ➔ ***Initial Conditions***
        ➔ ***Starting Concentrations*** - *Use Observed Values should be checked*
        <OK>

Finally, we need to check the simulation run time parameters and run the model:

    ➔ ***Simulator***
        ➔ ***Bioplume III***
            Data Set Heading [Static Piezometric Surface]
            Runtime Options
                ➔ ***Time Parameters***
                    Maximum No. of Time Steps [10]
                    Time Increment Multiplier [0]
                    Initial Time Step in Seconds [0]
                    Steady State Run ☻✓]
                ➔ ***Execution Parameters***
                    No. of Iteration Parameters [7]
                    Convergence Criteria [.001]
                    Maximum No. of Iterations [100]
                    Maximum Cell Distance per Move of Particles [0.50]
                    Maximum No. of Particles [3000]
                    No. Particles per Node [15] **<OK>**
                ➔ ***Program Options***
                    Time Step Interval for Complete Printout [1] *- All other input items in this submenu should be equal to zero.* **<OK>**
                ➔ ***Transport Subgrid*** *- Not used. Default values only* **<OK>**
                ➔ ***Biodegradation*** *- Not used in this simulation. Oxygen, nitrate, ferric iron, sulfate, and carbon dioxide all should be checked* **<Inactive> <OK>**

The WBIOP3 window will pop up to translate the graphics files into BIOPLUME III input stream. When the translation is complete the following message will appear "Program Terminated with exit code 0". Click **<Yes>**. The BIOPL3.EXE window will pop up indicating that BIOPLUME III is running. When the simulation is complete the black cursor square will begin to blink. When the simulation is completed close the BIOPL3.exe window (and the input/output window):

BIOPL3.exe
      → *File*
      <Exit> - *Exits the window*
      <No> - *Does not save the Input/Output window*

The window "PBIOP3" will pop up on the screen and begin scrolling a series of variable values. Upon completion the following message will appear "Program Terminated with exit code 0. Exit Window?." Enter **<Yes>**. The simulation is complete and model results can now be viewed graphically:

Main
      → *Results*
            → *Concentrations*
                  Hydrocarbon <2-D Contours>
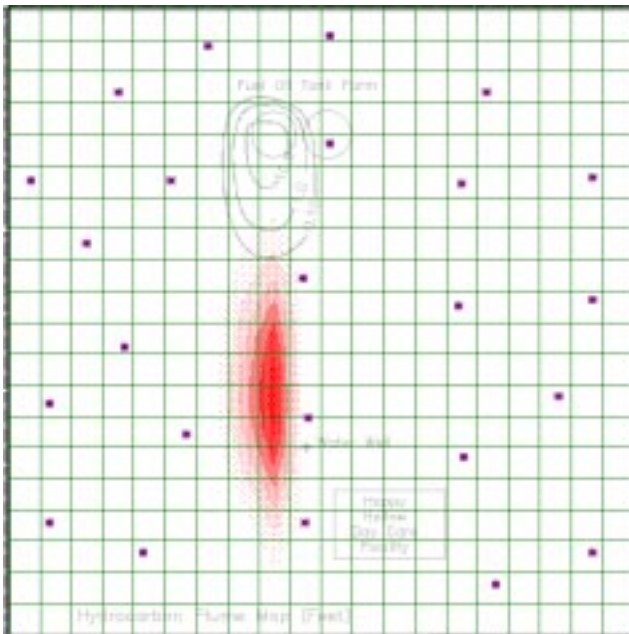
The initial view will be the predicted hydrocarbon concentration at 10 years which should look something like Figure 3.9. Various time steps can be viewed by clicking on the following buttons:

After viewing **<Main>**.

Figure 3.9 Simulated Hydrocarbon Plume in 10 Years.

3.4.3   Constant Source Addition

Now we will set up the model to simulate a constant contaminant source. If you do not already have *Test02* active then open that file now:

Main
> ➔ *File*
>> ➔ *Open* <Test02> <OK>

First, save this simulation to a new file name, as *Test03*:

Main
> ➔ *File*
>> ➔*Save As* <Test03> <OK> - *Saves current session as Test03.*

Next, we need to erase (delete) all existing hydrocarbon concentration values:

Main
> ➔ *Loading*
>> ➔ *Observed Concentrations*
>>> ➔ *Hydrocarbon*

Click on the shaded area concentration then press **<Delete>**. Click on each of the line concentration values and also press the delete button.   This will remove all observed concentration values from the grid. Return to the ***Main*** menu. Click on the source tool that looks like this:

The cursor will change to a "+" symbol. Trace around the 10 mg/L concentration contour. When you've finished double click to complete the polygon. Next, double click again on the shaded area to bring up the *Source 1* menu. Then:

Source1
> ➔ *Loading*
>> ➔ *Concentration*
>>> **[Hydrocarbon]** - *Defines the current source as being for hydrocarbon. Sources can be applied for each electron acceptor independently under this option.*
>>> ➔ *Set Value - A graph will appear. Click on the red dot and drag it vertically up to the 10 mg/L mark. This sets the constant source of hydrocarbon at 10 mg/L.*
>>> **<OK>**

<OK>

Main

➔ ***File* <Save>**

Figure 3.10 Simulated Hydrocarbon Plume as
Constant Source.

You're ready again to run the
simulation. Repeat the steps listed in
Section 3.4.2 above. This time the
results for a 10 year migration period
look like Figure 3.10.

3.5   Session 4: Simulated Microbial Attenuation

3.5.1   Addition of Electron Acceptors

We have previously developed a model simulating flow and non-attenuated hydrocarbon mass transport. Now we will take the process one step further by introducing biological degradation that will be stoichiometrically balanced against Oxygen and Sulfate reduction. First, create a new file:

Main
>   ➔ ***File***
>   ➔ ***Open*** **<Test02> <OK>**

Save this simulation to a new file name:

Main
>   ➔ ***File***
>   ➔***Save As*** **<Test04> <OK>**

For this simulation we assume that the original concentration of dissolved oxygen and sulfate in the ground water is 8 and 80 mg/L respectively. Additionally, here we assume that the general chemical equation for the hydrocarbon solute is C_7H_8 (toluene). Therefore, the stoichiometric expression for complete mineralization of toluene with oxygen is (for additional information see Section 4, "Theoretical Development," and Appendix B, "Air Force Intrinsic Remediation Protocol"):

$$C_7H_8 + 9O_2 \implies 7CO_2 + 4H_2O$$
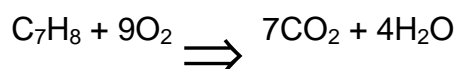
Here, 9 molar volumes of molecular oxygen are required to convert 1 mole of organic to carbon dioxide and water. <u>BIOPLUME III reactions are assumed to be on a mass per mass basis.</u> By conversion we see that:

$$C_7H_8 = 92 \text{ g/mole so } 92 \text{ g/mole} * 1 \text{ mole} = 92 \text{ g}$$
$$O_2 = 32 \text{ g/mole so } 32 \text{ g/mole} * 9 \text{ moles} = 288 \text{ g}$$

Therefore, the mass/mass ratio of oxygen to organic is 288 g/ 92 g = 3.1. In this case, 3.1 mg/L oxygen is needed to oxidize 1 mg/L hydrocarbon.

The stoichiometric expression for sulfate reduction, assuming hydrogen sulfide (H_2S) production, is:

$$C_7H_8 + 3.67SO_4 \Longrightarrow 7CO_2 + 3.67H_2S + 0.33H_20$$
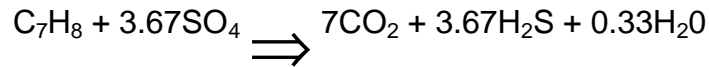
Here, 3.67 moles SO_4 oxidize 1 mole C_7H_8. Converting to a mass/mass basis yields 3.8 mg/L sulfate required to oxidize 1 mg/L toluene. Other assumptions used here are that:

- Oxygen is used before sulfate;
- Oxygen and sulfate concentrations are initially constant across the entire grid;
- Oxygen reacts instantaneously with hydrocarbon according to the stoichiometry expressed above;
- Sulfate reacts with hydrocarbon according to a first order rate constant of 0.001.

As with the sessions above, to begin the model we need to make some changes under the **Domain** directory related to electron acceptor reaction parameters:

➢ ***Domain***
    ➢ **Chemical Species**
        ➢ *Electron Acceptors*
            ➢ *Oxygen*
                ➢ *Reaction* **<No Sorption Isotherm> <No Decay> <No ion exchange> <OK>**
                ➢ *Interaction*
                    Stoichiometric Ratio of Electron Acceptor to Hydrocarbon [3.1]
                    Electron Acceptor Threshold [.50] - Sets minimum level that aerobic bacteria can remove oxygen to 0.50 mg/L
                    First Order Decay Rate [0]
                    Maximum Hydrocarbon Utilization [0]
                    Hydrocarbon Half-Saturation [0]
                    Electron Acceptor Half Saturation [0]
                    Microbial Concentration [0]
                    Retardation Factor for Microorganisms [0]
                    <OK>
            ➢ *Sulfate*
                ➢ *Reaction* **<No Sorption Isotherm> <No Decay> <No ion exchange> <OK>**
                ➢ *Interaction*
                      Stoichiometric Ratio of Electron Acceptor to Hydrocarbon [3.82]
                    Electron Acceptor Threshold [0]
                    First Order Decay Rate [.001]
                    Maximum Hydrocarbon Utilization [0]

Hydrocarbon Half-Saturation [0]
Electron Acceptor Half Saturation [0]
Microbial Concentration [0]
Retardation Factor for Microorganisms [0]
<OK>
<OK>

Next, we need to define the concentrations of oxygen and sulfate across the grid. This is done in two phases. First, the current concentration of oxygen and sulfate must be entered:

➔ *Loading*
    ➔ *Observed Concentrations*
        ➔ *Oxygen*

Select the Area Concentration Tool from the Tool Box:

Beginning in one corner of the grid draw a square encompassing the entire grid area. When complete, double click to end. Place the cursor on the shaded square and double click again. Then:

Concentration Zone 1
    Concentration
        Concentration [8.0] - *Enters a value of 8.0 mg/L for the concentration of oxygen across the entire grid.*
    <OK>
<Main>

Repeat the process for sulfate:

➔ *Loading*
    ➔ *Observed Concentrations*
        ➔ *Sulfate*

As with oxygen use the Area Concentration Tool in the Tool Box to enter the concentration attribute of 80.0 mg/L for sulfate then return to the **Main** menu.

The concentrations of oxygen and sulfate we just entered are mobile solutes. Without the addition of a source, oxygen and sulfate would "migrate" off the grid so that some areas near the grid boundary would have little or no electron acceptor concentrations over time. To eliminate that problem a source of electron acceptors must be added. In the **Main** menu click on the **Recharge** tool in the **Tool Box**:

The cursor will change to a "+" symbol. Draw a rectangular shape covering the top row of constant head cells. When finished, double click to end. Place the cursor on the shaded area and double click again to activate *Recharge Region 1*. From that point:

Recharge Region 1
       Loading
              ***Concentration* [Oxygen]** - *Selects oxygen as the source parameter*
                  ➔ *Set Values*
                      ***Concentration* [8.0]** **-** *Using the cursor you can click on the red dot and move it vertically up to the 8.0 mg/L level on the graph or you can directly enter 8.0 mg/L .*
                      <OK>
              ***Concentration* [Sulfate] -** *Selects sulfate as the source parameter.*
                  ➔ *Set Values*
                      ***Concentration* [80.0]** **-** *Using the cursor you can click on the red dot and move it vertically up to the 80.0 mg/L level on the graph also.*
                      <OK>
<OK>

Repeat this process by introducing recharge areas to the constant head cells on the bottom, left, and right grid cells. Define the concentration for each area as 8.0 mg/L oxygen and 80 mg/L sulfate. When finished the grid should look like Figure 3.11.
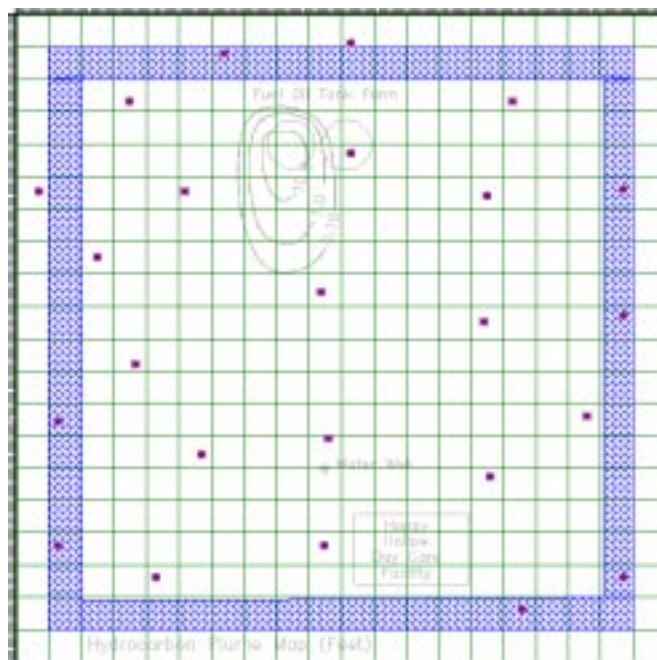
Figure 3.11 Addition of Electron Acceptor Source Areas.

Next, the Kriging Method needs to be selected for each electron acceptor:

> **➔ Grid**
> > **➔ Select Kriging**
> > > **➔ Observed Concentrations**
> > > > **➔ Oxygen <Quick Kriging> <OK>**
> **➔ Grid**
> > **➔ Select Kriging**
> > > **➔ Observed Concentrations**
> > > > **➔ Sulfate <Quick Kriging> <OK>**

> **➔ File <Save>** - *Saves and appends values entered for electron acceptor concentration to the grid.*

As above, we want to check the concentrations just entered to make sure there are correct:

> **➔ Grid**
> > **➔ Observed Concentrations**
> > > **➔ Oxygen**
> > > > **➔ 2-D Concentrations**

Click anywhere on the grid to see a cell concentration of 8 mg/L. **<Main>** Repeat the process to check sulfate:

> **➔ Grid**
> > **➔ Observed Concentrations**
> > > **➔ Sulfate**
> > > > **➔ 2-D Concentrations**

Click anywhere on the grid to see a cell concentration of 80 mg/L. **<Main>** Also, it's a good idea to check the hydrocarbon concentration and piezometric head distribution at this time under *Main* **➔** *Grid* **➔** *Observed Concentrations*. If these appear correct you're ready for the next step. If not, then re-Krig, save, and check the distribution again until correct.

3.5.2 Model Execution and Results

We are now ready to execute the simulation. As above, step through the Initial Conditions submenus in preparation for executing the simulation:

> **➔Initial Conditions**
> > **➔ Simulation Period <OK>**
> **➔ Initial Conditions**
> > **➔ Starting Heads <OK>**
> **➔ Initial Conditions**

➔ *Starting Concentrations* **<Use Observed Values> <OK>**

Finally, we need to check the simulation parameters and run the model:

    ➔ *Simulator*
       ➔ *Bioplume III*
          Data Set Heading **[Attenuated Hydrocarbon Model Test 04]**
         ➔**Runtime Options**
            ➔ *Time Parameters*
               Maximum No. of Time Steps [10]
               Pumping Period in Years [0]
               Time Increment Multiplier [0]
               Initial Time Step in Seconds [0] **<OK>**
            ➔ *Execution Parameters*
               No. of Iteration Parameters [7]
               Convergence Criteria [.001]
               Maximum No. of Iterations [200]
               Maximum Cell Distance per Move of Particles [0.50]
               Maximum No. of Particles [3000]
               No. Particles per Node [15] **<OK>**
            ➔ *Program Options*
               Time Step Interval for Complete Printout [1]
            ➔ *Transport Subgrid* **<OK>**
            ➔ *Biodegradation*
               Oxygen **<Instantaneous Reaction>**
               Nitrate **<Inactive>**
               Ferric Iron **<Inactive>**
               Sulfate **<First Order Decay>**
               Carbon Dioxide **<Inactive> <OK>**
       ➔ *Save Data and Run Simulation*
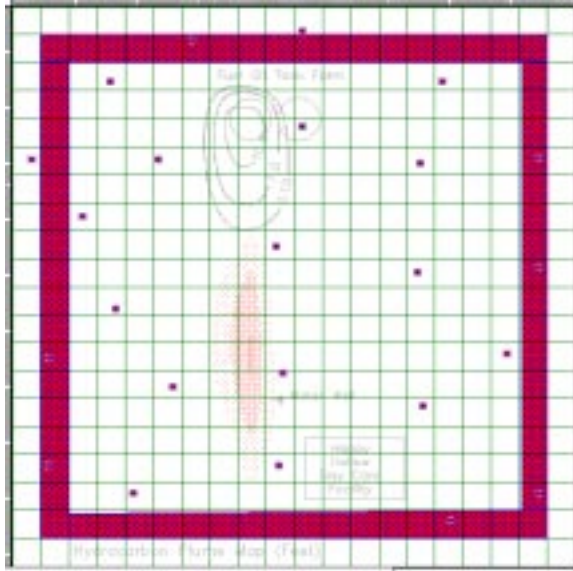
Figure 3.12 Simulated Hydrocarbon Plume at 10 Years Assuming Microbial Attenuation.

As discussed above, step through the WBIOP3, BIOPL3.EXE, and BIOPL3.exe windows. Model results can be viewed graphically under the Results menu. You'll note that the plume concentration for hydrocarbon is greatly diminished over the results obtained in Test02 (Figure 3.12). Additionally, you should see electron acceptor concentration sags for both oxygen and sulfate similar to those shown on Figures 3.13 and 3.14.
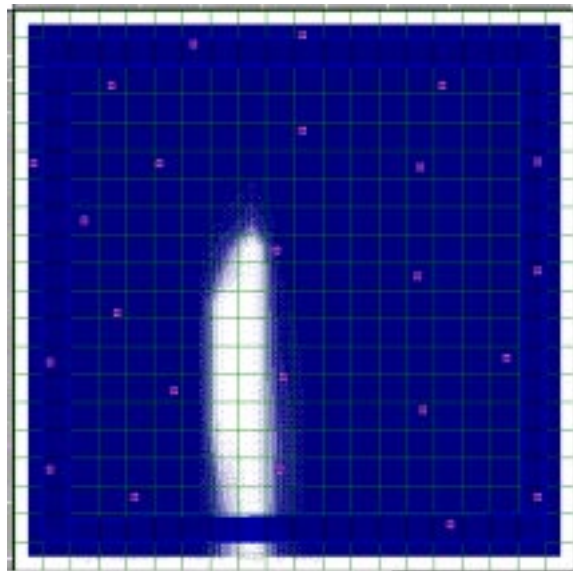
Figure 3.13 Oxygen Distribution Showing Reaction Sag.
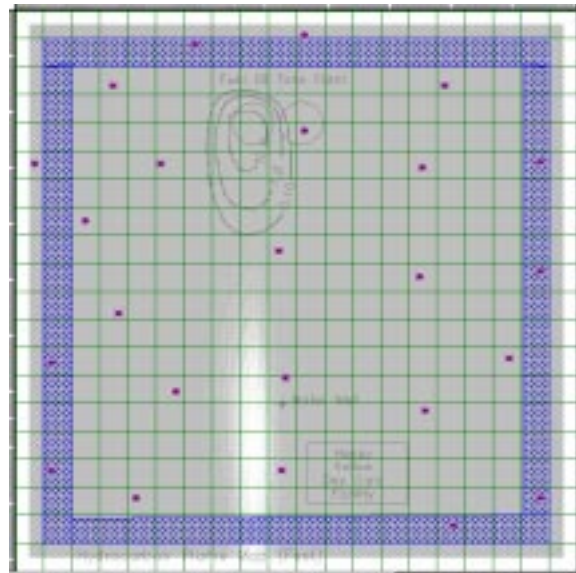
Figure 3.14 Sulfate Distribution Showing Reaction Sag.

3.6 Session 5: Special Features

A number of special features are available with the Graphical Platform that can be used to adapt a model to more closely simulate field conditions. In the *Main* menu, the *Tool Box* contains buttons that simplify the addition of lakes, rivers, and drains. The addition of these attributes to a simulation are discussed below. First, create a new file using the simulation developed in Session 2:

Main
> ➔ *File*
> > ➔ *Open* <Test02> <OK>

Save this simulation to a new file name:

Main
> ➔ *File*
> > ➔*Save As* <Test05> <OK>

3.6.1 Adding Wells

In this section we will examine the addition of a well to the simulation. It is necessary to define the pumping domain:

Main
> ➔ *Domain*
> > ➔ *Loading Domain*
> > > ➔ *Pumping Rates*
> > > > *Default* [0] - *Sets default pumping rate to 0 ft³/sec. <u>Note that all positive pumping rates are for pumping wells and negative rate numbers are for injection wells</u>*
> > > > *Minimum* [-0.1] - Sets default lower pumping rate on all well graphs to -0.1 ft³/sec.
> > > > *Maximum* [0.1] - Sets default maximum pumping rate on all well graphs to 0.1 ft³/sec (44.8 gpm).
> > > > *Ruler Tick Increments*
> > > > > *Major* [.1] - Sets one major tic increment at .1 ft³/sec.
> > > > > *Minor* [.02] - Divides the one major tick increment into 10 minor units for all pumping graphs
> > > > *Cursor Increments* [.02] - Permits graphical adjustment of pumping rates for all wells in increments of .02 ft³/sec.
> > ➔ *File* <Save>

On the button bar find and click on the well icon button that looks like this:

Note that the normal mouse pointer changes to a circle shape. Point the cell on the grid containing the water well at coordinates (1,510, 1,010) and click. The circle shape will be transferred to the grid and now represents a new injection or withdraw well. Note that the mouse cursor returns back to its normal configuration. Next, place the cursor on the well and double click which will open the *Well 1* menu.

For this example we'll set up two separate stress periods of five years each. For the first five year period the well will not be pumped. For years six through ten the well will be produced at 0.02 ft^3/sec. First we need to define the stress periods.

> *Well 1*
>> ➔ *Time Steps*
>>> ➔ *Add Timestep* **<Add> [5]** - *Defines a new stress period beginning after the fifth year.*
>> **<OK>**

Note: Although many stress periods can be added all must be of equal duration. For example, in the current simulation we could define five stress periods; however, each period would need to be set at two years. Considerable pumping versatility can be achieved by defining many stress periods and setting the same discharge rate for several sequential periods.

Next, the discharge rate for each time step must be specified. Continuing in the *Well 1* menu, click on *Pumping Rates.* It is possible to manually enter the pumping rates by clicking on the *Time* period desired then entering the discharge value under *Rate*. These values can also be easily entered graphically. On the displayed graph click on the small dot at time zero and hold down on the mouse button. While holding the button drag the dot to the zero pumping rate value. Next, click on the dot at time five and drag it up to 0.02. Click on **<OK><OK>** to return to the *Main* menu.

Though not needed in the current example, note that in the *Well 1* menu concentrations of contaminants and electron acceptors could also be introduced to the simulation by direct injection. Injection, however, requires a negative pumping rate.
We are ready to run the simulation again. First, update the current simulation by saving the file:

Main
> ➔ *File* **<Save**⟩

As always, it's a good idea to check the condition of the head and hydrocarbon distribution under *Main* ➔ *Grid* ➔ *Observed Heads or Observed Concentrations*. If all is correct proceed with the simulation:

Main
>*→Initial Conditions*
>>*→ Simulation Period <OK>*

Main
>*→ Initial Conditions*
>>*→ Starting Heads <OK>*

Main
>*→ Initial Conditions*
>>*→ Starting Concentrations <OK>*

Main
>*→ Simulator*
>>*→ Bioplume III*
>>>*Data Set Heading* **<Pumping well test with no biodegradation>**
>>>**→Runtime Options**
>>>>*→ Time Parameters*
>>>>>***Maximum No. of Time Steps*** [5] - Sets 5 time steps for each of the two stress periods or one time step per year for the 10 year duration of the simulation.
>>>>>***Pumping Period in Years*** [0]
>>>>>***Time Increment Multiplier*** [0]
>>>>>***Initial Time Step in Seconds*** *[0]* **<OK>**
>>>>*→ Execution Parameters*
>>>>>***No. of Iteration Parameters*** [7]
>>>>>***Convergence Criteria*** [.001]
>>>>>***Maximum No. of Iterations*** [200]
>>>>>***Maximum Cell Distance per Move of Particles*** [0.50]
>>>>>***Maximum No. of Particles*** [3000]
>>>>>***No. Particles per Node*** [15] **<OK>**
>>>>*→ Program Options*
>>>>>***Time Step Interval for Complete Printout*** [1]
>>>>*→ Transport Subgrid <OK>*
>>>>*→ Biodegradation*
>>>>>***Oxygen* <Inactive>**
>>>>>***Nitrate* <Inactive>**
>>>>>***Ferric Iron* <Inactive>**
>>>>>***Sulfate* <Inactive>**
>>>>>***Carbon Dioxide* <Inactive> <OK>**
>>>*→ Save Data and Run Simulation*

Follow the steps outlined above to run through the model. After processing is complete, view the dynamic piezometric head under *→Results* as described above. The piezometric surface for the first five years should look like Figure 3.3 in Session 1. A cone of depression like that shown in Figure 3.15 should be evident for the last five year time period. Plume distribution should also manifest pumping effects:

Main
    ➔ *Results*
        Concentrations ➔
            ➔ *Hydrocarbon*
                ➔ *2 D Contours*
                    ➔ ***Contour Range* \<Span Current Timestep\>** - *Sets the range of hydrocarbon concentration contours to span the current time step.*

After viewing plume distribution return to the ***Main*** menu.
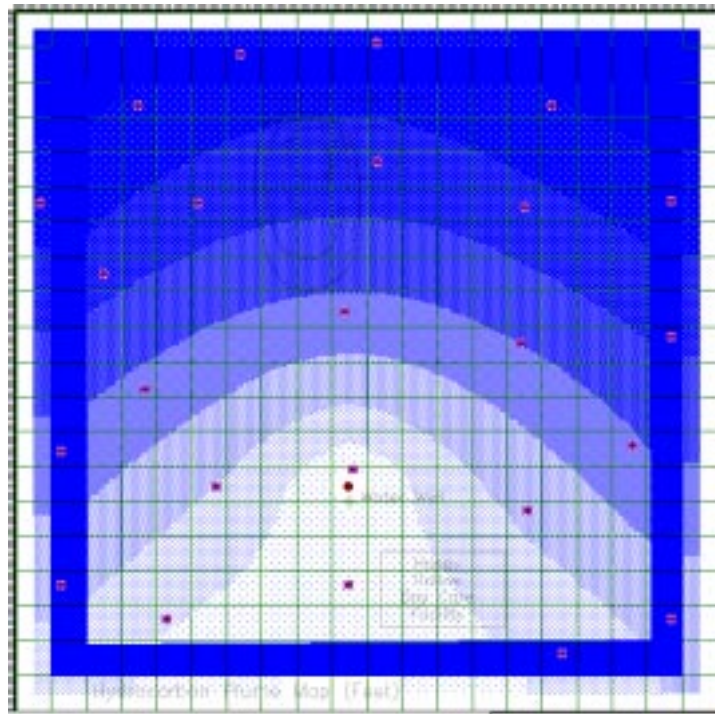
Figure 3.15 Head Distribution Under Pumping
Conditions.

3.6.2   Rivers, Drains, and Lakes

Rivers, drains, and lakes can easily be added to a simulation using special buttons located in the ***Tool Box***. These features are simulated by specifying designated cells to have constant head values and high hydraulic conductivity. Using special tools makes this application easier. For this example a river and lake will be added to the model. As in the examples above, start a new simulation based on Test02:

Main
    ➔ *File*
        ➔ *Open* **\<Test02\> \<OK\>**

Main
>➔ *File*
>>➔*Save As* **<Test06> <OK>**

Next, change the base image to Test04.bmp following the steps listed in Session 1. The new image should show the addition of a stream and lake.   Click on the *River Tool* in the *Tool Box* that looks like this:

The cursor should change to a "+" shape. Click on one end of Little Creek and continue clicking along the trace of the stream. When finished double-click exit the drawing mode. Place the cursor on the line you just drew and double click to activate the *River 1* menu:

River 1
>➔ *River Bed*
>>*Bed Level* [0] - Sets base of river at 0 but also diminishes the thickness of the aquifer concurrently. Therefore, value must be above the base of the aquifer.
>>*Thickness* [1]
>>*Hydraulic Conductivity* [.1]
>➔ *Loading*
>>➔ *Levels*
>>>*Surface Levels* [3] - Sets hydraulic elevation to 3. This item could also be set graphically.
>**<OK>**

A lake can be added in a simmilar manner. Click on the *Lake Tool* in the *Tool Box* that looks like this:

Again, the cursor should change to a "+" shape. Using the cursor, draw around Tiny Lake. When finished double click to end the drawing mode. Place the cursor on the lake area and double click again to activate the *Lake 1* menu. Then:

Lake 1
>➔ *Lake Bed*
>>*Bed Level* [4] - *Must be less than the thickness of the aquifer.*
>>*Thickness* [10]
>>*Hydraulic Conductivity* [.1]
>➔ *Loading*
>>➔ *Levels*

> **Surface Level** [6.5] - *Sets the hydraulic head to 6.5 feet defining the water surface of the lake.*

\<OK\>

We are now ready to run another simulation. Step through the Initial Conditions and Simulator menus as described in sections above. When the simulation is completed view the hydraulic heads under Results. A constant head value of 6.5 will be found in the lake area. Head contours will converge on the stream. An examination of the plume distribution with respect to time will show hydrocarbon intersecting and following the path of the creek.

3.7 Session 6: Video Animation

With the Windows 95 version of the Platform video animation of plume migration is possible. Through AVI animation, sequential time steps can be viewed in rapid succession.   To demonstrate this feature reopen Test04:

Main
>*➔ File*
>>*➔ Open* **[Test04]**

Go to *Main* *➔ Results*. If the Results submenu is inactive (grayed out) then:

Main
>*➔ File*
>>**\<Restore\>** - *Restores prior simulation results.*

If the *Results* submenu is still inactive you'll need to rerun the simulation. Now, assuming the *Results* submenu is now active view the hydrocarbon concentration plume:

Main
>*➔ Results*
>>*➔ Concentrations*
>>>*➔ Hydrocarbon*
>>>>*➔ 2 D Contours*
>>>>>*➔ Contour Range*
>>>>>>**\<Span Current Timestep\>**

Next, using the *Timestep* tool click back to view *Time 0*. Recall that the *Timestep* tool looks like this:
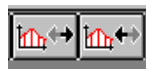
Next, capture this image by clicking on the ***Save Image*** tool in the ***Tool Box***. The save image tool looks like this:

The cursor will change to a large square shape. Identify a rectangular area on the grid of which you want to create an image. This area need not be the entire grid; however, the same area must be identified on successive time steps. So, whatever area you select to work with note the coordinates. For this session place the cursor over the cell in position (600, 300). Click and hold the mouse button. Drag down and to the right to the cell located at (1,800, 1,400) then release the mouse button. A shaded rectangle will appear over the blocked area and the ***Save Bitmap File As*** menu will pop up:

Save Bitmap File As
    ➔ ***File Name* [A.bmp] <OK>** - *Saves the designated grid area as a windows bit map under the file name "user00.bmp".*

Next, using the ***Timestep*** tool go to ***Time 1***. Click on the ***Save Image*** tool and block out the same grid range as before. This time save the image as "B.bmp". Repeat this process for each successive time step saving the images as "A.bmp" through "J.bmp". When finished return to the ***Main*** menu.

We are now ready to tie the sequential time steps together in a single video clip:

Main
    ➔ ***Results***
        ➔ ***Avi Animation***
            EIS Video Animation
                ➔ ***File***
                    ➔ ***Select Bitmap Files to Compile***
                    Select All Bitmap Files to Compile
                        ➔ ***Folders* <C:\eisbiop2\report>** **-** *Go to the designated subdirectory under the root of C: assuming \EISBIOP\Bioplume III was installed on the C: directory.*

While holding down on the "Ctrl" button on your keyboard use the mouse and click on the file names "A.bmp" through "J.bmp". When finished click on **<OK>.** The ***Save AVI Movie As*** menu will pop up:

Save AVI Movie As
    ***File Name* [Test.avi] <OK>**

The following message will appear "Done building AVI!" **<OK>.** To view the animation clip:

EIS\GWM Video Animation
➔ *File*
➔ *Open AVI* **[Test.avi]**
<OK>

The image of Timestep 0 will appear. To activate the animation sequence use the mouse to click on the "scissors" symbol in the lower left hand corner of the image.

4.0   BIOPLUME III THEORETICAL DEVELOPMENT

4.1   Overview

The BIOPLUME III model simulates aerobic and anaerobic biodegradation processes using oxygen, nitrate, iron (III), sulfate, and carbon dioxide as electron acceptors. In addition, the model simulates advection, dispersion, sorption, and ion exchange. The model solves the transport equation six times to determine the fate and transport of the hydrocarbons and the electron acceptors/reaction by-products. For example, in the case of iron (III), the model simulates the production and transport of iron (II) or ferrous iron. The following two sections describe in more detail the conceptual model for biodegradation used in BIOPLUME III and provides a summary of the limitations of the program. For more information on the processes of advection, dispersion, and sorption, the user is encouraged to consult Appendix A and Konikow and Bredehoeft (1978 & 1989).

4.1.2   Conceptual Model for Biodegradation

Recent research suggests that hydrocarbons are degraded both aerobically and anaerobically in subsurface environments. The main electron acceptors include oxygen for aerobic biodegradation and nitrate, iron (III), sulfate, and carbon dioxide for anaerobic biodegradation. Manganese has also been identified as an anaerobic electron acceptor; however, manganese has not been incorporated into the current version of BIOPLUME III.

The conceptual model used in BIOPLUME III to simulate these biodegradation processes tracks six plumes simultaneously: hydrocarbon, oxygen, nitrate, iron (II) , sulfate, and carbon dioxide. Iron (III) is input as a concentration matrix of ferric iron in the formation. Once ferric iron is used for biodegradation, BIOPLUME III simulates the production and transport of ferrous iron.

Biodegradation occurs sequentially in the following order:

$$\text{Oxygen} \rightarrow \text{Nitrate} \rightarrow \text{Iron (III)} \rightarrow \text{Sulfate} \rightarrow \text{Carbon Dioxide}$$

The biodegradation of hydrocarbon in a given location using nitrate, for example, can only occur if oxygen has been depleted to its threshold concentration at that location.

Three different kinetic expressions can be utilized for the biodegradation reaction for each of the electron acceptors:

  1.   First-order decay
  2.   Instantaneous reaction
  3.   Monod kinetics

These kinetic expressions are discussed in more detail in Section 4.2.3. The first-order decay model implemented in BIOPLUME III for any of the electron acceptors is limited by the

82

availability of the electron acceptor in question. In other words, the model allows the first-order reaction to take place up to the point that the electron acceptor concentration available in the aquifer has been depleted.

The Monod kinetic model used in BIOPLUME III assumes a constant microbial population for each of the aerobic and anaerobic reactions and does not simulate the growth, transport and decay of the microbial population in the subsurface.

4.1.3   BIOPLUME III Applicability and Limitations

The BIOPLUME III model has been mainly developed to simulate the natural attenuation of hydrocarbons using oxygen, nitrate, iron (III), sulfate, and carbon dioxide as electron acceptors for biodegradation. BIOPLUME III is generally used to answer a number of questions regarding natural attenuation:

1. How long will the plume extend if no engineered/source controls are implemented?

2. How long will the plume persist until natural attenuation processes completely dissipate the contaminants?

3. How long will the plume extend or persist if some engineered controls or source reduction measures are undertaken (for example, free phase removal or residual soil contamination removal)?

The model can also be used to simulate bioremediation of hydrocarbons in ground water by injecting electron acceptors (except for iron(III)) and can also be used to simulate air sparging for low injection air flow rates. Finally, the model can be used to simulate advection, dispersion, and sorption without including biodegradation.

As with any model, there are limitations to the use of BIOPLUME III. The assumptions used in the USGS MOC code include:

1. Darcy's law is valid and hydraulic-head gradients are the only driving mechanism for flow.

2. The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.

3. Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.

4. No chemical reactions occur that affect the fluid properties, or the aquifer properties.

5. Ionic and molecular diffusion are negligible contributors to the total dispersive flux.

6. Vertical variations in head and concentration are negligible.

7. The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

The limitations imposed by the biodegradation expressions incorporated in BIOPLUME III include:

1. The model does not account for selective or competitive biodegradation of the hydrocarbons. This means that hydrocarbons are generally simulated as a lumped organic which represents the sum of benzene, toluene, ethyl benzene or xylene. If a single component is to be simulated, the user would have to determine how much electron acceptor would be available for the component in question.

2. The conceptual model for biodegradation used in BIOPLUME III is a simplification of the complex biologically mediated redox reactions that occur in the subsurface.

4.1.4   Comparison of BIOPLUME III to Analytical Models

The testing program for BIOPLUME III was based on: i) previous modeling projects performed by several different researchers, ii) articles in the related literature, and iii) testing performed directly by the project team.

The BIOPLUME III model is based on the Method of Characteristics (MOC) code (Konikow and Bredehoeft, 1978 and 1989), which was first modified by Borden to develop the BIOPLUME model (Borden and Bedient, 1986a and 1986b). Rifai then modified the BIOPLUME model to develop the BIOPLUME II model (Rifai et al., 1987). BIOPLUME II formed the basis for the BIOPLUME III model, in part using source code from a research model developed by Rifai (Rifai and Bedient, 1990).

The following comparison/checking operations have been conducted throughout the development of the BIOPLUME models:

1. The MOC model was compared to an analytical solution (Konikow and Bredehoeft, 1978). This work is summarized in Appendix A.6 of the BIOPLUME III User's Manual.

2. BIOPLUME was successfully calibrated to a field site (Borden and Bedient, 1986b).

3. BIOPLUME II was successfully calibrated to a field site (Rifai et al., 1988).

4. An analytical solution supplemented by a superposition technique for the instantaneous biodegradation reaction was compared against BIOPLUME II by Connor et al. (1994), who concluded that "incorporation of the simple oxygen-superposition function into the Domenico model provides a steady-state plume prediction in close agreement with the BIOPLUME II model." In addition, Ollila (1996) performed a similar comparison and determined that the analytical solution was in "close agreement with BIOPLUME II."

5. BIOPLUME III was tested by comparing i) the results from BIOPLUME III simulations using a single electron acceptor against ii) BIOPLUME II runs with the oxygen concentrations adjusted to reflect the different utilization factors for each non-oxygen electron acceptor. These comparisons were performed for oxygen, nitrate, sulfate, and methane (because the iron reaction was based on dissolution from a solid, it could not be compared in the same way). The BIOPLUME III Monod biodegradation modules, originally developed by Rifai for a research code (Rifai and Bedient, 1990), were tested by reducing the half-saturation constants and increasing the maximum utilization rates until the results approached the instantaneous reaction solutions. There are no analytical solutions which include Monod kinetics that can be used for model testing.

6. As part of this project, the model was successfully calibrated to 8 field sites by the project team. After calibration, the simulated BTEX and electron acceptor/by-product concentrations matched observed conditions in the field.

4.2   Mathematical Model

4.2.1   Numerical Simulation of Oxygen Limited Biodegradation in BIOPLUME II

4.2.1.1 Equation Formulation. Borden and Bedient (1986) simulated the growth of microorganisms and removal of hydrocarbon and oxygen using a modification of the Monod function where:

$$\frac{dH}{dt} = - M_t \bullet k \bullet \left(\frac{H}{K_h + H}\right)\left(\frac{O}{K_o + O}\right) \tag{4.1}$$

$$\frac{dO}{dt} = - M_t \bullet k \bullet F \bullet \left(\frac{H}{K_h + H}\right)\left(\frac{O}{K_o + O}\right) \tag{4.2}$$

$$\frac{dM_t}{dt} = M_t \bullet k \bullet Y \bullet \left(\frac{H}{K_h + H}\right)\left(\frac{O}{K_o + O}\right) + k_c \bullet Y \bullet C - b \bullet M_t \tag{4.3}$$

where

H	=	hydrocarbon concentration
O	=	oxygen concentration
M_t	=	total microbial concentration
k	=	maximum hydrocarbon utilization rate per unit mass microorganisms
Y	=	microbial yield coefficient (g cells/g hydrocarbon)
K_h	=	hydrocarbon half-saturation constant
K_o	=	oxygen half-saturation constant

$$k_c \quad = \quad \text{first-order decay rate of natural organic carbon}$$

$$C \quad = \quad \text{natural organic carbon concentration}$$

$$b \quad = \quad \text{microbial decay rate}$$

$$F \quad = \quad \text{ratio of oxygen to hydrocarbon consumed}$$

Equations 4.1 through 4.3 were combined with the advection/dispersion equation for a solute undergoing linear instantaneous adsorption to result in:

$$\frac{\partial H}{\partial t} = \nabla \bullet (D\nabla H - vH)/R_h - M_t \bullet k \bullet \left(\frac{H}{K_h + H}\right)\left(\frac{O}{K_o + O}\right) \tag{4.4}$$

$$\frac{\partial O}{\partial t} = \nabla \bullet (D\nabla O - vO) - M_t \bullet k \bullet F \bullet \left(\frac{H}{K_h + H}\right)\left(\frac{O}{K_o + O}\right) \tag{4.5}$$

where

$$D \quad = \quad \text{dispersion tensor}$$

$$v \quad = \quad \text{ground water velocity vector}$$

$$R_h \quad = \quad \text{retardation factor for hydrocarbon}$$

The movement of naturally occurring microorganisms will be limited by the tendency of the organisms to grow as microcolonies attached to the formation. Borden and Bedient (1986) assumed that the transfer of microorganisms between the solid surface and ground water will be rapid and will follow a linear relationship with total concentration, thus allowing them to simulate the transport of microorganisms using a simple retardation factor approach:

$$\frac{\partial M_s}{\partial t} = \nabla \bullet (D\nabla M_s - vM_s)/R_m$$

$$+ M_s \bullet k \bullet Y \bullet \left(\frac{H}{K_h + H}\right)\left(\frac{O}{K_o + O}\right) + \frac{k_c Y C}{R_m} - bM_s \tag{4.6}$$

where

$$M_s \quad = \quad \text{concentration of microbes in solution}$$

$$Ma \quad = \quad \text{concentration of microbes attached to aquifer}$$

$$K_m \quad = \quad \text{ratio of microbes attached to microbes in solution}$$

$$R_m \quad = \quad \text{microbial retardation factor}$$

$$M_a \quad = \quad K_m \bullet M_s$$

$$M_t \quad = \quad M_s + M_a = (1 + K_m) * M_s = R_m \bullet M_s$$

Borden and Bedient (1986) conducted one-dimensional simulations with equations (4.4) - (4.6) and determined that there are three general regions where different processes control the rate and extent of degradation: near the contaminant source, in the heart of the plume and at the leading edge of the plume. Biodegradation rates will be very high near the source and will result in depleted oxygen levels. Biodegradation in the heart of the plume will be limited by the availability of oxygen. The primary mass transfer processes include horizontal mixing with oxygenated formation water, advective fluxes of oxygen and vertical exchange with the unsaturated zone. The limited oxygen supply to the heart of the plume will result in a region of reduced oxygen and hydrocarbon concentrations. At the leading edge of the plume, oxygen is present in excess and hydrocarbons will be absent or present in trace quantities.

Sensitivity analyses with the one-dimensional model indicated that the microbial parameters had little or no effect on the hydrocarbon concentration in the body of the plume and on the time to hydrocarbon breakthrough. This led Borden and Bedient (1986) to assume that the consumption of hydrocarbon and oxygen might be approximated as an instantaneous reaction between oxygen and hydrocarbon:

$$H(t+1) \quad = \quad H(t) - O(t)/F \qquad O(t+1) = 0 \text{ where } H(t) > O(t)/F \qquad (4.7)$$

$$O(t+1) \quad = \quad O(t) - H(t) \bullet F \qquad H(t+1) = 0 \text{ where } O(t) > H(t) \bullet F \qquad (4.8)$$

where $H(t)$, $H(t+1)$, $O(t)$, $O(t+1)$ are the hydrocarbon and oxygen concentrations at time t and $t+1$.

Borden and Bedient (1986) concluded that the instantaneous reaction assumption is a close approximation to equations (4.4) through (4.6). Their simulations indicate that the most significant errors using this assumption occur in the region near the source area especially when ground water velocities are very high or for poorly degradable hydrocarbons.

Borden and Bedient (1986) used the instantaneous reaction assumption to simplify the system of equations (4.4) - (4.6) to:

$$\frac{\partial H}{\partial t} \quad = \quad \frac{1}{R_h} \left(D_l \frac{\partial^2 H}{\partial x^2} + D_t \frac{\partial^2 H}{\partial y^2} - v \frac{\partial H}{\partial x} \right) - \delta \qquad (4.9)$$

$$\frac{\partial O}{\partial t} \quad = \quad D_l \frac{\partial^2 O}{\partial x^2} + D_t \frac{\partial^2 O}{\partial y^2} - v \frac{\partial O}{\partial x} - \delta F \qquad (4.10)$$

where
$$\delta \quad = \quad \min (H, O/F)$$
$$D_t \quad = \quad \text{transverse dispersion coefficient}$$
$$\alpha_t \quad = \quad \text{transverse dispersivity}$$
$$D_t \quad = \quad \alpha_t \bullet v$$
$$y \quad = \quad \text{coordinate orthogonal to the flow}$$

Two-dimensional simulations of equations (4.9) and (4.10) indicate that biodegrading plumes are generally less laterally spread than their non-degrading counterparts. Simulations also indicated that transverse mixing is the major source of oxygen to the plume.

Borden (1986) examined the vertical exchange of oxygen with the unsaturated zone. His simulations indicated that the effects of gas exchange with the unsaturated zone may be approximated as a first-order decay in space and time of hydrocarbon concentrations. Borden (1986) developed a regression function at the United Creosoting Company site to determine the reaeration first-order decay coefficient:

$$K' \quad = \quad 2611 \, D_V^{\,0.79} \, \exp\left(\frac{-10.5 \, B}{B + 1.04}\right) \tag{4.11}$$

where

B	=	saturated thickness
D_V	=	vertical dispersion coefficient

4.2.1.2 Development of the BIOPLUME II Model. Rifai et al. (1988) incorporated the conclusions developed by Borden and Bedient (1986) into the USGS two-dimensional solute transport model more commonly referred as the Method of Characteristics (MOC) model. The MOC model was modified from a single particle mover to a dual particle mover model to simulate the transport of hydrocarbon and oxygen. The system of transport equations solved in BIOPLUME II is given by:

$$\frac{\partial Hb}{\partial t} \quad = \quad \frac{1}{R_h} \left(\frac{\partial}{\partial x_i} \left(bD_{ij} \frac{\partial H}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bHV_i) \right) - \frac{H'W}{n} \tag{4.12}$$

$$\frac{\partial Ob}{\partial t} \quad = \quad \left(\frac{\partial}{\partial x_i} \left(bD_{ij} \frac{\partial O}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bOV_i) \right) - \frac{O'W}{n} \tag{4.13}$$

where

H	=	concentration of hydrocarbon
O	=	concentration of oxygen
H'	=	concentration of hydrocarbon in source or sink fluid
O'	=	concentration of oxygen in source or sink fluid
n	=	effective porosity
b	=	saturated thickness
W	=	volume flux per unit area
V_i	=	seepage velocity in the direction of x_i
R_h	=	retardation factor for hydrocarbon
D_{ij}	=	coefficient of hydrodynamic dispersion

$$x_i / x_j \quad = \quad \text{cartesian coordinates}$$

$$t \quad = \quad \text{time}$$

The hydrocarbon and oxygen plumes are combined using the principle of superposition and equations (4.7) and (4.8). The principle of superposition is best portrayed in Figure 4.1. It is noted from Figure 4.1 that wherever the hydrocarbon is present in relatively high concentrations, oxygen is absent. The oxygen plume forms an envelope for the hydrocarbon plume with oxygen concentrations gradually increasing to initial background levels as one moves away from the centerline of the hydrocarbon plume. In profile view, the hydrocarbon plume is less spread out, and has lower concentrations than the nonbiodegraded plume.

4.2.2   BIOPLUME III Equation Formulation

Much like the approach used in developing BIOPLUME II, the 1989 version of the MOC model was modified to become a six-component particle mover model to simulate the transport of hydrocarbon, oxygen, nitrate, iron(II), sulfate and carbon dioxide. Since the biodegradation of hydrocarbon uses iron (III) as an electron acceptor, iron (III) concentrations are simulated as an initial concentration of ferric iron that is available in each cell. Once the iron (III) is consumed, hydrocarbon concentrations are reduced and ferrous iron is produced. The resulting ferrous iron is then transported in the aquifer. The BIOPLUME III equations include:

$$\frac{\partial Hb}{\partial t} \quad = \quad \frac{1}{R_h} \left(\frac{\partial}{\partial x_i} \left(b D_{ij} \frac{\partial H}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bHV_i) \right) - \frac{H'W}{n} \tag{4.14}$$

$$\frac{\partial Ob}{\partial t} \quad = \quad \left(\frac{\partial}{\partial x_i} \left(b D_{ij} \frac{\partial O}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bOV_i) \right) - \frac{O'W}{n} \tag{4.15}$$

$$\frac{\partial Nb}{\partial t} \quad = \quad \left(\frac{\partial}{\partial x_i} \left(b D_{ij} \frac{\partial N}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bNV_i) \right) - \frac{N'W}{n} \tag{4.16}$$

$$\frac{\partial Fb}{\partial t} \quad = \quad \left(\frac{\partial}{\partial x_i} \left(b D_{ij} \frac{\partial F}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bFV_i) \right) - \frac{F'W}{n} \tag{4.17}$$

$$\frac{\partial Sb}{\partial t} \quad = \quad \left(\frac{\partial}{\partial x_i} \left(b D_{ij} \frac{\partial S}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bSV_i) \right) - \frac{S'W}{n} \tag{4.18}$$

$$\frac{\partial Cb}{\partial t} \quad = \quad \left(\frac{\partial}{\partial x_i} \left(b D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (bCV_i) \right) - \frac{C'W}{n} \tag{4.19}$$

where

$$N \quad = \quad \text{concentration of nitrate}$$

$$N' \quad = \quad \text{concentration of nitrate in source or sink fluid}$$
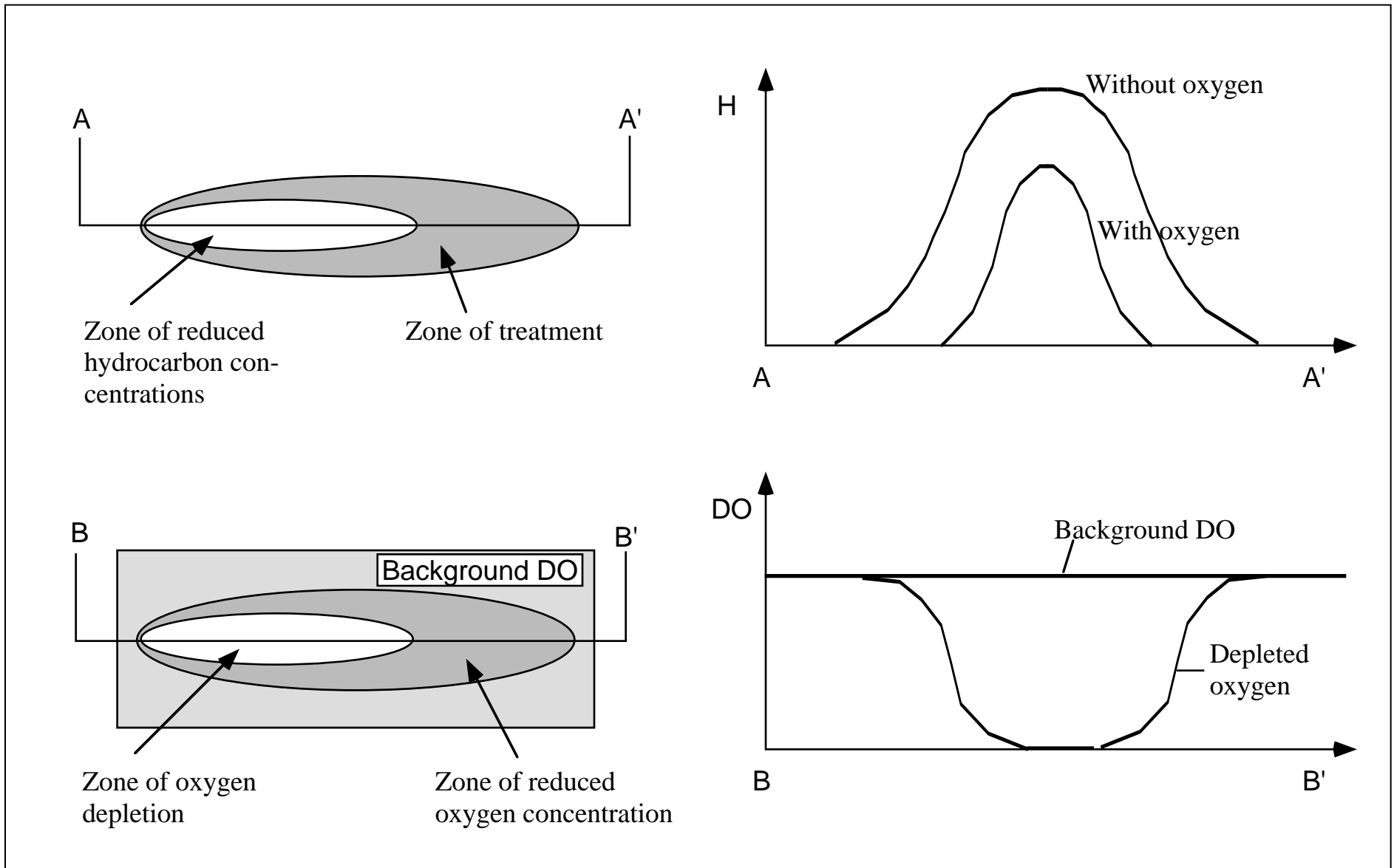
Source: Bedient, Rifai, and Newell (1994)

Figure 4.1. Principle of Superposition for Combining the Hydrocarbon
and Oxygen Plumes in BIOPLUME II

F $\quad$ = $\quad$ concentration of iron (II)

F' $\quad$ = $\quad$ concentration of iron (II) in source or sink fluid

S $\quad$ = $\quad$ concentration of sulfate

S' $\quad$ = $\quad$ concentration of sulfate in source or sink fluid

C $\quad$ = $\quad$ concentration of carbon dioxide

C' $\quad$ = $\quad$ concentration of carbon dioxide in source or sink fluid

All other parameters as defined previously.

The biodegradation of hydrocarbon using the aerobic and anaerobic electron acceptors is simulated using the principle of superposition and the following equations:

$$H(t+1) \quad = \quad H(t) - R_{HO} - R_{HN} - R_{HFe} - R_{HS} - R_{HC} \tag{4.20}$$

$$O(t+1) \quad = \quad O(t) - R_{OH} \tag{4.21}$$

$$N(t+1) \quad = \quad N(t) - R_{NH} \tag{4.22}$$

$$Fe(t+1) \quad = \quad Fe(t) - R_{FeH} \tag{4.23}$$

$$F(t+1) \quad = \quad R_{FeH} \tag{4.24}$$

$$S(t+1) \quad = \quad S(t) - R_{SH} \tag{4.25}$$

$$C(t+1) \quad = \quad C(t) - R_{CH} \tag{4.26}$$

where R_{HO}, R_{HN}, R_{HFe}, R_{HS}, R_{HC} are the hydrocarbon concentration losses due to biodegradation using oxygen, nitrate, ferric iron, sulfate and carbon dioxide as electron acceptors, respectively. The terms R_{OH}, R_{NH}, R_{FeH}, R_{SH}, R_{CH} are the corresponding concentration losses in the electron acceptors. These reaction terms are computed using one of the three biodegradation expressions: first-order, instantaneous or Monod. For example, and for the instantaneous model, the reaction terms are computed as follows:

$$
\begin{aligned}
R_{HO} \quad &= \quad O(t)/F_O \\
R_{HN} \quad &= \quad N(t)/F_N \\
R_{HFe} \quad &= \quad Fe(t)/F_{Fe} \\
R_{HS} \quad &= \quad S(t)/F_S \\
R_{HC} \quad &= \quad C(t)/F_C
\end{aligned}
\tag{4.27}
$$

$$
\begin{aligned}
R_{OH} \quad &= \quad H(t) \bullet F_O \\
R_{NH} \quad &= \quad H(t+1)^1 \bullet F_N \\
R_{FeH} \quad &= \quad H(t+1)^2 \bullet F_{Fe} \\
R_{SH} \quad &= \quad H(t+1)^3 \bullet F_S \\
R_{CH} \quad &= \quad H(t+1)^4 \bullet F_C
\end{aligned}
\tag{4.28}
$$

where F_O, F_N, F_{Fe}, F_S, and F_C are the stoichiometric ratios for each of the electron acceptors, respectively and $H(t+1)^1$, $H(t+1)^2$, $H(t+1)^3$, and $H(t+1)^4$ are the hydrocarbon concentrations modified by loss due to the reaction with oxygen; oxygen and nitrate; oxygen, nitrate and iron; and oxygen, nitrate, iron and sulfate; respectively in the given time step.

For each of the electron acceptors, the following constraints are applied:

$$
\begin{aligned}
H(t+1)^1 &= 0 \qquad \text{where } O(t) > H(t) \bullet F_O \\
O(t+1) &= 0 \qquad \text{where } H(t) > O(t)/F_O
\end{aligned}
\tag{4.29}
$$

$$
\begin{aligned}
H(t+1)^2 &= 0 \qquad \text{where } N(t) > H(t+1)^1 \bullet F_N \\
N(t+1) &= 0 \qquad \text{where } H(t+1)^1 > N(t)/F_N
\end{aligned}
\tag{4.30}
$$

$$
\begin{aligned}
H(t+1)^3 &= 0 \qquad \text{where } Fe(t) > H(t+1)^2 \bullet F_{Fe} \\
Fe(t+1) &= 0 \qquad \text{where } H(t+1)^2 > Fe(t)/F_{Fe}
\end{aligned}
\tag{4.31}
$$

$$
\begin{aligned}
H(t+1)^4 &= 0 \qquad \text{where } S(t) > H(t+1)^3 \bullet F_s \\
S(t+1) &= 0 \qquad \text{where } H(t+1)^3 > S(t)/F
\end{aligned}
\tag{4.32}
$$

$$
\begin{aligned}
H(t+1) &= 0 \qquad \text{where } C(t) > H(t+1)^4 \bullet F_c \\
C(t+1) &= 0 \qquad \text{where } H(t+1)^4 > C(t)/F_C
\end{aligned}
\tag{4.33}
$$

Furthermore, these reaction terms are subject to additional constraints. For first-order decay, instantaneous and Monod kinetic models:

$$
R_{HN} = 0 \quad \text{if} \quad O(t+1) > O
\tag{4.34}
$$

$$
\begin{aligned}
R_{HFe} = 0 \quad &\text{if} \quad O(t+1) > O_{min} \\
&\text{or} \quad N(t+1) > N_{min}
\end{aligned}
\tag{4.35}
$$

$$
\begin{aligned}
R_{HS} = 0 \quad &\text{if} \quad O(t+1) > O_{min} \\
&\text{or} \quad N(t+1) > N_{min} \\
&\text{or} \quad Fe(t+1) > Fe_{min}
\end{aligned}
\tag{4.36}
$$

$$
\begin{aligned}
R_{HC} = 0 \quad &\text{if} \quad O(t+1) > O_{min} \\
&\text{or} \quad N(t+1) > N_{min} \\
&\text{or} \quad Fe(t+1) > Fe_{min} \\
&\text{or} \quad S(t+1) > S_{min}
\end{aligned}
\tag{4.37}
$$

where O_{min}, N_{min}, Fe_{min}, S_{min}, C_{min} are the threshold concentrations for the corresponding electron acceptor below which no biodegradation will take place.

For the first-order decay and Monod kinetic models the reaction terms are compared to the concentration of the electron acceptor:

$$R_{HO} \leq O(t)/F_O \tag{4.38}$$

$$R_{HN} \leq N(t)/F_N \tag{4.39}$$

$$R_{HFe} \leq Fe(t)/F_{Fe} \tag{4.40}$$

$$R_{HS} \leq S(t)/F_S \tag{4.41}$$

$$R_{HC} \leq C(t)/F_C \tag{4.42}$$

4.2.3   Biodegradation Kinetic Models in BIOPLUME III

The BIOPLUME III model simulates three types of kinetic reactions to represent the aerobic and anaerobic biodegradation of the hydrocarbon: first-order decay, instantaneous reaction and Monod kinetics. These expressions are described in the following sections.

4.2.3.1 First-Order Decay Model. One of the most commonly used expressions for representing the biodegradation of an organic compound involves the use of an exponential decay relationship:

$$C = C_o \bullet e^{-kt} \tag{4.43}$$

where C is the biodegraded concentration of the chemical, C_o is the starting concentration, and k is the rate of decrease of the chemical. First-order rate constants can be expressed in terms of a half-life for the chemical:

$$t_{1/2} = \frac{0.693}{k} \tag{4.44}$$

The general literature contains a large number of studies that have determined the half-lives of many organics detected in ground water. For example, literature values for the half-life for benzene range from 10 to 730 days while those for TCE range from 10.7 months to 4.5 years (Howard et al., 1991).

The first-order decay model does not account for site-specific information such as the availability of electron acceptors. This explains, in part, why the reported half-lives for a given chemical vary over a broad range of values. Another consideration is the fact that the reported values for first-order decay rates may have been derived from laboratory experiments conducted under a specific set of conditions. There has been very little work done to correlate first-order decay rates developed from laboratory experiments to an equivalent rate that would apply at the field scale. A number of investigators have alternatively developed methods for estimating first-order decay rates from natural attenuation field data (Wiedemeier et al., 1995b and Buscheck et al., 1993).

4.2.3.2 Instantaneous Reaction Model. The instantaneous reaction expression, an expression first proposed by Borden and Bedient (1986), assumes that microbial biodegradation kinetics are fast in comparison with the transport of oxygen, and that the growth of microorganisms and utilization of oxygen and organics in the subsurface can be simulated as an instantaneous reaction between the organic contaminant and oxygen.

From a practical standpoint, the instantaneous reaction model assumes that the rate of utilization of the contaminant and oxygen by the microorganisms is very high, and that the time required to mineralize the contaminant is very small, or almost instantaneous. Using oxygen as an electron acceptor, for example, biodegradation is calculated using the expression:

$$\Delta C_R = -\frac{O}{F} \tag{4.45}$$

where ΔC_R is the change in contaminant concentration due to biodegradation, O is the concentration of oxygen, and F is the ratio of oxygen to contaminant consumed. The instantaneous reaction model has the advantage of not requiring kinetic data. The model, however, is limited to situations where the rate of biodegradation is fast relative to the rate of ground water flow.

4.2.3.3 Monod Kinetic Model. One of the most common expressions for simulating biodegradation is the hyperbolic saturation function presented by Monod (1942) and referred to as Monod or Michaelis-Menten kinetics:

$$\mu = \mu_{max} \frac{C}{K_c + C} \tag{4.46}$$

where μ is the growth rate (time^{-1}), μ_{max} is the maximum growth rate (time^{-1}), and C is the concentration of the growth-limiting substrate (mg/L). The term K_c is known as the half-saturation constant or the growth-limiting substrate concentration which allows the microorganism to grow at half the maximum specific growth rate.

The rate equation describing μ as a function of C contains first-order, mixed-order, and zero-order regions. When $C >> K_c$, $K_c + C$ is almost equal to C, and the reaction approaches zero-order with:

$$\mu = \mu_{max} \tag{4.47}$$

and μ_{max} becomes the limiting maximum reaction rate. When $C << K_c$, Equation (4.46) reduces to:

$$\mu = \frac{\mu_{max}}{K_C} \bullet C \tag{4.48}$$

and the reaction approaches first-order with $\dfrac{\mu_{max}}{K_C}$ equal to the first-order rate constant.

In ground water, the Monod growth function is related to the rate of decrease of an organic compound. This is done by utilizing a yield coefficient, Y, where Y is a measure of the organisms formed per substrate utilized. The change in substrate concentration can then be expressed as follows:

$$\frac{dC}{dt} = \frac{\mu_{max} \, M \, C}{Y \, (K_C + C)} \tag{4.49}$$

where M is the microbial mass in mg/L. Because of the relationship between substrate utilization and the growth of microbial mass, Equation (4.49) is accompanied by an expression of the change in microbial mass as a function of time:

$$\frac{dM}{dt} = \mu_{max} \, M \, Y \, \frac{C}{(K_C + C)} - b \bullet M \tag{4.50}$$

where b is a first-order decay coefficient that accounts for cell death.

The advantage of using Monod kinetics is that the constants K_C and μ_{max} uniquely define the rate equation for mineralization of a specific compound. The ratio $\dfrac{\mu_{max}}{K_C}$ also represents the first-order rate constant for degradation when $C \ll K_C$. This rate constant incorporates both the activity of the degrading population and the substrate dependency of the reaction. It therefore takes into account both population and substrate levels, and provides a theoretical basis for extrapolating laboratory rate data to the environment.

The reduction of contaminant concentrations using Monod kinetics can be expressed as:

$$\Delta C = M_t \, \mu_{max} \left(\frac{C}{K_c + C} \right) \Delta t \tag{4.51}$$

where C = contaminant concentration, M_t is the total microbial concentration, μ_{max} = maximum contaminant utilization rate per unit mass microorganisms, K_c = contaminant half saturation constant, and Δt is the time interval being considered.

Incorporating Equation (4.51) into the one-dimensional transport equation, for example, results in:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - M_t \, \mu_{max} \left(\frac{C}{K_c + C} \right) \qquad (4.52)$$

where v is the seepage velocity, and D_x is the dispersion coefficient.

One of the main difficulties with the Monod kinetic model is estimating the necessary biodegradation parameters for using the model (the maximum growth rate and the half-saturation constants).

4.3　Application of BIOPLUME III to Sites

Sufficient field data are essential when using the BIOPLUME III model for simulating existing flow and/or contaminant conditions at a site or when using the model for predictive purposes. However, it may be desirable to model a site even when little data exist. The modeling in this case may serve as a method for identifying those areas where detailed field information needs to be collected.

Applying an appropriate modeling methodology will increase the confidence in modeling results with BIOPLUME III. Anderson and Woessner (1992) propose a general modeling protocol that can be applied to any site. Specific steps which apply to BIOPLUME III include:

1. Establish the purpose of the model;
2. Develop a conceptual model of the system;
3. Calibrate the site model;
4. Determine the effects of uncertainty on model results;
5. Verify the calibrated model;
6. Predict results based on the calibrated model;
7. Determine the effects of uncertainty on model predictions;
8. Present modeling results;
9. Postaudit and update model as necessary.

Stating the purpose of the modeling effort with BIOPLUME III helps focus the study and determine the expectations from the analysis. Typical objectives include:

1. Determining the effectiveness of natural attenuation for remediating a given site; and
2. Designing a ground water pump-and-treat and/or bioremediation system.

Formulating a conceptual model of the site is essential to the success of a BIOPLUME III effort. A conceptual model is a pictorial representation of the ground water flow and transport system, frequently in the form of a block diagram or a cross-section. The nature of the conceptual model will determine the dimensions of the BIOPLUME III model and the design of the grid.

Formulating a conceptual model for the BIOPLUME III model includes: (1) defining the hydrogeologic features of interest, i.e., the aquifers that will be modeled; (2) defining the flow system (including boundary and initial conditions) and sources and sinks of water in the system such as recharge from infiltration, and pumping; and (3) defining the transport system (velocity, dispersion, sorption and biodegradation) and sources and sinks of chemicals in the system (including boundary and initial conditions).

4.3.1   Calibration, Verification and Prediction

Calibrating the BIOPLUME III model is the process of demonstrating that the model is capable of producing field-measured values of the head and concentrations at the site. For the case of ground water flow, for example, calibration is accomplished by finding a set of parameters, boundary and initial conditions, and stresses that produces simulated values of heads that match measured values within a specified range of error.

The procedure for calibrating the BIOPLUME III model is by manual trial-and-error selection of parameters. The main parameters that are used for calibrating the flow at a site include: transmissivity, thickness, recharge and boundary conditions. The main parameters that are used to calibrate the transport and fate of chemicals at a site include: source definition, dispersion, sorption, and biodegradation parameters. In addition, the transmissivity, thickness and recharge data used in calibrating the flow solution determine the transport velocity and should be checked for accuracy against observed field velocities.

Obtaining the information necessary for the BIOPLUME III model is a process that involves interpreting field data to estimate the values for the model parameters. This process, while not straight forward in some cases, is crucial to the modeling effort. In general, the site hydrogeologic and water quality data are analyzed with the objective of predicting trends and estimating the parameter values for BIOPLUME III. The subsurface geologic data are usually interpreted to yield values for transmissivity, thickness, and porosity. The water level or potentiometric surface data are analyzed to determine the direction of ground water flow and the water level contours. Water quality data are analyzed to determine the spatial and temporal trends in contaminant distributions at the site.

An emerging tool in spatial data analysis that should be mentioned here is *geostatistics*. Geostatistics can be viewed as a set of statistical procedures for describing the correlation of spatially distributed random variables and for performing interpolation and aerial estimation of these variables (Cooper and Istok, 1988). *Kriging*, for example, is one of the most widely used geostatistical methods to determine spatial distributions of the hydraulic conductivity (or transmissivity and thickness) at a site. Contouring data using other statistical methods can also be used as an alternative to kriging.

A quantitative evaluation of the calibration process involves an assessment of the *calibration error*. The calibration error is determined by comparing model predicted values to observed values of the heads and concentrations. Two equations are commonly used for this purpose:

$$\text{Mean Error} = \frac{1}{n} \sum_{i=1}^{n} (x_m - x_s)_i \qquad (4.53)$$

Root Mean Squared (RMS) Error

$$= \left[\frac{1}{n} \sum_{i=1}^{n} (x_m - x_s)^2_i \right]^{0.5} \qquad (4.54)$$

where x_m and x_s are the measured and simulated values, respectively.

It should be noted that the calibration error is very different and distinct from the *computational error* which is a result of the numerical approximation procedures used in the BIOPLUME II model. Computational errors are discussed in more detail in Section II.5.

Verifying the calibrated site model is the process of using the calibrated model to predict a second set of measured data from the site. The purpose of this step is to ensure that the calibrated model is indeed capable of simulating observed site conditions. If the modeling results for the verification step do not match within reasonable error the observed field data, the model might require fine-tuning and "re-calibration".

Prediction is the process of using the calibrated/verified model to determine site conditions in response to an anticipated set of future events. The prediction process is often associated within a sensitivity analysis similar to that completed with the model after calibration. This is necessary to determine which parameters specifically impact the predicted results.

4.3.2 Sensitivity Analysis

The purpose of a sensitivity analysis is to quantify the effects of uncertainty in the estimates of model parameters on model results. During a sensitivity analysis, calibrated values for transmissivity, thickness, recharge, dispersivity, etc. are systematically changed within a prescribed range of applicable values. The magnitude of change in heads and concentrations from the calibrated model is a measure of the sensitivity of the model results to the particular parameter. The results of this analysis are expressed as the effects of the parameter change on the spatial distribution of heads and concentrations.

The sensitivity of BIOPLUME III model results to the input parameters is a key analysis that the user should perform for each site application. This section will present in general the relative sensitivity of the model to various input parameters using a hypothetical case study scenario. The user is encouraged to repeat some of these analyses for their specific sites.

The hypothetical site "base case" scenario used in the sensitivity simulations was set-up as follows:

Grid Size	9 x 10
Cell Size	900' x 900'
Aquifer Thickness	20 ft
Transmissivity	0.1 ft^2/s
Porosity	0.3
CELDIS	0.5
Longitudinal Disp.	100 ft
Transverse Disp.	30 ft
Simulation Time	2.5 yrs
Source of Contamination	1 injection well @ 0.1 cfs and 100 mg/L source conc.
Recharge	0 cfs
Boundary Conditions	Constant head, upgradient and downgradient
Chemical Reactions	None
Biodegradation Reactions	None

Three categories of parameters were analyzed: hydrogeologic, chemical and biodegradation model parameters. In each category and for each parameter analyzed, the value of the parameter was changed by a factor of up to one order of magnitude from the "base case" scenario. The associated model results were then analyzed to determine the impact of the changed parameter values on the contaminant plume shape, size and concentrations.

Hydrogeologic Parameters. Five hydrogeologic parameters were evaluated: porosity, aquifer thickness, transmissivity, longitudinal and transverse dispersivity. Overall, model results were most sensitive to changes in porosity, thickness and transmissivity. This is to be expected since the three parameters affect the seepage velocity for the aquifer. The data in Table 4.1 indicate that model results are most sensitive to changes in the transmissivity and aquifer thickness.

Chemical Parameters. Two variables, linear sorption and radioactive decay, were used in this analysis to illustrate the sensitivity of the model to selected chemical parameters. The user is encouraged to determine the sensitivity of model results to the remaining chemical parameters (Langmuir and Freundlich sorption parameters and ion exchange) if they apply to their site.

Both linear sorption and radioactive decay have a substantial impact on the model results as can be seen in Table 4.2. A retardation factor of 2 caused plume concentrations to decline by 27% from the "base case" scenario and a half-life of 2 x 10^7 seconds or 231 days caused plume concentrations to decline by over 50%.

Biodegradation Parameters. The BIOPLUME III model simulates biodegradation using two basic methods. The first method involves specifying an overall first-order decay rate to simulate both aerobic and anaerobic processes. The second method involves specifying the background electron

Table 4.1. Sensitivity of Model Results to Changes in Hydrogeologic Parameters

Variable		Max. Plume Concentration (mg/l)	Plume Length (# cells)	Plume Width (# cells)
	0.15	75	6	5
Porosity	0.3 *	67	4	3
	0.45	80	4	3
	10	75	6	5
Thickness	20 *	67	4	3
(ft)	40	47	2	2
	0.01	90	3	3
Transmissivity	0.1 *	67	4	3
(sq. ft. / sec)	0.2	57	5	3
Longitudinal	10	70	3	3
Dispersivity	50	69	4	3
(ft)	100 *	67	4	3
Transverse	10	68	4	3
Dispersivity	30 *	67	4	3
(ft)	60	66	4	3

*   Base Case

Table 4.2. Sensitivity of Model Results to Linear Sorption and Radioactive Decay

Variable		Max. Plume Concentration (mg/l)	Plume Length (# cells)	Plume Width (# cells)
	1 *	67	4	3
R	2	49	3	2
	5	28	2	1
	0 *	67	4	3
THALF	10^7	20	2	2
(sec)	2×10^7	33	2	3

*   Base Case

acceptor concentrations in the aquifer and the selecting an associated kinetic model for the analysis.

The sensitivity analyses conducted for the biodegradation parameters involved simulating the impact of using an overall first-order decay parameter as well as the impact of specifying electron acceptor concentrations with instantaneous kinetics. The results from the analyses are shown in Table 4.3.

The data in Table 4.3 illustrates that model results are very sensitive to biodegradation parameters. Regardless of the modeling methodology and biodegradation kinetics, the simulated concentrations using biodegradation are likely to differ substantially from their counterparts without biodegradation.

4.3.3   Impact of Non-BTEX Constituents on BIOPLUME III Modeling

BTEX constituents only comprise a small percentage of the total organic mass in gasoline and JP-4 mixtures. However, the best available information suggests that most JP-4 and gasoline plumes will be dominated by BTEX components, and that only a small fraction of the plumes contain dissolved non-BTEX compounds. This is due to the BTEX compounds having very high solubilities relative to the remaining fraction of organic mass in these fuel mixtures. In other words, most of the non-BTEX constituents of gasoline and JP-4 are relatively insoluble, creating dissolved-phased plumes that are dominated by the BTEX compounds. The following calculations support this conceptual model of BTEX-dominated plumes from JP-4 and gasoline releases.

Gasoline composition data presented by Johnson et al. (1990a and 1990b), and JP-4 composition data presented by Stelljes and Watkin (Stelljes and Watkin, 1993; data adapted from Oak Ridge National Laboratory, 1989) were used to determine the effective solubility of these hydrocarbon mixtures in equilibrium with water (effective solubility = mole fraction x pure phase solubility; see Bedient et al., 1994). The total effective solubility of all the constituents was then compared to the effective solubility of the BTEX constituents. The following tables show this calculation for fresh gasoline, weathered gasoline, and virgin JP-4:

FRESH GASOLINE
(data from Johnson et al., 1990)

Constituent	Mass Fraction	Mole Fraction	Pure-Phase Solubility (mg/L)	Effective Solubility (mg/L)
Benzene	0.0076	0.0093	1780	17
Toluene	0.055	0.0568	515	29
Ethylbenzene	0.0	0.0	152	0
Xylenes	0.0957	0.0858	198	17
TOTAL BTEX	0.16	0.15	152 - 1780 (range)	63
58 Compounds	0.84	0.85	0.004 - 1230 (range)	30
TOTAL	**1.00**	**1.00**	-	**93**

% BTEX = (63 mg/L) $\prod$ (93 mg/L) = 68 %

WEATHERED GASOLINE # 1
(data from Johnson et al., 1990a)

Constituent	Mass Fraction	Mole Fraction	Pure-Phase Solubility (mg/L)	Effective Solubility (mg/L)
Benzene	0.01	0.0137	1780	24
Toluene	0.1048	0.1216	515	63
Ethylbenzene	0.0	0.0	152	0
Xylenes	0.1239	0.1247	198	25
TOTAL BTEX	0.24	0.26	152 - 1780 (range)	112
58 Compounds	0.76	0.74	0.004 - 1230 (range)	14
TOTAL	**1.00**	**1.00**	-	**126**

% BTEX = (112 mg/L) $\prod$ (126 mg/L) = 89 %

WEATHERED GASOLINE #2
(data from Johnson et al., 1990b)

Constituent	Mass Fraction	Mole Fraction	Pure-Phase Solubility (mg/L)	Effective Solubility (mg/L)
Benzene	0.0021	0.003	1780	5
Toluene	0.0359	0.043	515	22
Ethylbenzene	0.013	0.014	152	2
Xylenes	0.080	0.084	198	15
TOTAL BTEX	0.13	0.14	*152 - 1780 (range)*	44
64 Compounds	0.87	0.86	*0.004 - 1230 (range)*	21
TOTAL	**1.00**	**1.00**	-	**65**

% BTEX = (44 mg/L) $\prod$ (65 mg/L) = 68 %

VIRGIN JP-4
(data from Stelljes and Watkin, 1993; Oak Ridge N. Lab, 1989)

Constituent	Mass Fraction	Mole Fraction	Pure-Phase Solubility (mg/L)	Effective Solubility (mg/L)
Benzene	0.005	0.023	1780	42
Toluene	0.0133	0.053	515	27
Ethylbenzene	0.0037	0.013	152	2
Xylenes	0.0232	0.080	198	16
TOTAL BTEX	0.045 (4.5%)	0.168	152 - 1780 (range)	87
13 Compounds	0.27 (27%)	0.832	0.004 - 1230 (range)	4
TOTAL	**0.315 (31.5)%**	**1.000**	-	**91**

% BTEX = (87 mg/L) $\prod$ (91 mg/L) = <u>95 %</u>

In each of these four fuel samples, BTEX compounds comprise the majority of the dissolved organic mass in equilibrium with water. The non-BTEX components represent a much smaller portion of the dissolved mass. As expected, the theoretical dissolved-phase concentrations from these samples are much higher than what is typically observed in groundwater samples due to factors such as dilution, the heterogeneous distribution of non-aqueous phase liquids, and the low level of mixing occurring in aquifers (see Bedient et al., 1994 for a more complete discussion).

Note that the total effective solubility of weathered gasoline #1 (125.4 mg/L) is greater than the total effective solubility of the fresh gasoline (92.8 mg/L). A comparison of the two samples indicates that the fresh gasoline includes a significant mass of light, volatile compounds that have pure-phase solubilities that are much lower than that of the BTEX compounds (e.g., isopentane with a vapor pressure of 0.78 atm and a solubility of 48 mg/L, compared to solubilities of 152 - 1780 mg/L for the BTEX compounds). When these light compounds are weathered (probably volatilized), the mole fractions of the BTEX components (the only remaining components with any significant solubility) increase, thereby increasing the total effective solubility of the weathered gasoline. On the other hand, weathered gasoline #2 has a total effective solubility that is significantly lower than fresh gasoline (65.0 mg/L vs. 92.8 mg/L), suggesting that this gasoline has weathered to the point where there has been significant removal of both volatile and soluble components from the gasoline.

In their analysis, Stelljes and Watkin (1993) identified only 17 compounds representing 31% by mass of a complete JP-4 mixture. However, a comparison of the relative make-up of the quantified mixture to the reported make-up of JP-4 (also from Stelljes and Watkin, 1993) shows the various classes of organic compounds to be equivalently represented in both mixtures. The quantified mixture can therefore be assumed to be generally representative of the complete JP-4 mixture.

Table 4.3. Sensitivity of Model Results to First Order Decay and
Instantaneous Reaction Biodegradation Kinetics

Variable		Max. Plume Concentration (mg/l)	Plume Length (# cells)	Plume Width (# cells)
	0 *	67	4	3
DEC1	0.116×10^{-7}	58	4	3
(1/sec)	0.116×10^{-6}	43	2	1
	0 *	67	4	3
O_2	3	67	4	3
(mg/l)	12	66	2	3
O_2, NO_3	0, 0, 0, 0, 0 *	67	4	3
Fe, SO_4,				
CO_2	3, 3, 3, 3, 3 **	62	2	2

*   Base Case
** Threshold Conc. = 0.5 mg/L for all; Stoichiometric Coefficients
    in order shown = 3, 5, 22, 5, 2

% benzenes, alkylbenzenes in identified compounds:	14%	*(note: equals 4.5% of 31.5%)*
% benzenes, alkylbenzenes in complete JP-4 mixture:	18%	*(from Stelljes and Watkin, 1993)*
% branched alkanes in all identified compounds:	26%	
% branched alkanes in complete JP-4 mixture:	31%	
% cycloalkanes in all compounds identified:	7%	
% cycloalkanes in complete JP-4 mixture:	16%	
% naphthalenes in all compounds identified:	6%	
% naphthalenes in complete JP-4 mixture:	3%	
% normal alkanes in all compounds identified:	47%	
% normal alkanes in complete JP-4 mixture:	32%	

Finally, it is important to note that there is considerable variability among different fresh fuels, and even more variation among weathered fuels. Therefore, these results should only be used as a general indicator that the BTEX compounds comprise the majority of the soluble components in plumes originating from JP-4 and gasoline releases. These results should not be used as absolute, universal values for all sites.

With regards to biodegradation modeling, however, it is probably appropriate to assume that BTEX compounds exert the majority (i.e. ~ 70% or greater) of the electron acceptor demand at JP-4 and gasoline sites. To make modeling BTEX more accurate, however, the total concentrations of available electron acceptors can be reduced by some fraction to account for the electron acceptor demand posed by biodegradable non-BTEX organics in groundwater. Two examples of how to account for the impact for non-BTEX components is to multiply all electron acceptor/by-product concentrations used in the model by either i) the ratio of BTEX/TOC concentrations, or ii) the ratio of BTEX/BOD concentrations (if TOC and BOD data are available). If these data are not available, a conservative approach would be to reduce all available electron acceptor/by-product concentrations used in the model by 30% to account for the possible impacts of non-BTEX organics in groundwater.

4.3.4   Mass Balance Assessments

The output from the BIOPLUME III Model includes a hydraulic mass balance and a chemical mass balance assessment (see Section A.5 in Appendix A). These mass balance assessments inform the user of how well the numerical techniques are performing in terms of simulating the specific site conditions. In general, water balances of less than 1% and chemical mass balances of less than 15% are desirable.

It is the authors' experience that high mass balance errors (for the contaminant) generally arise from:

1. Unreasonably high pumping or injection rates for the particular site conditions; or
2. A relatively high seepage velocity in the system; or
3. An inadequate grid that does not accommodate the plume being modeled.

Chemical mass balance errors can be possibly lowered by adjusting the parameters associated with the above listed reasons. The user should be cautioned, however, that changing these

parameters in some instances does not produce the desired effect on mass balance results. The authors attribute this to the nature of the method-of-characteristics and to the specific algorithm used in estimating chemical mass balance errors in the model.

5.0   PLATFORM USER'S GUIDE

5.1   User's Guide Overview

This is the Platform User's Guide which continues on the themes introduced in Section 2, "Getting Started." It provides further details on the Platform operations in conjunction with the modeling requirements of Intrinsic Remediation (Natural Attenuation) studies and the most commonly used menu options and controls. This document serves to:

- Highlight the basic modeling requirement of Intrinsic Remediation making a smooth transition from theory to practice.

- Highlight the unique editing tools of the Platform that greatly facilitate the mandatory creation and validation activities, which are an integral part of the modeling process.

The Platform provides the scientist and engineer the means to work in an interactive computer graphics environment where the remediation model under consideration (study) is continuously displayed on the screen. The user navigates through the various parts of the Platform by means of menus which are always displayed next to the model abstraction. Menu choices are selected and interaction with the model is performed by pointing with a mouse. By pointing to the screen, rather than typing commands, a natural dialogue is developed between the user and the platform. In this perspective, the different Menus become sophisticated graphical editors that speed up the various steps (chores) of the modeling process.

It is therefore natural to start with a quick review of the modeling steps given in Section 5.2, followed by the detailed description of the available menus, controls and input parameters given in Sections 5.3 and 5.4.   Finally, for the demanding user who wants to have a deeper insight of the Platform operations, Section 5.5 offers a brief description of the software architecture, a file description and details of auxiliary video technologies supported by the platform.

Framework

The Platform uses a hierarchical menu system using a main menu (parent menu) which, in turn, activates a series of secondary menus (child menus). For many applications, input is required in several secondary menus (child menus).   To simplify the description of the different input requirements and quickly navigate through the User's Guide we summarize the various procedures in a general framework starting with the basic requirements of the modeling process, gradually introducing the Platform tools needed to implement the model, and finishing with the detailed input data necessary to run the problem. This approach is illustrated below.
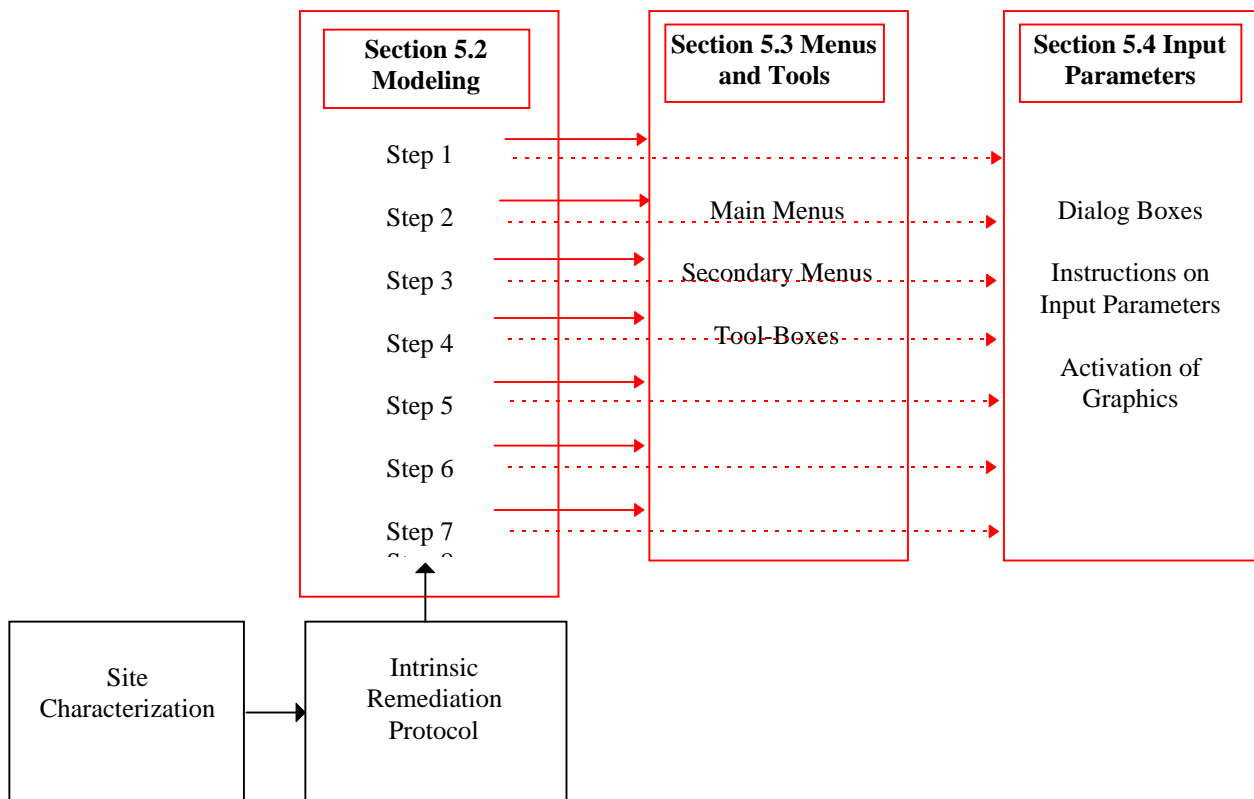
As it can be observed, "Raw Data" from the site characterization (site investigation) should be processed and sorted according to the Intrinsic Remediation Protocol before using the Platform. These data must be categorized in different modeling steps as indicated in Section 5.2 to speed up computer implementation. In each modeling step a detailed reference is given to the entry points of the Platform through the main and secondary menus introduced in Section 5.3 and the corresponding dialog boxes given in Section 5.4.

5.2   Modeling Steps Using the Platform

A model is a word description of the components of a contaminated aquifer system, the "loads" or "forcing" to the system, and the processes operative on the system. This description is made on the basis of preexisting data, regional aquifer atlases, or previous site studies. Pictures complement word descriptions (proverbially "worth a thousand words"). A graphical representation of the contaminated aquifer is part of the conceptual model.   Figure 5.1 illustrates a typical representation of a contaminated aquifer system with hydrocarbons. Present in the conceptual model shown in Figure 5.1 are a source of contamination, a fuel tank farm leaking at the surface; the vadose or unsaturated zone through which the 'free product' seeps; the mass of free product that "floats" atop the water table, i.e. that portion of the aquifer is saturated with fuel; a vapor zone, i.e. unsaturated zone filled with fuel vapors; and a zone of contact between free product and water table, where the fuel is dissolved into the saturated aquifer. The dissolved contaminant creates a plume which is advected and dispersed by the flow of the aquifer. In most instances, the immediate concern is about the quality of the aquifer and therefore how to control the level of concentration of the dissolved contaminant. The rest of the phases, leaking source, free product, characterize the release mechanism.

In this typical case study the Platform allows a quick simulation of the dissolved plume, its origin, its evolution, its migration and biodegradation. The program deals only with light hydrocarbons (LNAPLs -light non-aqueous phase liquids).
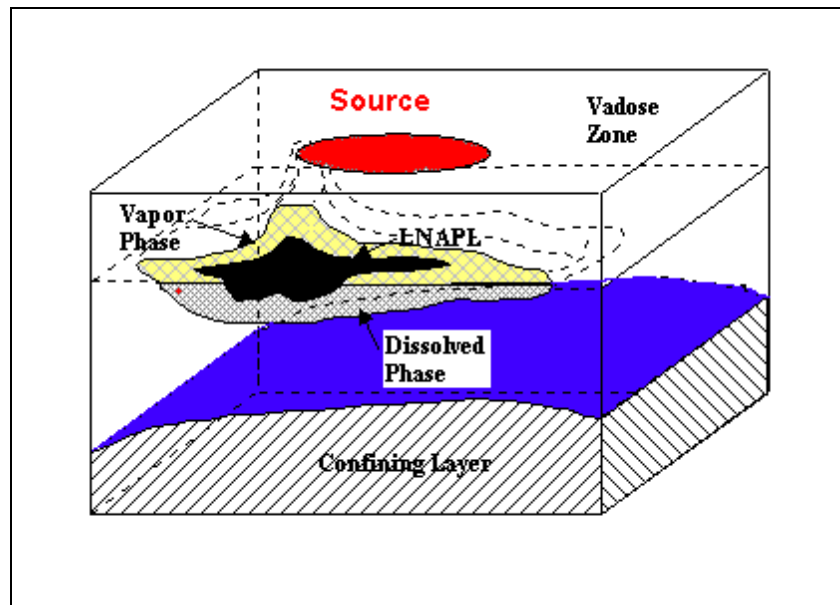

Figure 5.1 Conceptual Model.

Most of the steps that go into preparing for a model using the Platform are grouped in their logical sequence shown in Figure 5.2. They are as follows:

Step1:

The first thing that needs to be done is the determination of the modeling domain, that is the geographic extent of the simulation area. Typically this domain will start from the area of interest (for example a waste site or a well field) and extend to where secure boundary conditions may exist (that is conditions that are unaltered by forcing that may be imposed within the simulation domain), or beyond the radius of influence of anticipated forcing mechanisms. The element to consider in defining the simulation domain is a bitmap of the site showing as many features as available, including topographic contour lines, surface features, lakes, rivers, drains, observed piezometric heads and plume delineation. This bitmap is imported in the platform and "registered" to the scales of the simulation domain defined earlier. It provides the canvas on which to build the ground water biodegradation model using the platform tools.

Platform Implementation:

Menu "Domain" and its various options is the 'Domain Editor' allowing to enter all of the above mentioned parameters (see Figure 5.2 for the parameters that need to be defined in this step).

Recommended Approach:

- *Recognize the impact of the advective process in the migration of the Hydrocarbon plume for the given flow regime. Select a grid domain that covers the anticipated migration of the plume.*

- *Combine all possible bioremediation processes to reproduce the observed contaminant plume (e.g. within a period of 365 days).*

Step 2:

Define an optimum grid for the simulation. Grid definition is automated in the Platform and offers absolutely no inconvenience to the user on two counts:

1. It is drawn by specifying the number of cells in the x (top) and y (left) axes spanning the simulation domain. Note that the simulation domain can be any rectangular area inside the topographic domain.

2. The aquifer properties (conductivities, porosity, dispersion) are interpolated to the grid centers from observed data points by Kriging. A complete assortment of advanced kriging options are available for the user to control the geostatistical interpolation error. In fact this is one of the strong points of the Platform because once the raw data are entered the user does not ever have to revisit them although he/she may test a wide variety of different grid configurations.
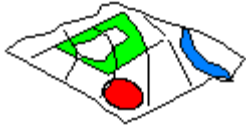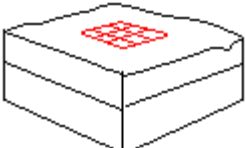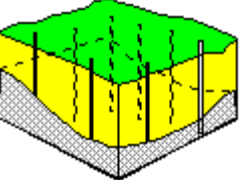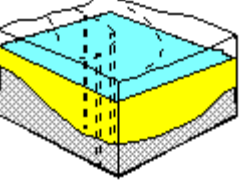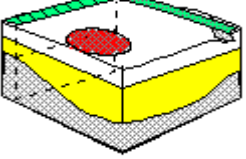
Modeling Steps	Modeling Activity	Bioplume III Editors Menu/Option
	Step1: Register the site map with contours of observed heads and concentrations. Define surface bounds (left and right), max and min elevations. Register raster background image if available.	Domain/Surface Domain Domain/Elevation Domain/Base Image
	Step 2: Define grid to better capture contaminant plume migration. (Define computational bounds and grid size number of columns and number of rows)	Grid/Generate
	Step 3: Define Properties of simulation domain delineated by the grid extent. Define constitutive properties of modeled strata. (Hydraulic conductivities, transport properties, and others). For a better refinement use Log-points and Kriged zones.	Domain/Define Strata Edit/Features (log-points, kriged zones)
	Step 4: Define Simulation Loadings Hydraulic Heads, Concentrations, and models features (wells, rivers, lakes, ponds)	Loading/Heads Loading/Concentrations Tool-Box -Edit/Features (log-points, kriged zones)
	Step 5: Define Boundary Conditions and Recharge at the boundaries.	Grid/Edit
	Step 6: Define simulation period and initial conditions	Initial Conditions/Simulation Period
	Step 7: Select simulation parameters and activate run	Simulator/Bioplume III
	Step 8: View graphics of output results	Results/Heads Results/Concentrations

Figure 5.2 Required Steps for a Groundwater Contaminant Migration Simulation.

Platform Implementation of Step 2:

Menu "Grid" and its different options is the 'Grid Editor' allowing to enter the number of required cells to create the grid. In this step you define the grid to better capture the contaminant plume migration. You need to define the computational bounds and the grid size number of columns and number of rows.

Step 3:

In this step you need to define the properties of the simulation domain delineated by the grid extent. Then you need to define the constitutive properties of the simulation strata. Such parameters are the hydraulic conductivities and the transport properties. For a better characterization of the strata in-homogeneities, if they exist at a particular site, use the Log-points and the Kriged zones available in the tool box. Then edit these features entering the appropriate constitutive parameters.

Platform Implementation of Step 3:

The menu "**Domain**" and the toolbox are the program controls to enter the values of these parameters.

Step 4:

Now it is time to define the time dependent "loads" for the simulation. These are the site measurements of the hydraulic heads, hydrocarbon contours, well pumping schedules, source mechanisms and other modeling features. The best way to enter these parameters in the program is to trace actual water and contour level isopleths shown on the site map image. Different modeling features such as wells, sources, rivers and lakes are external effects that are considered also as loads to the simulation. These features are created with the help of the toolbox.

Platform Implementation of Step 4:

The menu "**Loading**" and the toolbox are the program controls to enter the values of these loading parameters.

Step 5:

Boundary conditions are required so that the numerical model can approximate the flow and contaminant migration across the grid. BIOPLUME III supports three types of boundary conditions, inactive, constant head, and constant flow. Constant flow cells produce the effects of pumping wells and should be used with caution (in many cases they are not justified). All the cells around the perimeter of the grid must be defined as inactive for the models MOC and BIOPLUME III. They are automatically set to inactive in the Platform. The constant head condition prescribes water table elevations at a constant value in certain cells over the entire simulation. Boundary conditions must also be specified for concentrations, specifically for electron acceptors when recharging conditions prevail at the boundary of the grid.

Platform Implementation of Step 5:

The menu "**Grid**" and the toolbox are the program controls to enter the values of these boundary conditions.

Step 6:

At this stage we need to select the initial conditions to run the simulation. In that respect we need to enter the simulation period (usually several years) and the starting heads and concentrations.

Platform Implementation of Step 6:

Menu "**Initial Conditions**" allows you to select the above parameters.

Step 7:

We are now ready to run the model. However, you need first to select the time, and execution parameters as well as the program run time options and the biodegradation parameters. Depending on the size of the model several minutes are needed to complete the run.

Platform Implementation of Step 7:

Menu "**Simulator**" includes all the controls needed to run the program.

Step 8:

This is the most enjoyable step of the simulation. The output results come to live in a variety of graphics. The computed hydraulic heads and the concentrations of the hydrocarbon and the various electron acceptors can be visually inspected in two-dimensional maps or three-dimensional oblique views of the two-dimensional data. The calibration errors can also viewed as well as the results at the observation wells.

Platform Implementation of Step 8:

Menu "**Results**" allows to view the output graphics.

The conceptual model development is arguably the most important phase for a simulation study where experience counts the most. The automated/integrated Platform breaks rank with this tradition in two important ways:

1. Because data entry and model setup are performed by the Platform very efficiently, the user can concentrate on the physical, chemical, and biological aspects of the problem and gain experience very quickly.

2. The user does not need to switch from simple to more complicated models: all entered data are immediately accessible for use in testing new model setups, adjusted numerical grids, boundary conditions etc.

The Menus of the program are in fact sophisticated text and graphical editors that simplify the model creation. These editors include a variety of objects (e.g. a modeling feature) that take into account their event-driven nature. These objects have a context that determines their relationship to other objects, a set of properties that determine their characteristics, and built-in methods that determine their behavior in response to events.

Objects in the Platform are self-contained. You can change the behavior of one object in the model without changing the behavior of the remaining objects in the model. This object-oriented design offers great advantages. Features like recharge and pumping wells, interaction with rivers, drains, ponds, lakes and aquifers can now be included in the model graphically on the spot with a click of the mouse. No more hassle trying to input and track the simulation parameters. No need to blindly edit ASCII files to readjust input parameters. Instead the user can now focus on the model conceptualization without the need to micromanage input and output files. However, complete reports on the output results can be found in several output files that reside in the sub-directory of the case study.

All the details of the input modeling procedures are given in Section 5.3, following the framework of the above presented modeling steps. Each Menu and its options is considered as a graphical editor that allows the user to implement particular parameters and features in the program.

Along with the information provided in the next section the user should also consult the Tutorial (Section 3) which gives several examples, starting with simple cases and ending with the computer implementation of a real case study.

For the implementation of real case studies pertaining to Air Force Base Sites across the U.S. also consult Appendix B, "Implementing the Air Force I. R. Protocol Using the Graphical Platform," which explains how to analyze 3D field data and extract 2D information for the purpose of running BIOPLUME III.

5.3 Reference on Menus and Toolboxes

This is the Reference Section to which you will refer every time you have a question or need a detailed description of a particular feature of the Platform. You have a working knowledge of the various program graphical capabilities if you have read **Section 2**, "Getting Started". This Reference Section lists complete and definitive information on all program features.

In particular, you will find a detailed description of:

- The Menus (Editors) and menu options appearing in different Windows.

- The dialog boxes and their input parameters appearing on the screen when a particular menu option is invoked at various stages of the modeling process.

5.3.1 Description of Menus and Menu Options

As described in the Getting Started section, the Platform has ten basic Menus. Each of the main menus is associated with secondary pull-down menus which give access to various Platform options, allowing the user to generate pertinent input data, and activate different tasks of the program. There is a logical sequence to activating these menus. A particular case study necessitates several iterations, starting from a simple model and adding more refinements until we reach the desired accuracy. The Menus in the program are designed to facilitate the user in the difficult tasks of calibrating the model and validating the results. The description of the Menus is given in Table 5.1.

Table 5.1 Description of the Platform Menus.

Menu Name	Menu Function
File	Performs all file management operations, open, save, restore, delete, close, view file content.
Domain (Editor of Global Parameters)	Control parameters defining the geometry of the groundwater problem and the time domain. Appropriate selection of the cursor resolution.
Loading (Editor of Heads and Concentrations)	Defining all existing loading (Hydraulic heads, & concentrations) as a function of time.
Edit (Editor of Modeling Features, Wells, Sources, Lakes…)	All editing capabilities for the modeling features given in the toolbox for the groundwater contaminant migration problem.
Grid (Editor of Boundary Conditions and all Distributed parameters inside the Modeling Grid Area)	Definition and generation of the grid geometry used for different resolution processes. Editing of cell properties, constant/variable flow, inactive cells.
Initial Conditions (Editor of Simulation Period and initial Conditions)	Selecting initial conditions for the simulation.
Simulator	Selecting appropriate Simulation module to run.

Results **(Graphical Editor of Simulation Results)**	Visualization of all relevant data, input as well as results of various analysis options.
View **(Editor of Viewing Configurations)**	Select/Remove features appearing on the screen of the "BIOPLUME III" program.
Annotation	Activating/deactivating Annotations in all graphical options.

Each of the above main menus is associated with secondary pull-down menus which give access to the various Platform options, allowing the user to generate pertinent input data, and activate different tasks of the program. The complete Description of these options (secondary pull down menus) follows for each Menu Individually.

Menu "File"

On screen you get the following display:
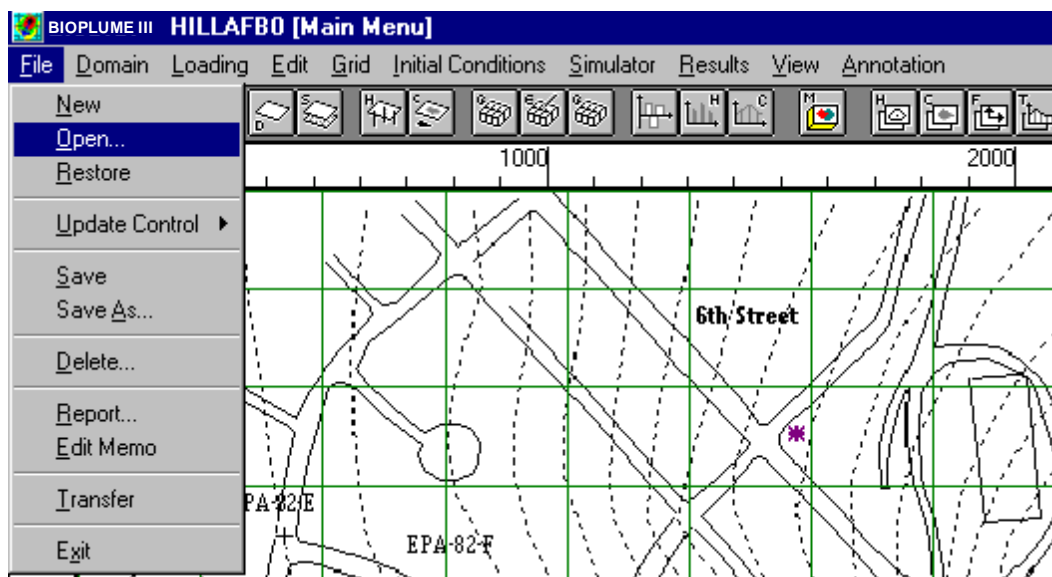
Menu Option	Description
New	Generate a new File which can be saved under option *Save_As*
Open	Open an existing file from the existing Data Base
Restore	Restore output files of a previous simulation (run)
Save	Save the active Input file
Save_As	Save the active case under a different name
Delete	Delete existing files

| Report	Browse or Print existing Input or Output ASCII files
Edit Memo	An "Editor" to report on the simulation
Transfer	Transfer via "Modem" selected files to another installation of "BIOPLUME III"
Exit	Exit the "BIOPLUME III" program

Menu "Domain"

On screen you get the following display:
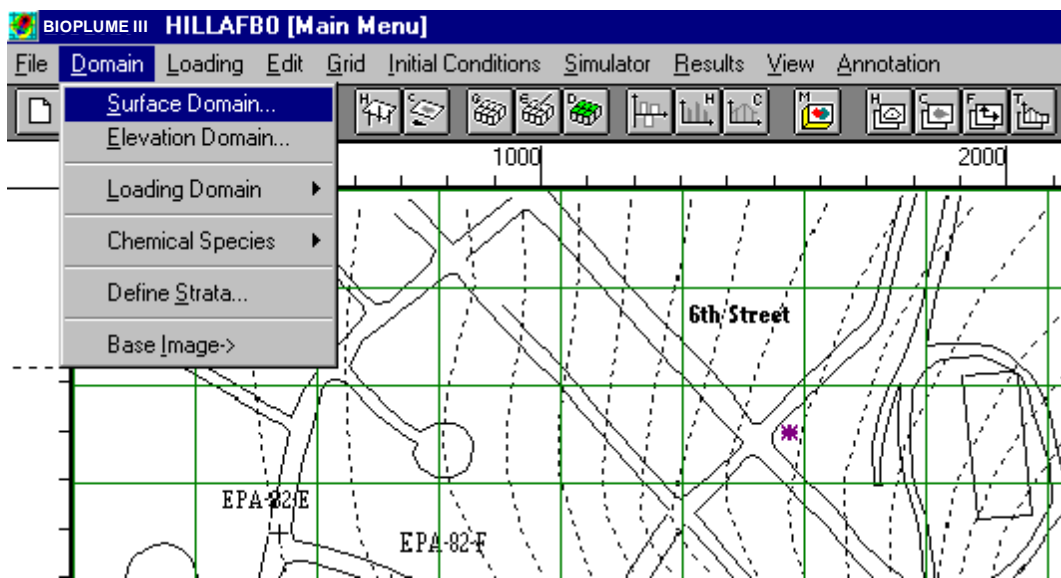
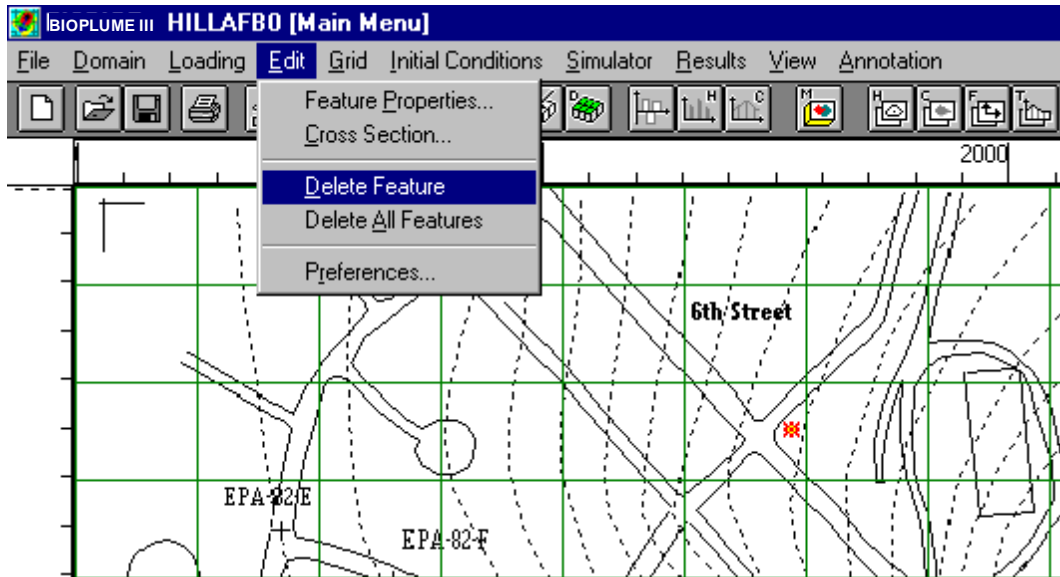| Menu Option	Description
Surface Domain	Global control data defining surface features of the problem
Elevation Domain	Global control data defining vertical scale features of the problem
Loading Domain	Bounds of the "Loading" parameters
Chemical Species	Define parameters of Electron Acceptors
Define Strata	Input data defining properties of layered geologic medium
Show Layers	Organization of strata into Computational layers
Base Image	Import of raster image of surface domain (BMP format)

Menu "Loading"

On screen you get the following display:
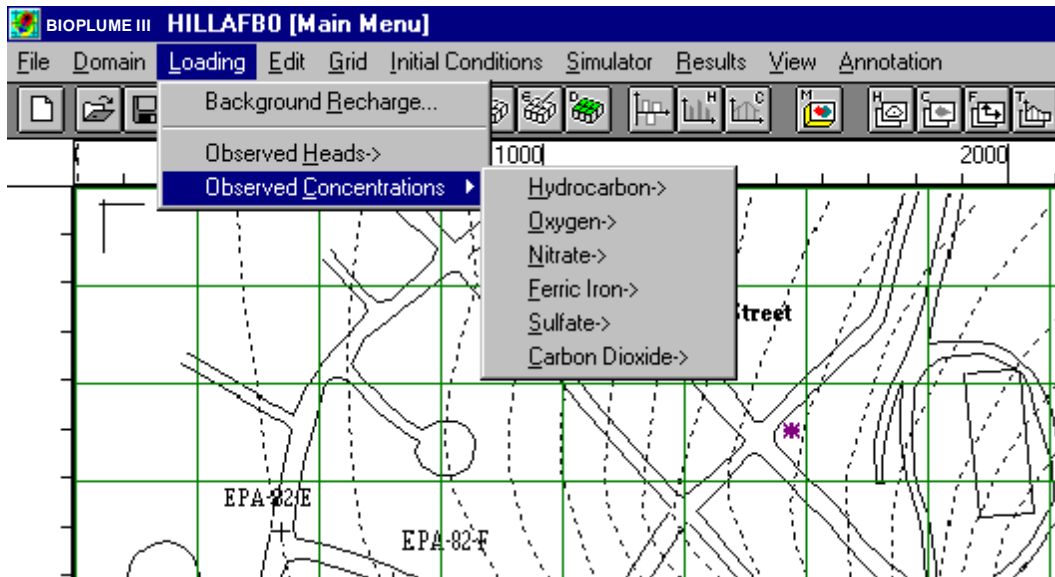
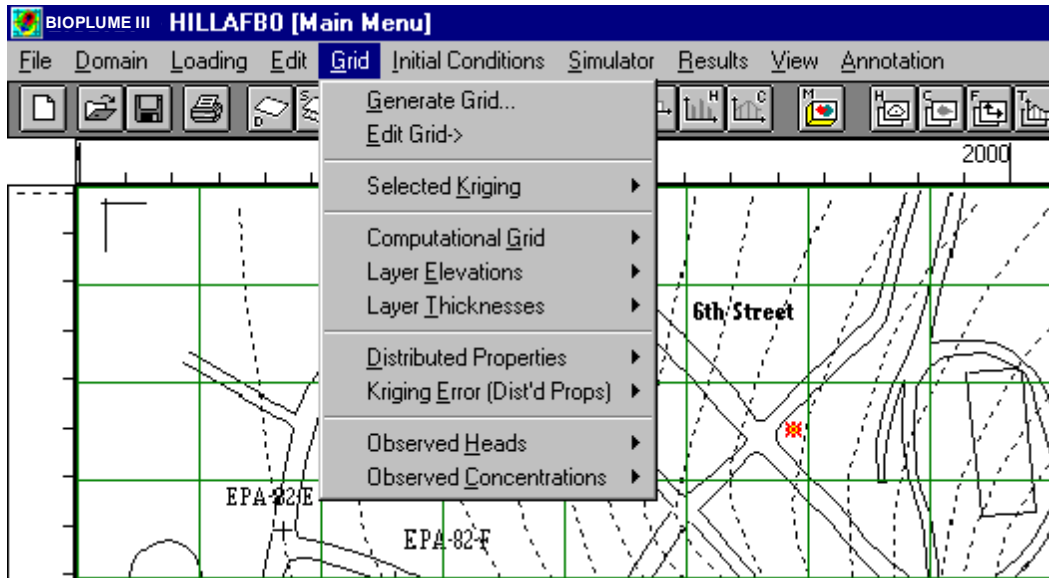| Menu Option	Description
Background Recharge	Defining the characteristics of the background recharge
Observed Heads	Locating the Observed Heads in the background of the simulation domain
Observed Concentrations	Locating the Observed Concentrations in the background of the simulation domain

Menu "Edit"

On the screen you get the following display:

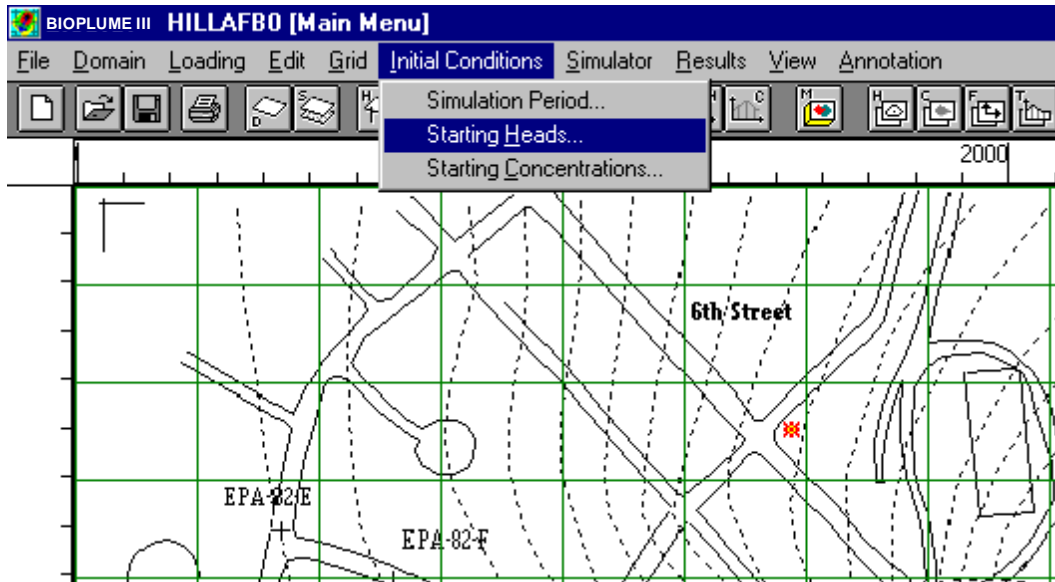| Menu Option	Description
Properties	Input characteristics of modeling features selected with smartIcons
Cross Section	Stratum properties of selected cross-section
Delete Feature	Delete selected modeling feature
Delete All Features	Delete all selected modeling features
Preference	Parameters for copying and pasting

Menu "Grid"

On the screen you get the following display:

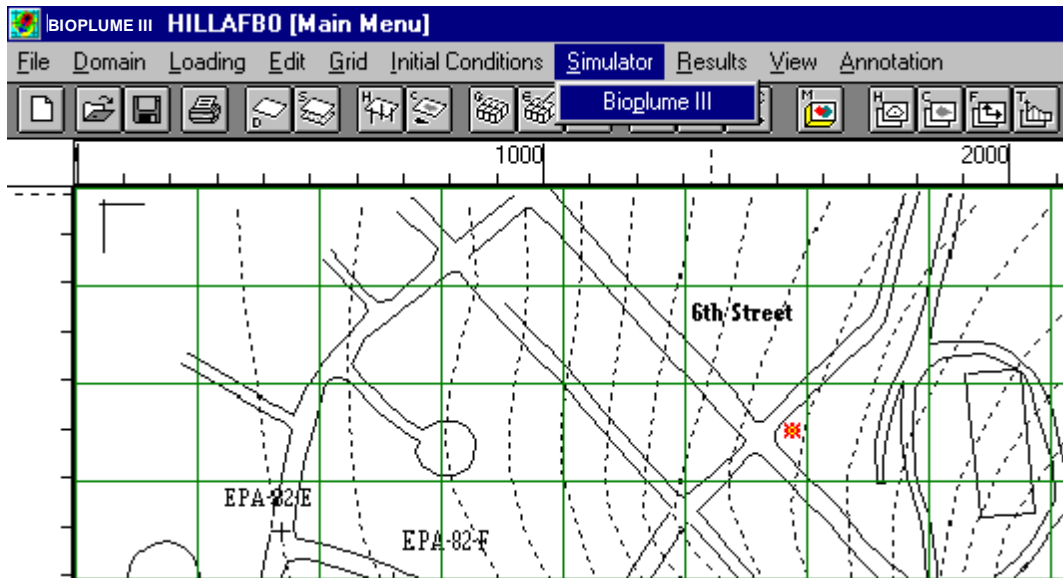| Menu Option	Description
Generate Grid	Automatic generation of the grid according to specified increments
Edit Grid	Refined editing of the grid, its boundary and initial conditions
Selected Kriging	Full "Kriging" procedure of selected properties of geologic medium
Computational Grid	View 3D display of computational grid
Layer Elevations	Show contours of layer elevations
Layer Thickness	Show contours of layer thickness
Distributed Properties	Complete "Kriging" procedure for all properties of geologic medium
Kriging Error (Dist'd Props)	Show contours of kriging error distribution
Observed Heads	Contours of observed Heads
Observed Concentrations	Contours of observed concentrations

Menu "Initial Conditions"

On the screen you get the following display:

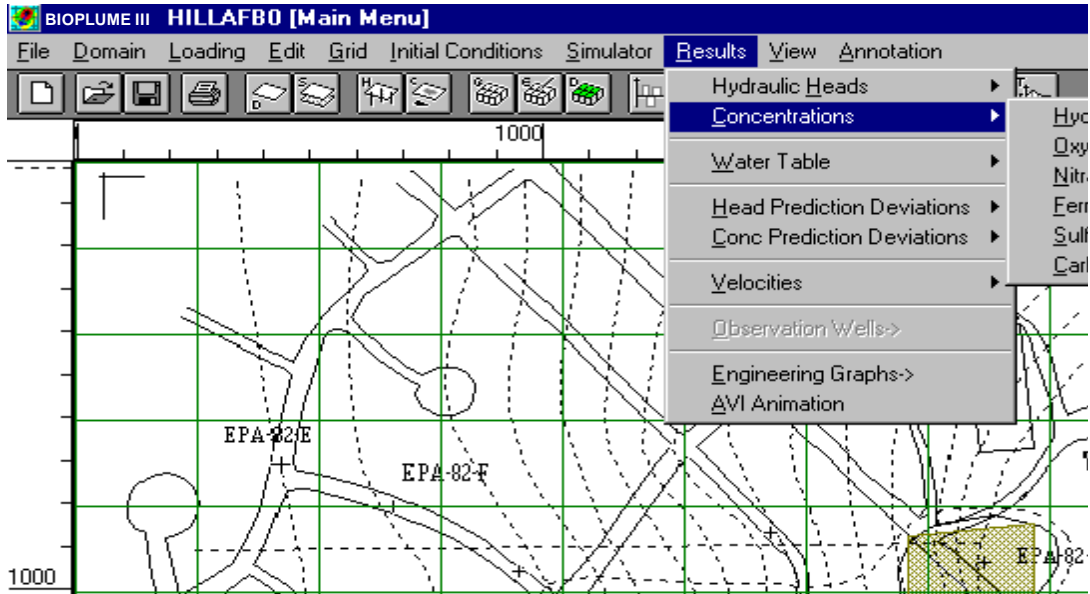| Menu Option	Description
Simulation Period	Define starting and end time for the simulation
Starting Heads	Select starting head conditions for the simulation
Starting Concentrations	Select starting concentrations for the simulation

Menu "Simulator"

On the screen you get the following display:

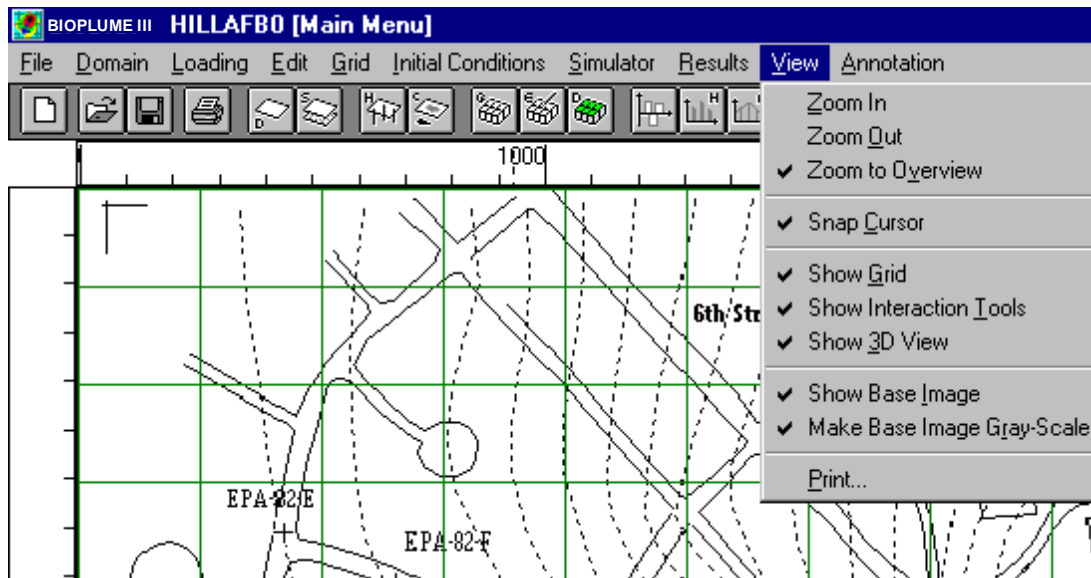| Menu Option	Description
Bioplume III	Activation of Bioplume III model

Menu "Results"

On the screen you get the following display:

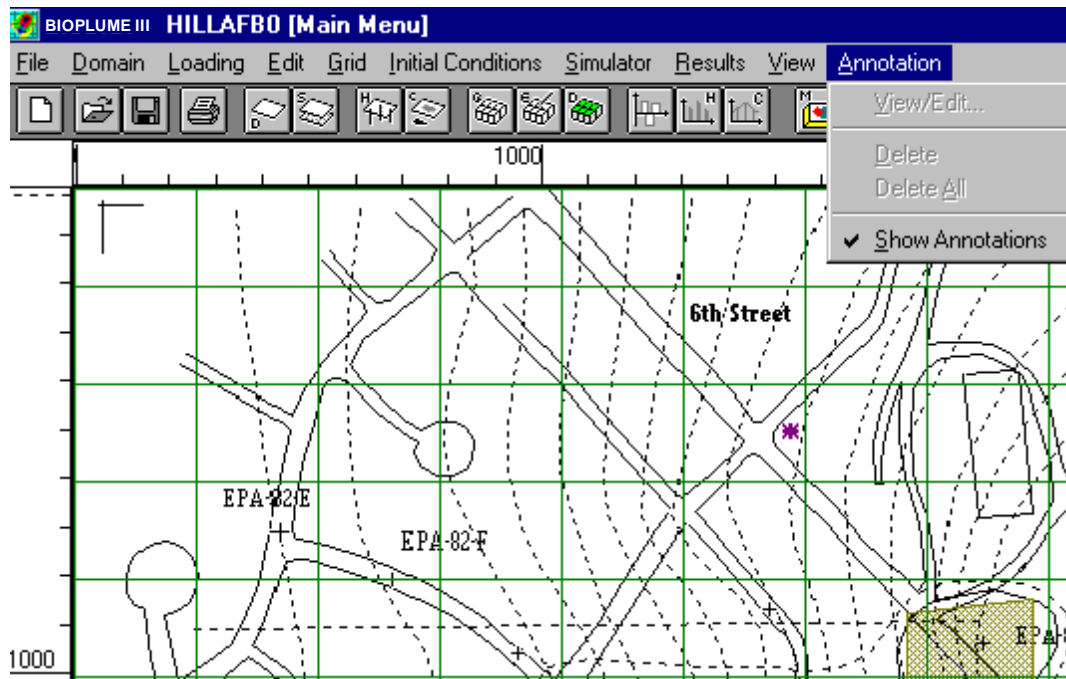| Menu Options	Description
Hydraulic Heads	Contours of computed Heads
Concentrations	Contours of computed Concentrations
Water Table	Contours of water table
Head Prediction Deviations	Contours of the computational error on the Heads
Concentration Prediction Deviations	Contours of the computational error on the Concentrations
Velocities	Graphical vector representation of computed "Velocities"
Observation Wells	Graphical representation of Observed variables
Engineering Graphs	Graphs of Concentrations
AVI Animation	Animation of plume migration

Menu "View"

On the screen you get the following display:

| Menu Options	Description
Zoom In	Reduce viewing scale
Zoom Out	Enlarge viewing scale
Zoom to Overview	Zoom to fit the image in the Window of working area
Snap Cursor	Activate resolution of the cursor movement
Show Grid	Show generated grid
Show Interaction Tools	Show box with smart-Icons (toolbox)
Show 3D View	Show 3D View window of simulated domain
Show Base Image	Show selected raster image in the background
Make Base Image Gray	Show selected raster image in gray scale
Print	Printing the Screen/Window

Menu "Annotation"

On the screen you get the following display:


Menu Options	Description
View/Edit	View or Edit Annotation Window in working area
Delete	Delete particular Annotation (Highlighted)
Delete All	Delete all Annotations in current simulation case
Show Annotation	Display Annotation Marks in working area

5.3.2   Secondary Menus

In the previous section were described the full list of primary menu options. Several menus such as: "**Loading**", "**Grid**", and "**Results**" lead to submenus that are specifically designed to support graphical interactive procedures: a small arrow next to the menu option indicates the existence of such secondary menu as show below.
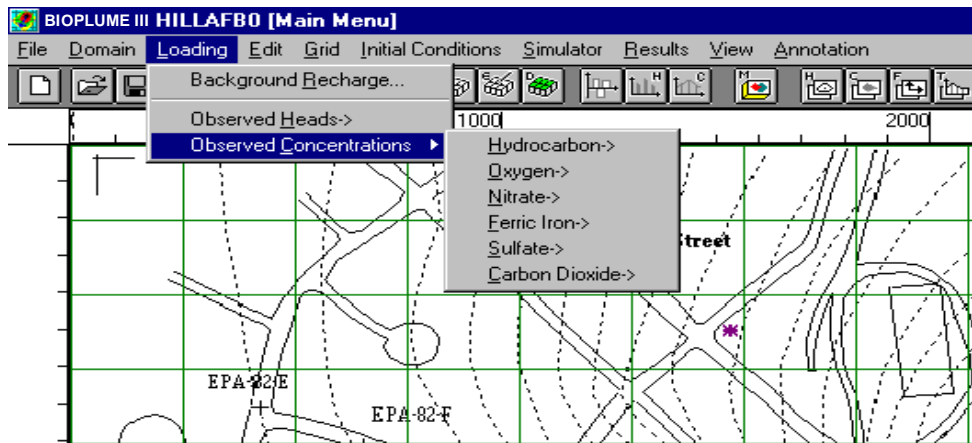
For example, in menu **"Loading"** option **"Observed Concentrations/Hydrocarbons"** has an arrow to the right indicating that it accesses a secondary menu. Click with the mouse at this type of menu option and automatically you move to a Secondary Menu, or "Sub-Menu" domain as shown in the figure below.
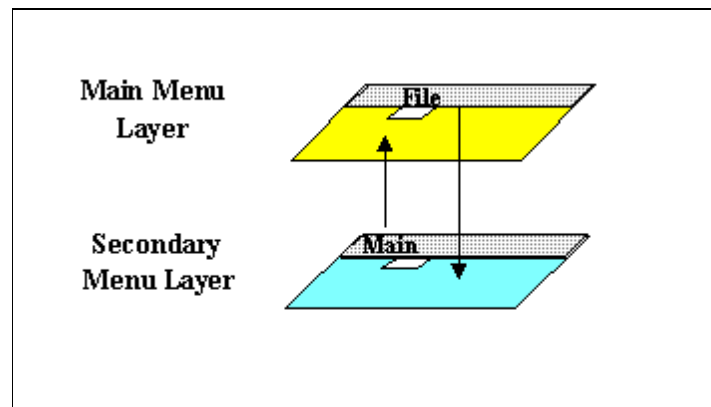
To move from the "Secondary" menu back to the main menu clicck on the submenu "**Main**". The complete list of the secondary menus follows.

Note that the calling option appears in the title bar of the window display for your reference. A total of 120 graphical options are offered in the Platform allowing you to view the results in 2D and 3D

(perspective) configurations. As you may have noticed most of these secondary menus (Sub-menus) belong to one of five categories as shown below:

Category 1(Base Image Operations)	"Main" " Select" "Edit" "View"
Category 2 (Loading Conditions)	"Main" "Edit" "Time" "View" "Annotation"
Category 3 (Grid Editing)	"Main" "Edit" "Layer" "View" "Annotation"
Category 4(Input Graphics)	"Main" "Contour range" "Layer" "View" "Annotation"
Category 5(Output graphics)	"Main" "Contour range" "Time" "Layer" "View" "Annotation"

The submenus are activated from all menus that are followed by a small arrow (➜). The list of the basic items of these "Submenus" is given in the following tables. (The result of their activation is self descriptive).

Category 1 (Base Image Operations)

Main	Select	Edit	View
	From File	ImageCenter	Zoom In
		Copy to Clipboard	Zoom Out
	From Cilpboard	Register Image	Zoom to Overview
	Deselect		Snap Cursor
			Show Features
			Show InteractionTools
			Print

Category 2 (Loading Conditions)

Main	Edit	Time	View	Annotation
	Properties	Previous Time-step	Zoom In	View/Edit
	Delete Load Object	Next Time-step	Zoom Out	Delete
	Delete All Load Objects	Select Time-step	Zoom to Overview	Delete All
		Edit Time-step	....	Show Annotations

Category 3 (Grid Editing)

Main	Edit	Layer	View	Annotation
	Edit Head Boundaries	Previous layer	Zoom In	View/Edit
	Edit Concentration Boundaries	Next layer	Zoom Out	Delete
	Delete grid-line	Select layer	Zoom to Overview	Delete All
			....	Show Annotations

Category 4 (Input Graphics)

Main	Contour Range	Layer	View	Annotation
	Span current layer	Previous layer	Zoom In	View/Edit
	Span all layers	Next layer	Zoom Out	Delete
	Set number of levels	Select layer	Zoom to Overview	Delete All
			....	Show Annotations

Category 5   (Output time dependent graphics)

| Main	Contour Range	Time	Layer	View	Annotation
	Span current layer	Previous Time-step	Previous layer	Zoom In	View/Edit
	Span all layers	Next Time-step	Next layer	Zoom Out	Delete
	Set number of levels	Select Time-step	Select layer	Zoom to Overview	Delete All
		Edit Time-step		....	Show Annotations

5.3.3   Available Menu Options in the Icon Bar

The **'Icon Bar'** which is located below the **'Menu Bar'** contains different sets of "**SmartIcons**" that can enhance the interactive operations. These **"**SmartIcons" are mouse shortcuts of the most commonly used menu options. A brief description of their function is provided in the following graphs.

For the Primary Menu System
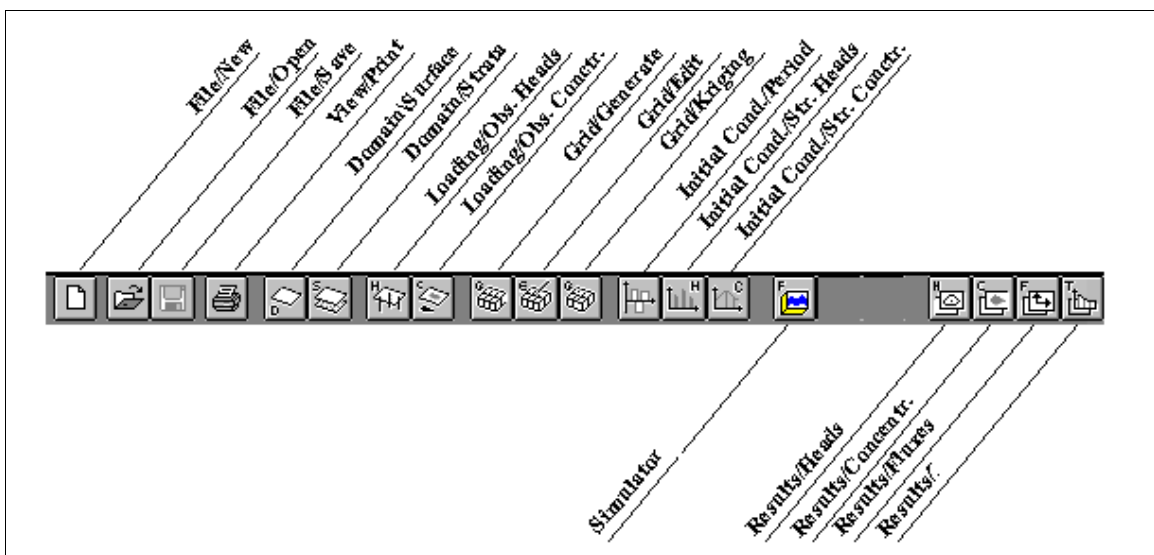
For the Secondary Menu System
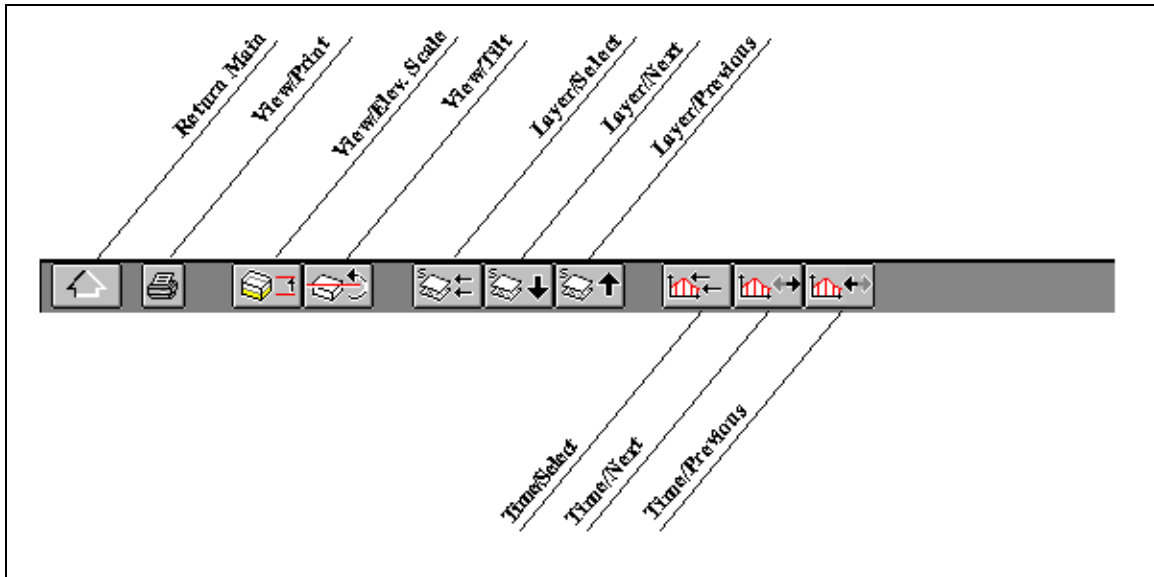
5.3.4   Tool-Box Features

The **tool-box** provides to the user all necessary tools to build a model or to select a particular graphical mode (function).   These tools cover the basic modeling features such as the **log-points**, **wells**, **contaminant sources**, **rivers**, **ponds** and **lakes**.   They are all contained in the tool-box for easy access. All the user has to do is point, click and drag. The selected modeling feature is created on the spot. Once a feature is created in the working area of the screen (highlighted), the user proceeds to the menu item "Edit" to input its properties. The feature edit option is also accessible by double-clicking on the feature (well, lake, river) in the working domain. Similar Tools are also available for editing the computational grid and specifying boundary conditions (constant head, concentrations).
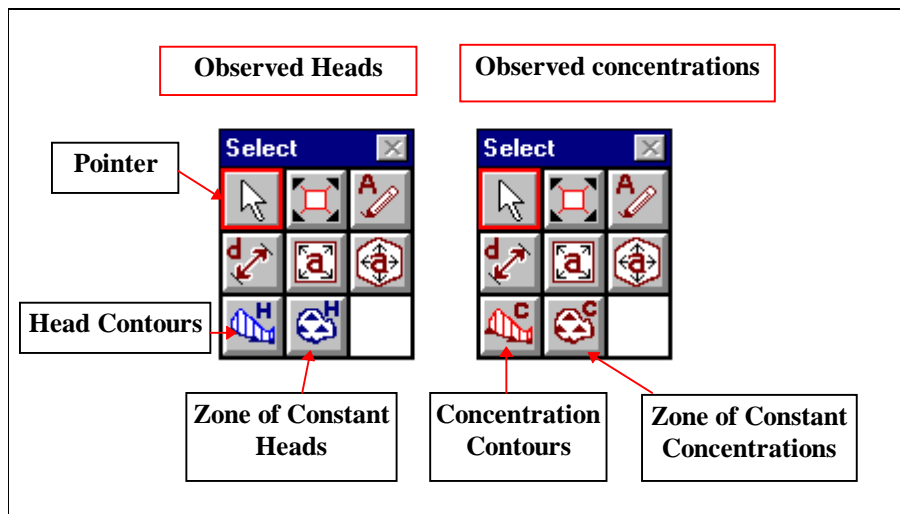
The tool-box also features tools that allow the evaluation of linear and polygonal distances and areas graphically on the screen using point-and-click procedures. These tools are useful to quickly evaluate contaminant extent and migration rates. The tables below offer the description of all features in the various tool-boxes.

Tool-Box in Main Menu Layer
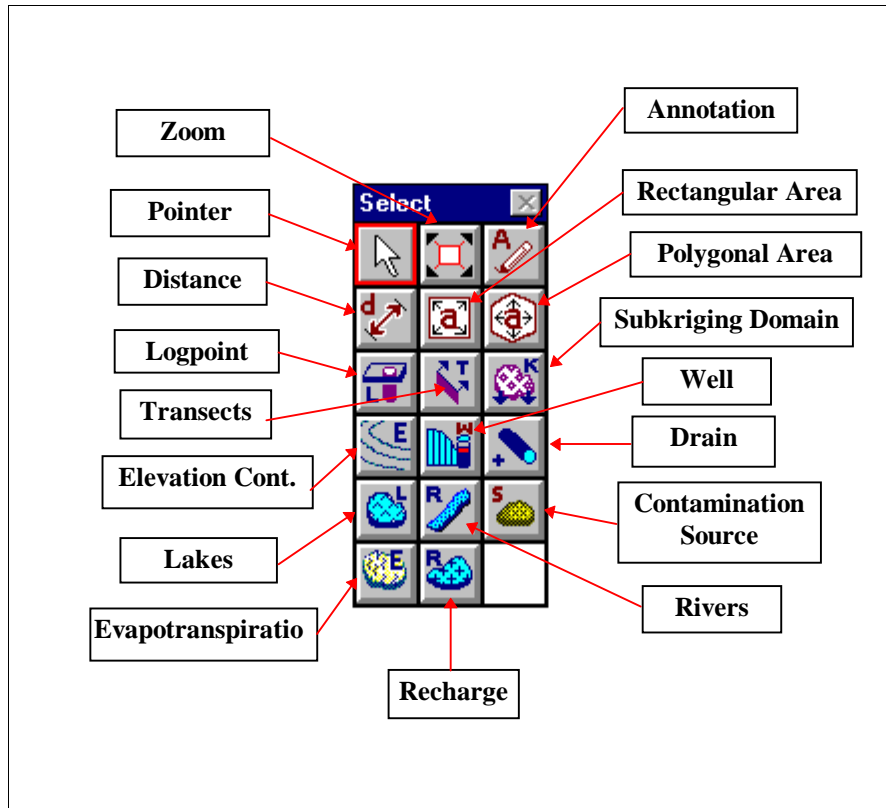
For more details on how to use these tools you can refer to Section 2, 'Tutorial' and the next section.
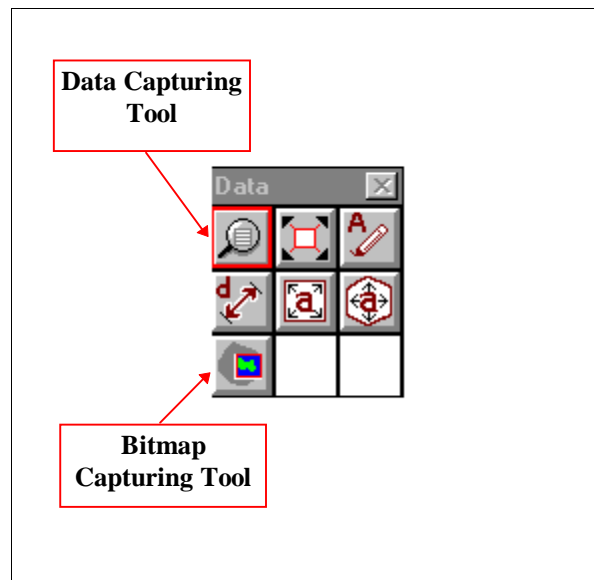
Tool-Box in Secondary Menu (Activated by "Loading/Observed Heads, or Concentrations)

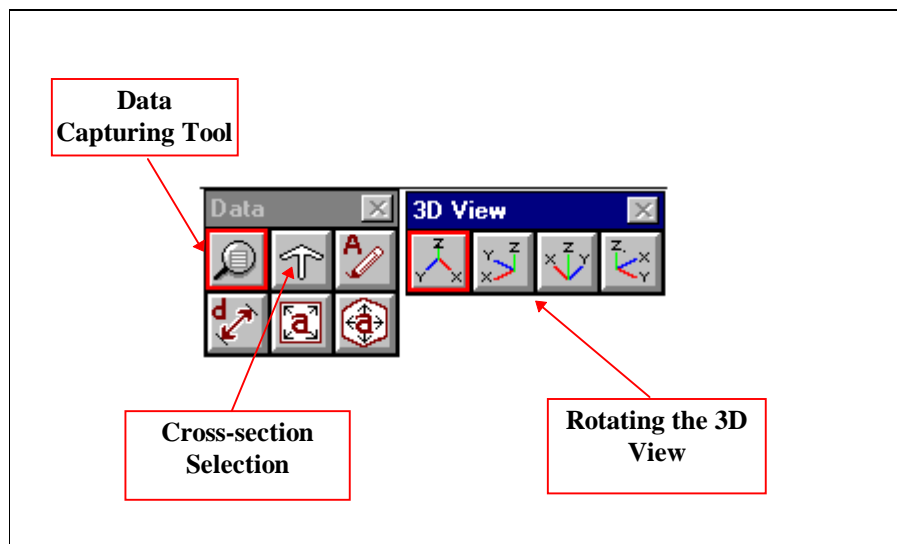**Tool-Box in Secondary Menu (Activated by "Grid Editor for Hydraulic Heads")**

Pointer

Constant
Head/
Concentr.

Variable
Head/
Concentr.

Inactive
Head/
Concentratr.
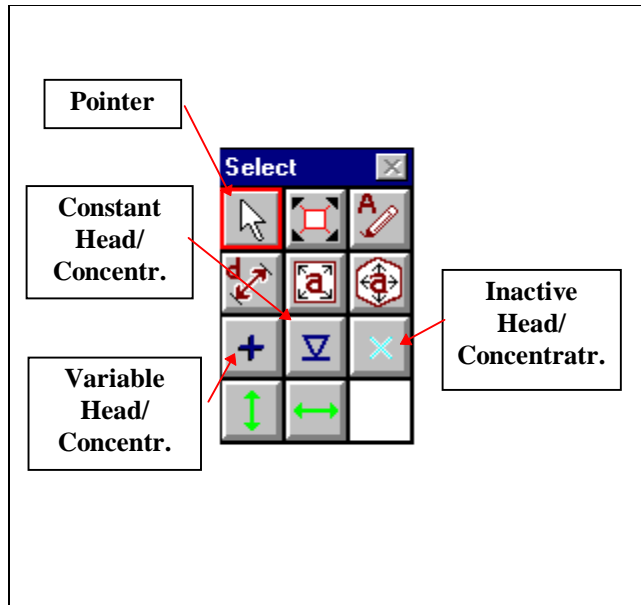
Tool-Box in Secondary Menu For 2D Contour Maps

Data Capturing
Tool

Bitmap
Capturing Tool

Tool-Box in Secondary Menu For 3D Elevations

(BIOPLUME III supports only 2D modeling)

With the presentation of the tool-box features we conclude the description of the basic operations of the program that allow an entry point to the implementation of the modeling steps introduced in Section 5.2. In the next section we continue with the definition of the input parameters that are required to run the BIOPLUME III simulation.

5.4 Reference on Dialog Boxes and Input Parameters

This is the Reference Section to which you will refer every time you have a question or need a detailed description on a dialog box and its corresponding input parameters appearing on the screen when a particular menu option is invoked at various stages of the modeling process. All necessary data needed to build and validate a simulation are easily handled using only a few dialog boxes that are properly managed from the main menu as shown below:

Operation	Detailed Modeling Activity	Corresponding Menu
File Manipulation	New, Open, Save	*"File"*
Simulation Domain	Define area, limiting values of basic parameters, & electron acceptors	*"Domain"*
Loading Parameters (Heads, Concentrations)	Define Heads and Concentrations at different times.	*"Loading"*
General Input Data	Define numerical grid and associated distributed properties of the soil media	*"Edit", "Grid"*
Initial Conditions	Define simulation period, select initial Heads and Concentrations	*" Initial Conditions"*
Numerical Simulation	Select running options and run the case study	*"Simulator"*
Graphics of Results	View different graphics of output results	*"Results"*

All input data required to run BIOPLUME III is prompted from the user by the Platform in a completely interactive manner. The error-prone formatting chores of editing input streams are totally eliminated. Furthermore, the user is guided by the appropriate dialog boxes as to what type of input is expected, the default value, and the range of values that are expected. The details on how to use these dialog boxes are discussed in the following pages. To facilitate the presentation, we show the input parameters of the dialog boxes exactly as they appear on the screen. Most of these dialog boxes are self explanatory. However, where needed you will find a brief explanation and description on the nature of these parameters. You can also consult Section 2, 'Tutorial' which has examples on how to use these tools.

5.4.1 Dialog Boxes Associated with Menu 'File'

Menu Item: "New"

This item initializes the Platform for a new case study.

Menu Item: "Open"

It allows the user to open an existing case study. It will retrieve all the files found in sub-directory ..\EISBioplume\Data\"Case Name" bearing the name of the case study. These files are automatically loaded into the system.

Use the mouse to open an existing case by double-clicking on the selected application name. Now you can access these files, to upgrade the case or view existing graphics and output results.

Menu Item: "Restore"

If for some reason the changes that you have made into an application case are not satisfactory you can restore the files to the original case (prior to the last change) by activating this menu option.

Menu Item: "Save"

It allows the user to save an existing case including the changes affected (edited) on that file. However, be aware that in this case all existing (simulation) output files will be deleted. A warning screen appears and gives you the option to "Cancel". As a rule, it is advisable to maintain simulation results in the original case name and to give the new version a new name using the "Save_As" menu option.

Menu Item: "Save_As"

It allows the user to change the name of an existing case by typing the new name in the appropriate box.

Menu Item: "Delete"

This item deletes all data and output files of the specified case. A warning screen appears on the screen that allows you to backtrack by "Canceling". BE AWARE, this is a strong command: all files

from the case, input and output will be deleted from the system for good! (at least consider making a back up tape).

Menu Item: "Report"

This option allows the user to view the ASCII (output) file from a BIOPLUME III simulation. See Section 4, 'Theoretical Development' and Appendices for more information on the contents of this file.
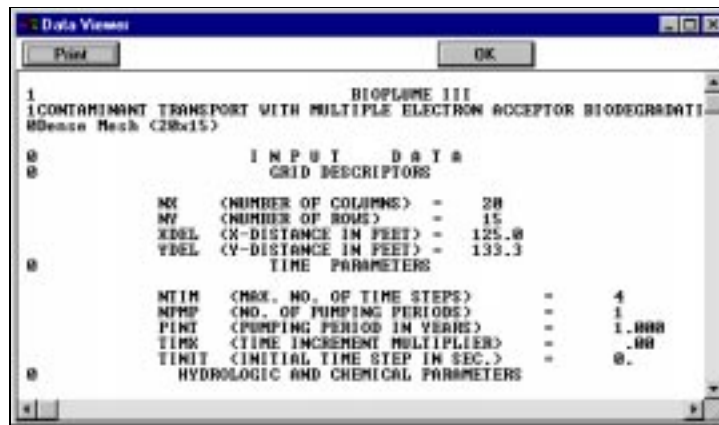
Menu Item: "Edit Memo"

A small editor to report on the simulation. Simple editing tools are supported.

Menu Item: "Transfer"

A simple module allowing you to transfer selected files via modem to another installation of the Platform.

Menu Item: "Exit"

Exit command to close out the Platform Windows application.

5.4.2   Dialog Boxes Associated with Menu 'Domain'

Menu Item: "Surface Domain"

This item allows the user to define the domain of interest for the simulation. It also allows the user to determine the scaling of the vertical and horizontal rulers and cursor resolution. The cursor resolution controls the "snap" cursor action. Use a consistent set of units for length. For your reference the values displayed in the dialog box are taken from the case study "Hillafb1". In this case the coordinates of the origin at the top left corner of the domain are (0., 0.), while the coordinates at the

bottom right corner are (2500.,2000) in feet. Note, however that any pair of coordinates can be selected at the origin.


Menu Item: "Elevation Domain"

This item allows the determination of vertical (elevation) domain, Ruler increments, and cursor resolution. Top and bottom elevations of the aquifer layer vary between 4560 ft and 4690 ft. above sea level in the example.

Menu Item: "Loading Domain"

This menu option allows the user to select the bounds (Upper and lower limits) of the following simulation parameters.

> **Time**
> **Pumping Rates**
> **Concentrations**
> **Infiltration**
> **Hydraulic Heads**

Each item activates a dialog box to enter pertinent input information. These dialog boxes are shown below.
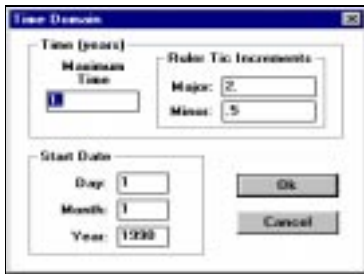
The ruler tic increments in all of these boxes determine the appearance of the rulers in all corresponding graphical displays. Note that if the increment is too small, the numerical characters will be difficult to read.

Menu Item: "Chemical Species"

This is an option that allows the user to enter the properties of the hydrocarbon contaminant and potential "Electron Acceptors" used in the simulation. The dialog box for the hydrocarbon is shown below.
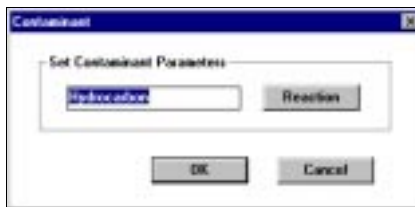
To enter the reaction properties for the hydrocarbon click on the "Reaction" button as shown below.
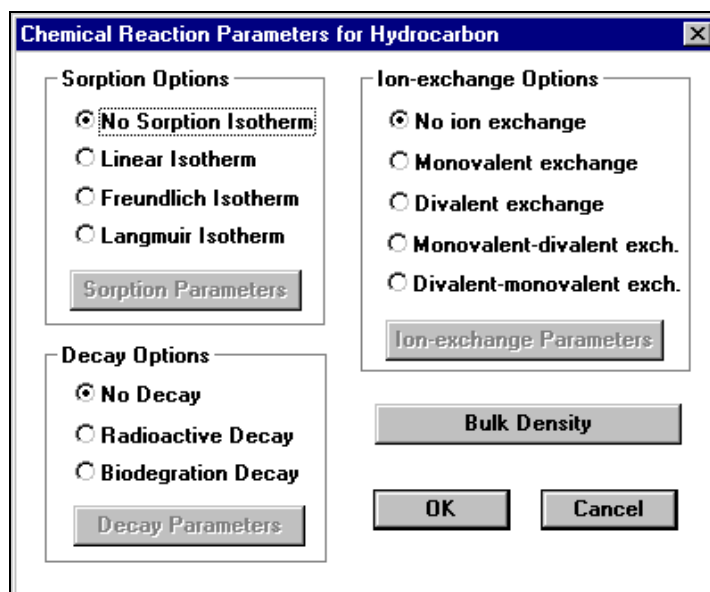
This is where you input the "Chemical Reaction Parameters"; for selection of chemical reaction type among Sorption, Decay, and Ion-exchange; Parameters buttons activate the next dialog box. **Note that all relevant parameters are entered once. Selection of chemical reaction type, if any to include in the simulation is done at "Run Time Option" dialog box discussed in menu "Simulator".** The next three dialog boxes show the editing boxes of the "Sorption", "Ion Exchange", and "Decay" parameters.
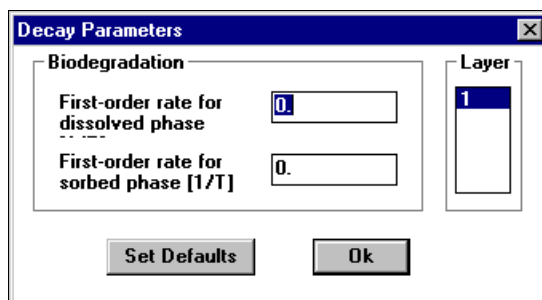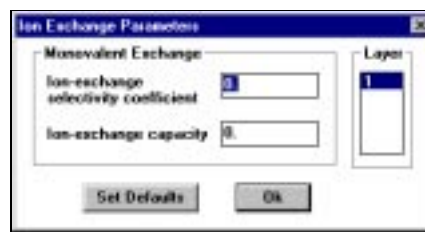
The same dialog boxes also appear for the reaction parameters of the "Electron Acceptors".

To enter the reaction and interaction properties for the **"Electron Acceptors"** click on **"Domain\Chemical Species\Electron Acceptors** to obtain the dialog box shown below.
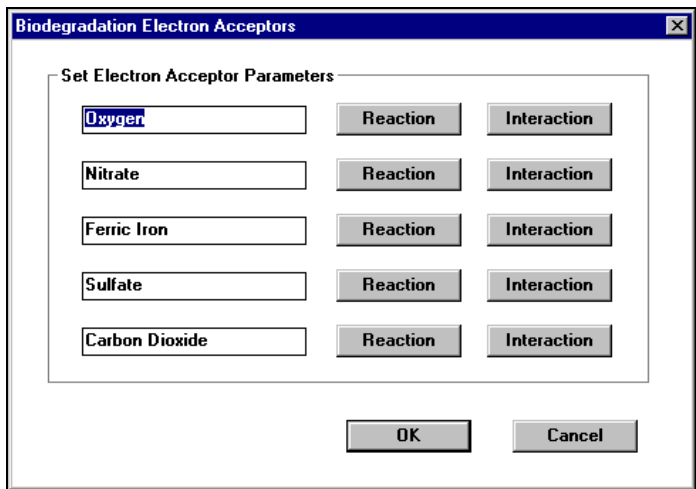
This dialog box includes all the electron acceptors supported by BIOPLUME III. Since the reaction parameters are the same as for the hydrocarbon, we illustrate here only the "Interaction" parameters shown in the dialog box below.
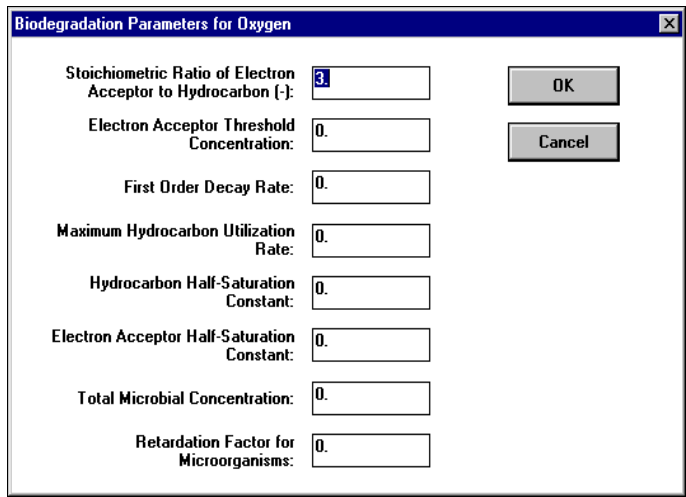
This dialog box shows the parameters for oxygen only; the list of Interaction parameters is the same for all "Electron Acceptors".

For further information on the nature and impact of these parameters on the simulation of "Intrinsic Remediation" consult Section 2, "Tutorial," and Appendix B, "Intrinsic Remediation Protocol".

Menu Item: "Define Strata"

The "Strata Definition" Box is provided for specification of background (constant, default) properties of the computational layer. The "Transport Properties" activates the screen for the dispersion coefficient.
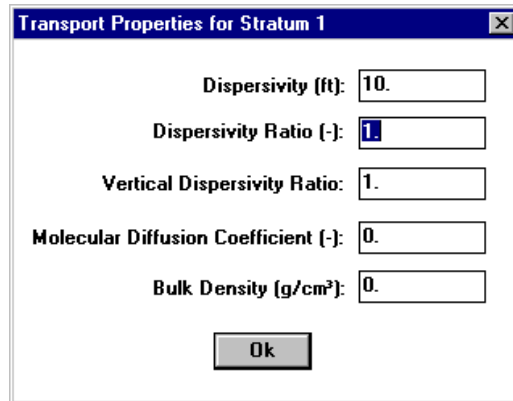
Menu Item "Base Image"

This option allows the selection and identification of the base image on top of which the modeling features will be defined using the tool-box. Upon activation of this option a secondary menu appears on the screen as shown below.
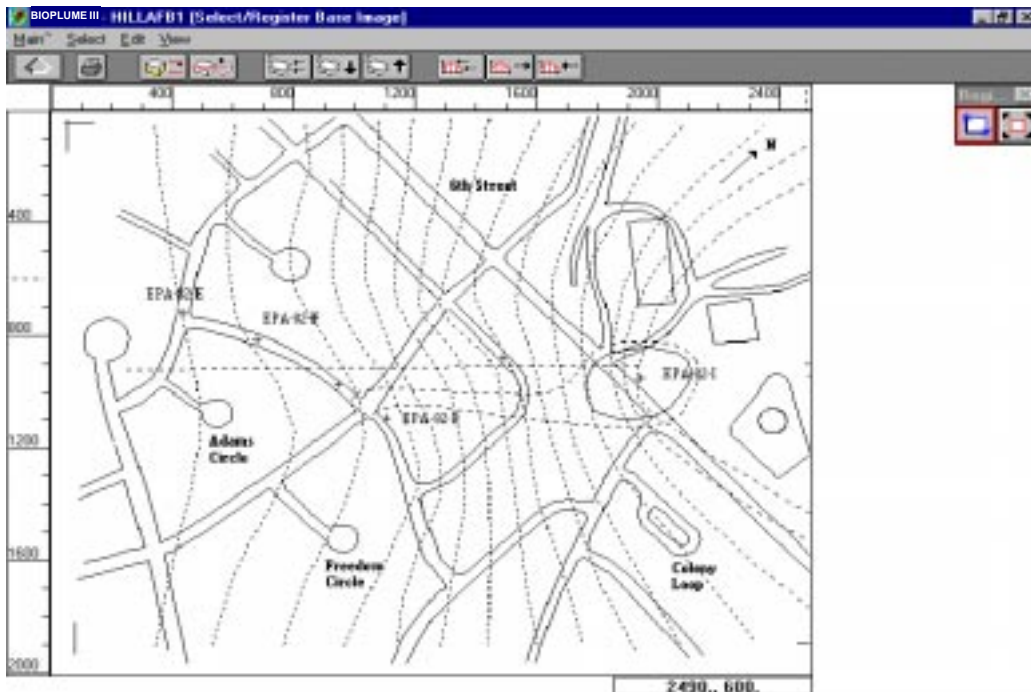
The big "Up Arrow" in the upper left corner of the screen indicates that you are in a Secondary Menu (Child Menu). The displayed image is obtained in two steps. In the first step we load an existing bitmap from the bitmap files stored in Sub-directory "..\EIS\Bioplume\Image\". This is done by activating menu option "Select\Image File" and enter in the editing box the name of the required bitmap file (files with extension .BMP). In a second step register the image that is displayed on the screen.

To register the image select the appropriate icon from the toolbox (the button adjacent to the zooming tool) and click on the working area to define the top left corner of the simulation domain. Then drag the mouse to the bottom right corner to register the area for the simulation. Releasing the mouse causes a dialog box to appear. Now all you need to do is enter the coordinates of these two points and the registration is completed.

The background image can be used to fulfill different objectives within the framework of the same application. For example, the background can be used to:
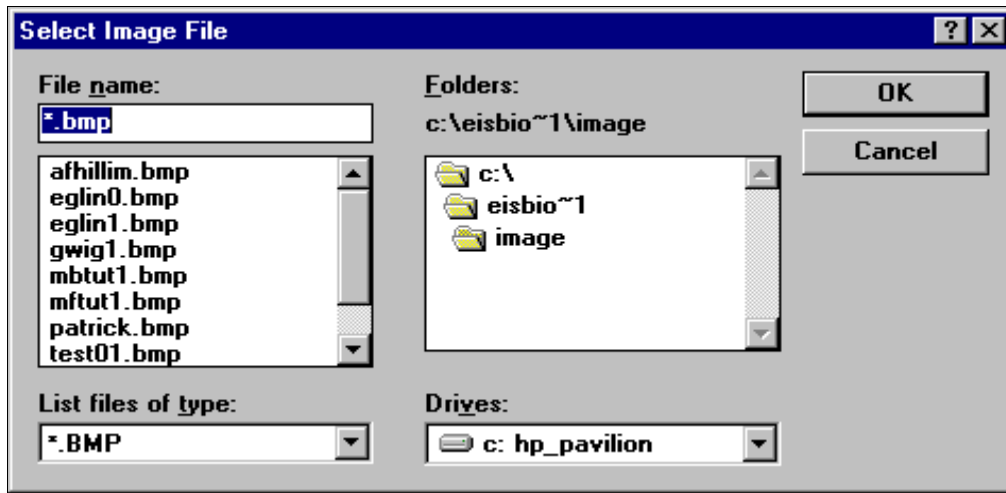
- locate the modeling features for a particular simulation

- graphically enter the initial and observed hydraulic heads, and

- graphically enter the initial and observed concentrations

The Platform allows interchanging of the background image. However, the user should check that the image registration points are the same in all background images for compatibility.

5.4.3   Dialog Boxes Associated with Menu 'Loading'

This menu allows the user to enter all known observed (measured) data from a monitoring activity. In that respect all the parameters that are edited with this menu are time dependent.

Menu Item "Background Recharge"

This option allows to impose a specified recharge rate (flux) and concentrations (hydrocarbon and electron acceptors) throughout the simulation domain at all known times as illustrated below.
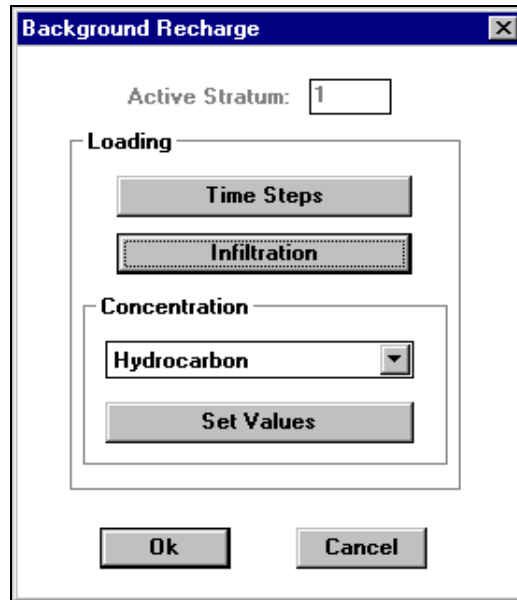
Desired time-steps in which site recharges are known can be entered by pressing on the "Timesteps" button. This activates the following screen.
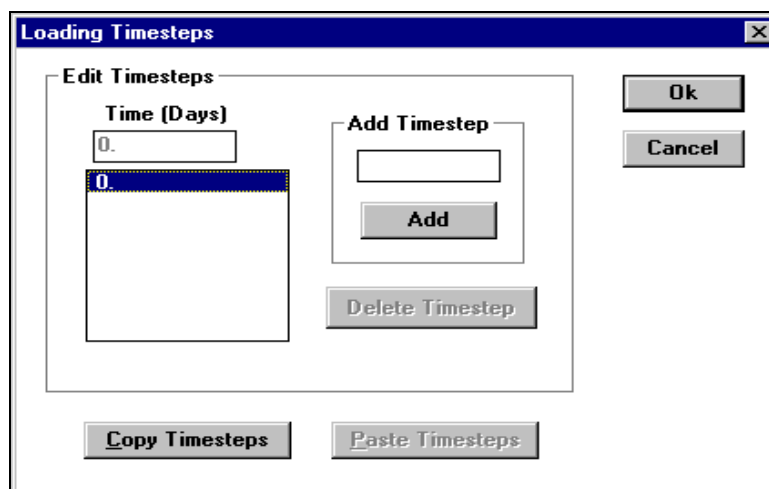
Note that you can add , copy, paste and delete different times.

To enter the observed fluxes click on the "Infiltration" button and specify the recharge rate (fluxes) at all specified times. Copy and Paste buttons allow to duplicate previous record. The entry is numerical and/or graphical as shown below.
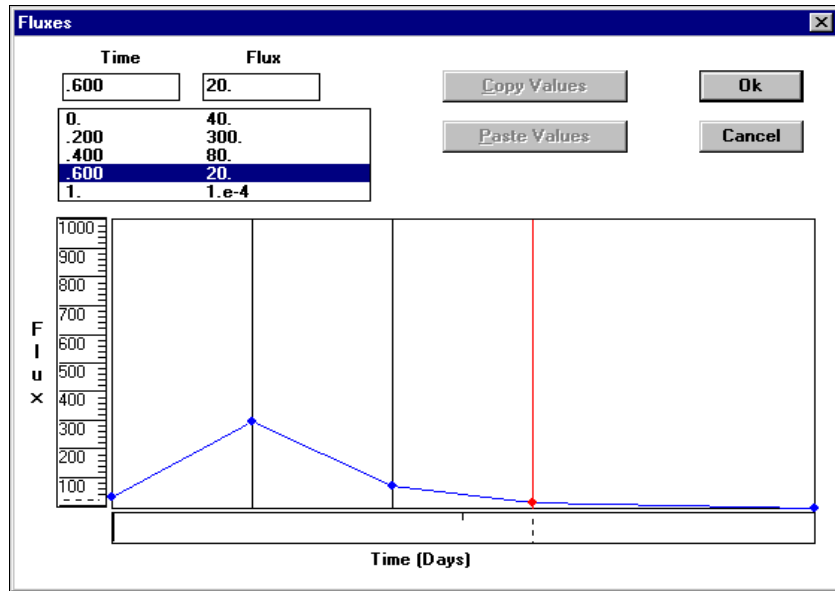
You can either enter the values at different times in the editing box or with the mouse by clicking and dragging the nodes for each specified time at the desired level. Follow the same procedure to specify "Recharge Concentrations" as shown below.
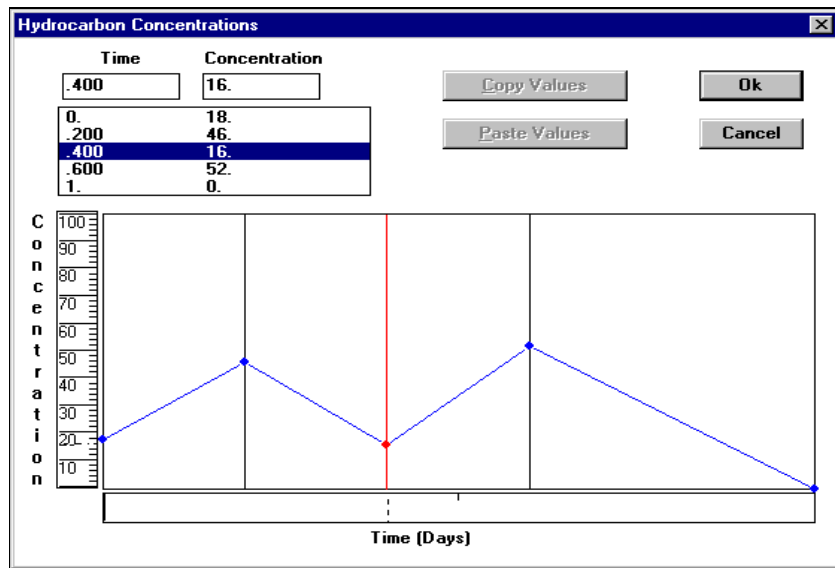
The previous three dialog boxes are typical of all time-dependent parameters. The same dialog boxes are encountered in many other parts of the program. Note that you can also specify "Recharge Concentrations" for all "Electron Acceptors".

Menu Item "Observed Heads"

This item allows specification of known hydraulic heads at all specified times in a secondary menu environment shown below. You can input the hydraulic head contours (e.g. as shown on the background bitmap) using the appropriate tool from the tool box. Just point and click.
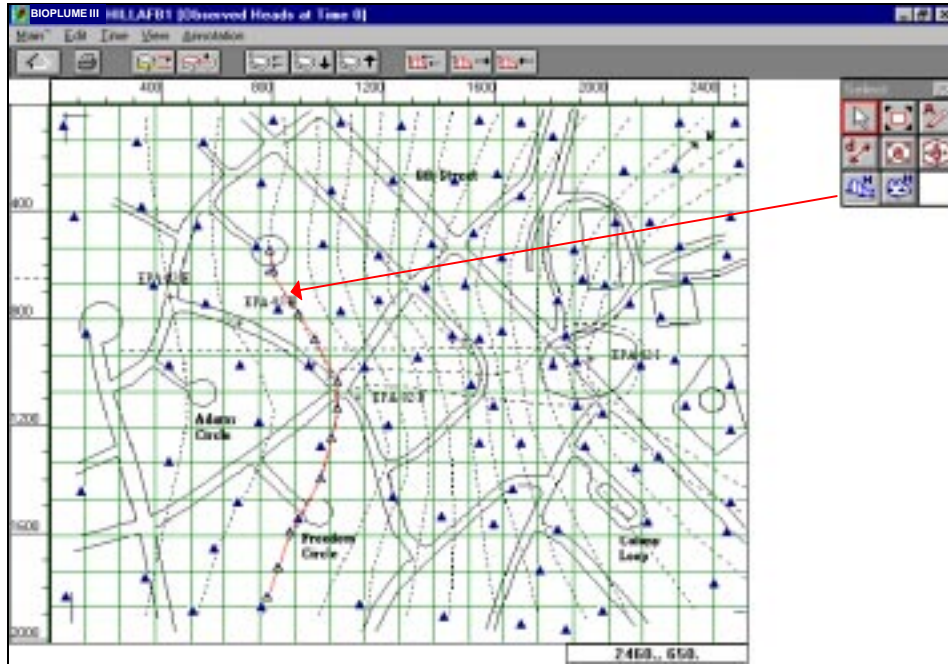
Once a contour is placed on the map, double click or edit this feature through menu edit to enter the contour level using the following dialog box.

You then proceed with the next contour of hydraulic heads. This procedure takes only a few minutes and the rest is taken care of by the Platform. The hydraulic heads will be automatically distributed at each grid cell where it is needed. Note also that the contours for the starting time can automatically be considered as initial conditions for your simulation. Subsequent times are considered as target values

for your calibration. The platform automatically tracks down the error between the observed and simulated values, (see option "Head Prediction Deviations" in Menu "Results").

Menu Item "Observed Concentrations"

This item allows specification of known concentration of the hydrocarbon and the various electron acceptors at all specified times in the secondary menu environment shown below. You can input the concentration levels (e.g. as shown on the background bitmap) using the appropriate tool from the tool box. Just point and click.
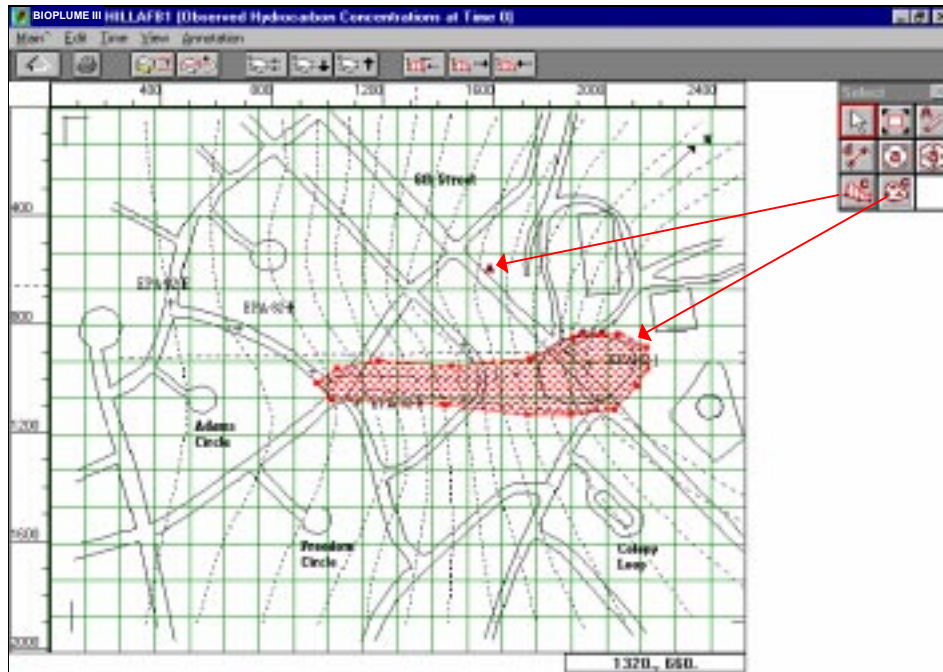
Once a Concentration zone is placed on the map, double click or edit this feature through menu edit to enter the concentration level using the following dialog box.
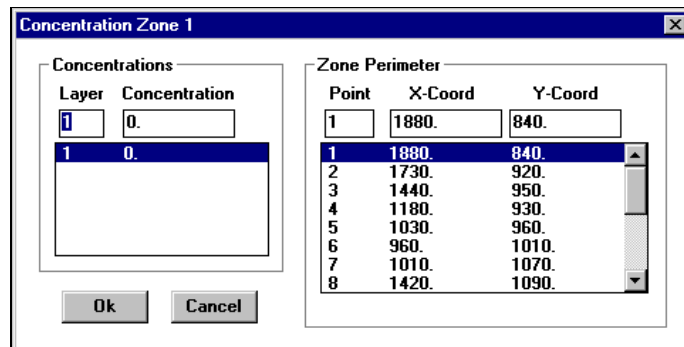
Note that with the concentration zone you need also to specify a logpoint with zero or background concentration to trigger the kriging module. The concentrations will be automatically distributed at each grid cell where needed. Note also that the contours for the starting time can automatically be considered as initial conditions for your simulation. Subsequent times are considered as target values

for your calibration. The platform automatically tracks down the error between the observed and simulated values (see option "Concentration Prediction Deviations" in Menu "Results").

5.4.4　Dialog Boxes Associated with Menu 'Edit'

This menu allows the user to input the appropriate input data (properties) associated with the modeling features that are available in the toolbox. In the Platform these modeling features are:

■ Recharge Zone,	■ Evapotranspiration zone,
■ Contaminant Source,	■ Subkriging Domain,
■ Wells,	■ Logpoints,
■ Rivers,	■ Transects
■ Drains,	

Note that these features must be activated in the graphics working area. You activate a feature by setting the mouse in the pointer mode and by clicking on the feature with the mouse. Bioplume III responds by highlighting this feature. Now you are ready to activate the appropriate dialog box to enter the input parameters of this feature by either double-clicking on the highlighted feature or pressing option "Properties in menu "Edit".

Log-points, wells and recharges are the most commonly used modeling features and are described in details herein.

Log-points

Several successive dialog boxes are needed to edit its parameters as shown below.
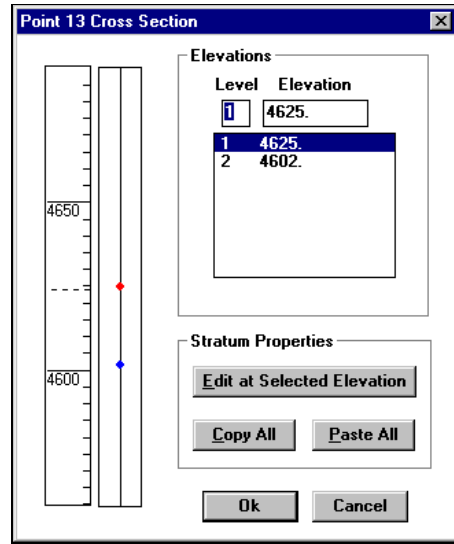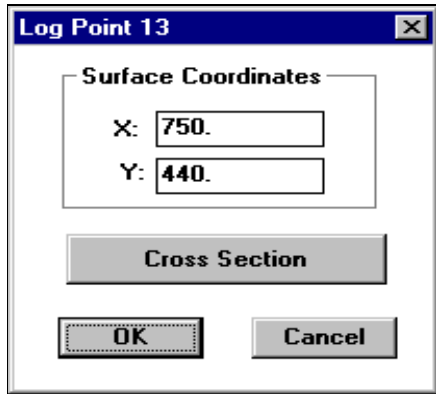
The cross section properties show the thickness of the computational layer at this particular location. To enter the parameters for the aquifer click on the button "Edit at Selected Elevation". You will get the dialog box shown below to enter the Horizontal Conductivities, Storage Coefficient, Effective Porosity and Longitudinal Dispersivity.
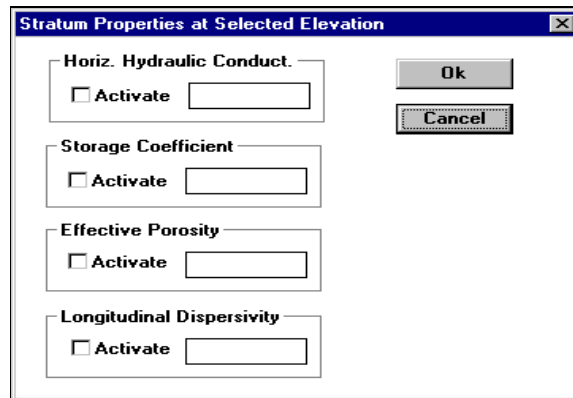
Wells

The dialog box for editing a well is shown below.

149
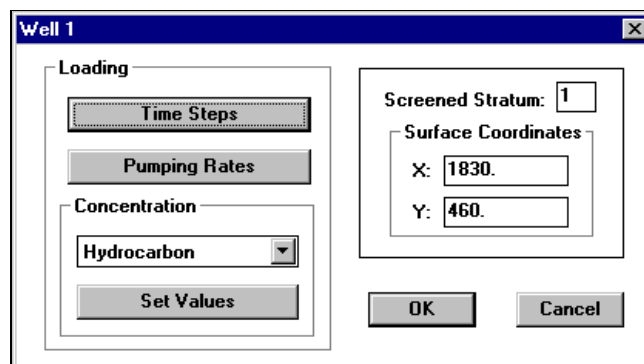
You start again by specifying the time steps in which the pumping rates changes and then enter the Pumping rates and various concentrations as shown in the next three dialog boxes.
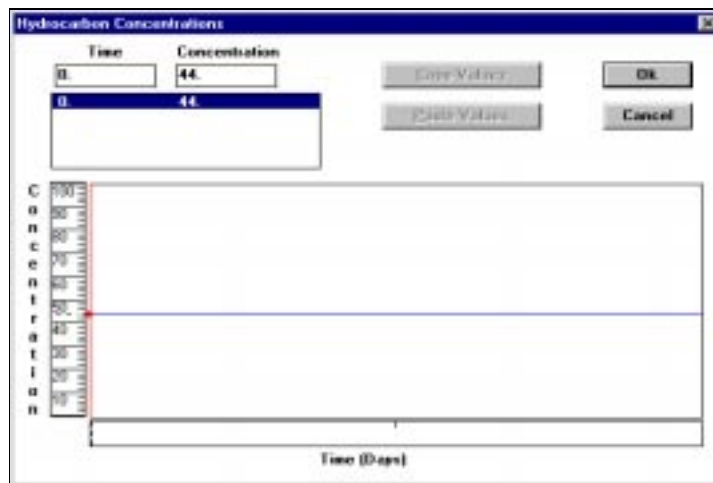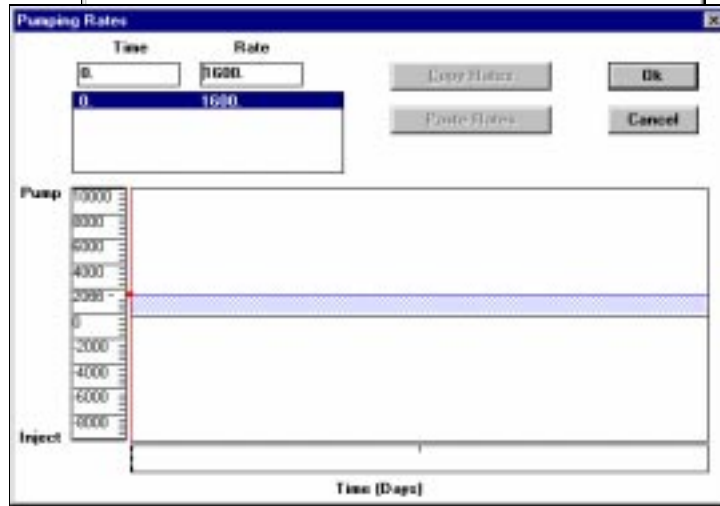
Recharge

For the recharge zone the procedure is the same: double-click on the recharge zone to obtain the following dialog box.
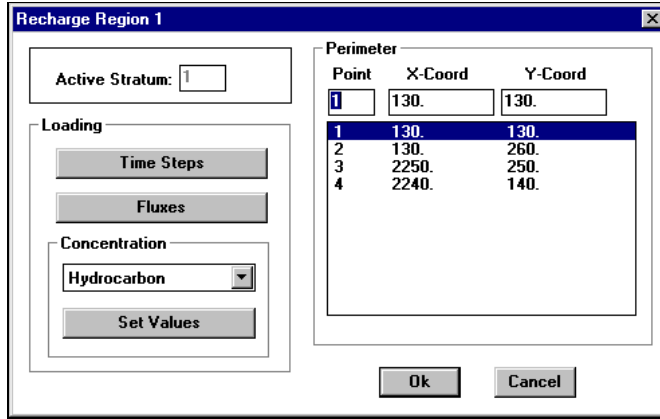
To enter the recharge parameters the procedure is the same as before. Enter the Time steps followed by the input recharges and concentrations.

The other modeling features have similar requirements that the user will find easy use.

Menu Item "Cross Section"

Cross Sections are defined by two points in the working area. The "Cross Section" button brings up the 2-D graph of the cross section (transect). New log-points are added mid-way to the right of an active log-line. Move it to its exact location by clicking on the vertical line and holding until properly placed. Adjust the thickness of the computational layer and input layer properties. The dialog box below shows a typical cross section along with the buttons to enter its properties.
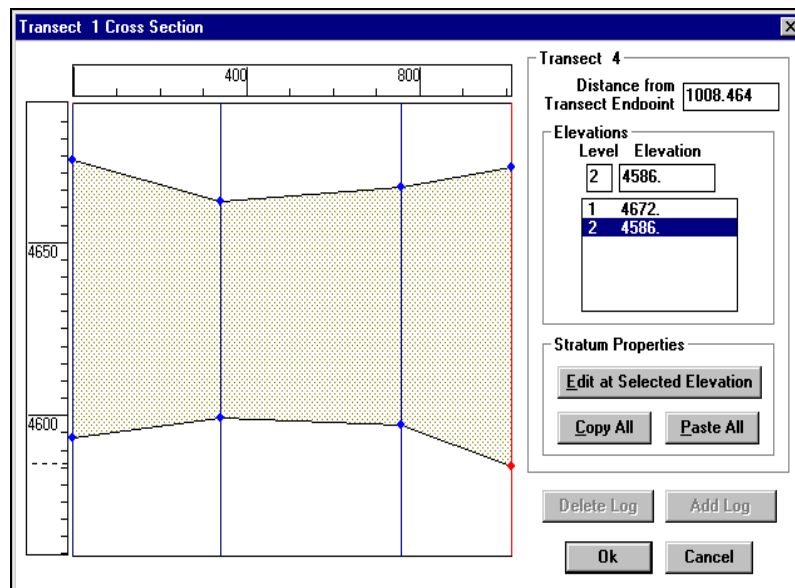
Clicking on the button "Strata Properties" activates a new dialog box to enter aquifer's properties as shown below.
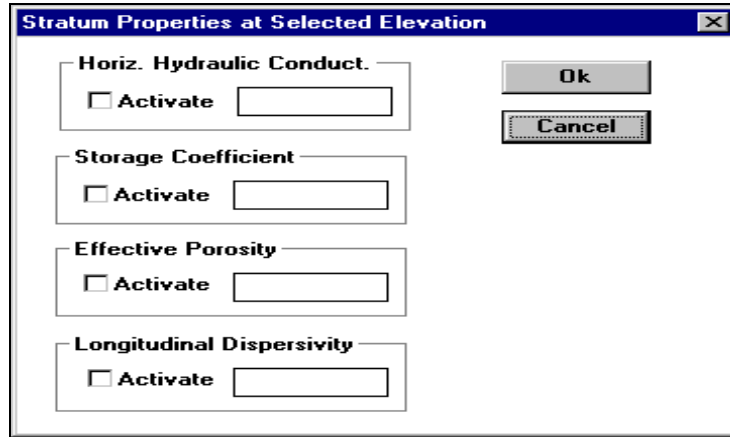
Menu Item "Delete"

Activating this option will delete the feature that is highlighted in the working area.

Menu Item "Delete All Features"

Activating this option will delete all the existing features of the simulation model. **Beware, this is a very drastic command.**

Menu Item "Preference"

This option allows the selection of different copying and pasting parameters.
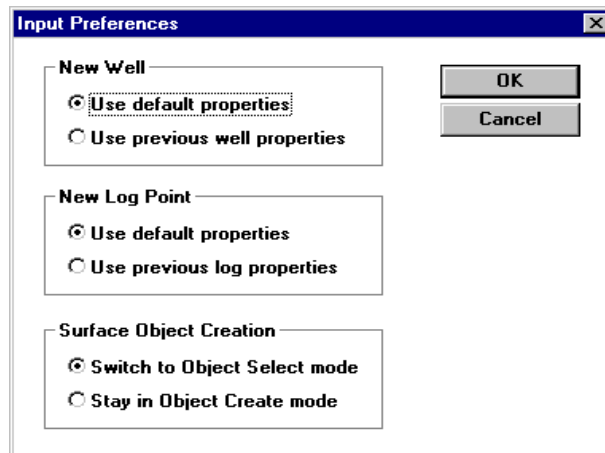
There are three sets of parameters. The first set allows the user to change the properties of the new well (pasted) from the default values to the properties of the previously created well. The same effects have the other two sets that are dealing with logpoints and selected contour levels.

5.4.5 Dialog Boxes Associated with Menu 'Grid'

This menu allows the definition and generation of the grid which is used to discretize the aquifer. It allows to access and use an enhanced "Kriging" procedure to infer aquifer properties at grid points.

Menu Item "Generate Grid"

The user defines a computational grid, either by increments, or by number of columns and rows. Note that the computational domain can also be narrower than the base map domain. These grid parameters are shown in the following dialog box.

Once the "**Generate Grid**" button is clicked the new grid appears in the working area of the screen.

Menu Item "Edit Grid"

This option is for editing grid features, specifying constant head/concentration cells, inactive cells and observation points. Clicking on the button "**Edit Grid**" spawns a secondary menu as shown below.

To select an observation well point just double click on a location in the working area as shown above and activate this option using the prompted dialog box. To select an inactive or constant head grid cell, use the tool box and the mouse to graphically edit the grid.
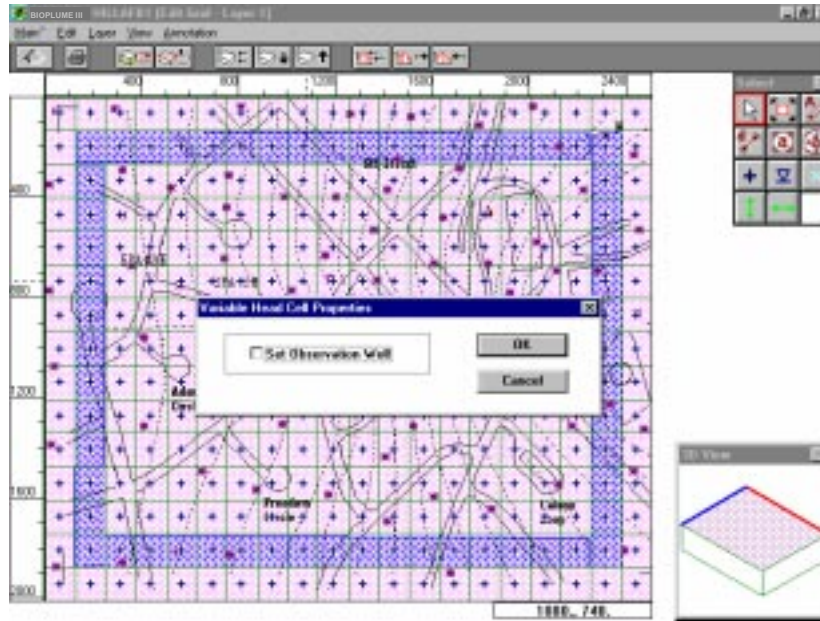
Menu Item "Selected Kriging"

All input parameters such as material properties, hydraulic heads and concentrations of hydrocarbons and electron acceptors are usually given at particular locations (logpoints). Therefore they need to be distributed throughout the computational grid. This is done automatically in the Platform whenever a "**Save**" procedure is activated. A default simple kriging procedure is used. However, for better accuracy you need to explicitly activate the "**Quick Kriging**" algorithm. This is the case when this particular menu option is activated. First select the type of parameter you need to re-krig and you will obtain the following screen (in this example the observed Hydraulic Heads).
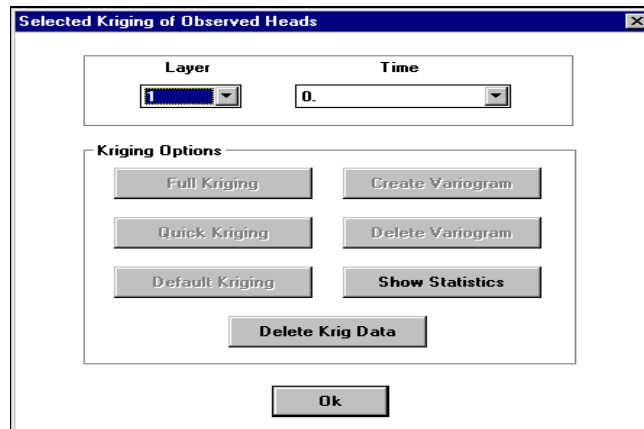
To re-adjust the parameter distribution obtained by the default kriging click on the "**Delete Krig Data**" button and activate option "**Quick Kriging**". After a few seconds the operation is completed and you can proceed with the re-adjustement of another parameter. After "Saving" the case, the new distribution will be available to inspect graphically. The demanding user may also want to inspect the

154

statistics of the examined parameter. All you need to do is to click on "**Show Statistics**" to obtain the dialog box below.

This allows the user to quickly validate the selection and orientation of the computational grid. The Platform computes the variogram of the parameter (e.g. observed hydraulic heads) in all pertinent directions. In the example the Northing variogram (y-direction) is flat showing little variation, while the Easting (x-direction) variogram is smooth with exponential growth. "**Show Variogram**" displays the graphics below. The variogram in the "Easting" direction confirms that the predominant flow regime is in the "x" direction.
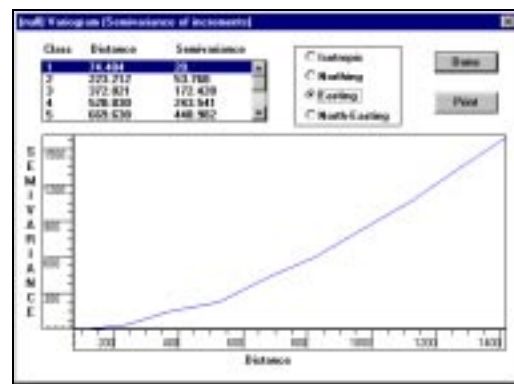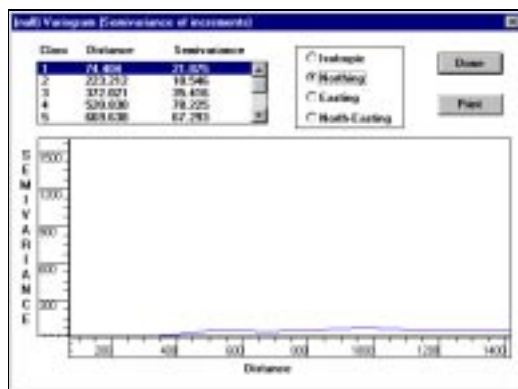
Menu Item "Computational Grid"

This is an option that allows the user to display a perspective view of the computational grid and the node wells.

Menu Item "Layer Elevations"

This is also an option that displays the computational layers in a perspective configuration. Cross Sections are obtained on the fly using the appropriate tool from the toolbox. Just point and click along the red or blue line to get the cross section below.
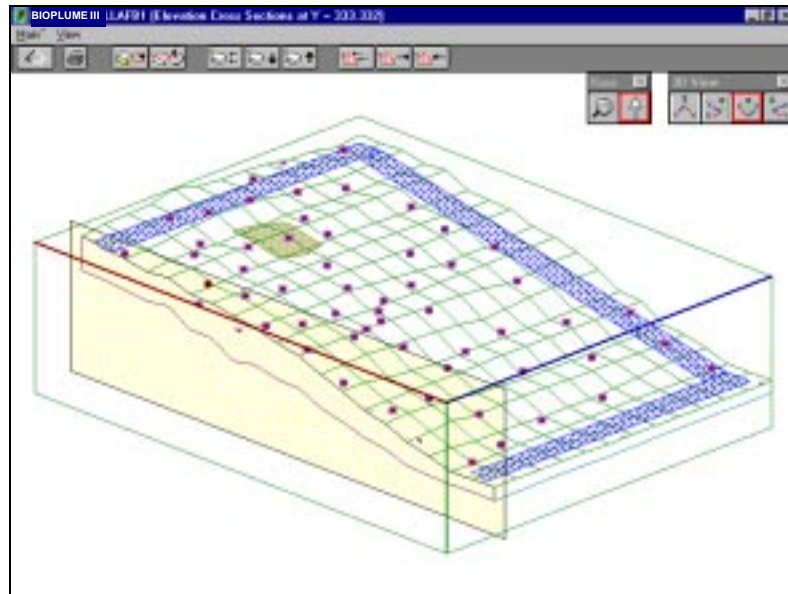
Menu Item "Layer Thickness"

The distribution of the thickness of the computational layer across the simulation domain can also be obtained using this option. Contours of the layer thickness are shown below.
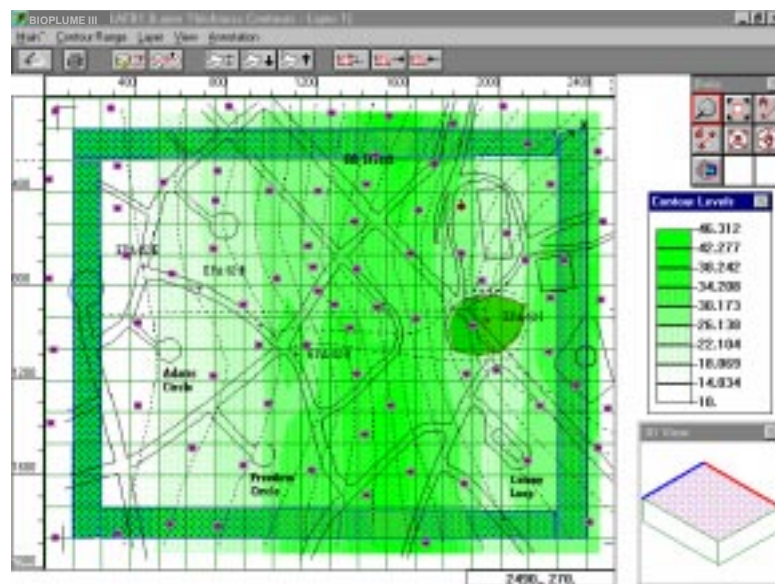
Menu Item " Distributed Properties"

Essentially, this option displays on the screen the results of the kriging procedures on the various distributed parameters (input parameters). The distribution of the hydraulic conductivity is shown in the example below.
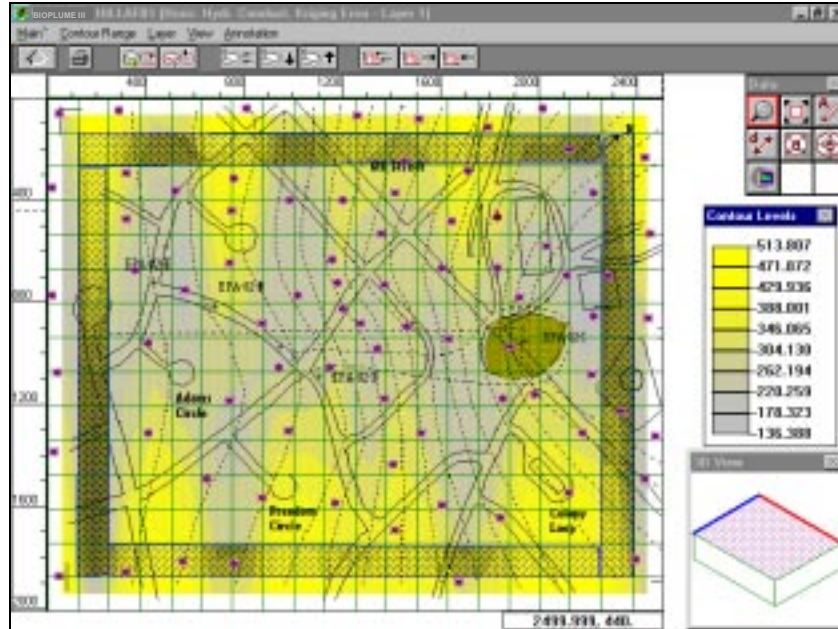
Menu Item "Observed Heads"

The results of the kriged observed heads at different times are shown in this option as shown below.
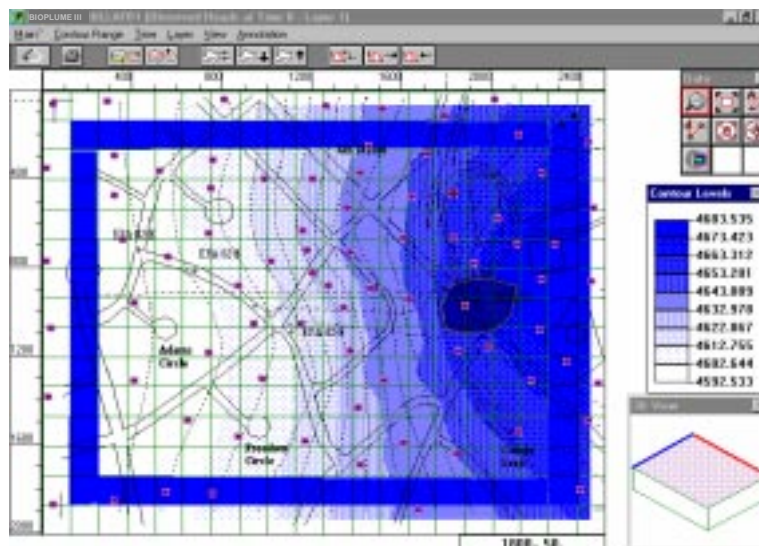
Menu Item "Observed Concentrations"

The results of the kriged observed concentrations at different times are also displayed in this option.

5.4.6   Dialog Boxes Associated with Menu 'Initial Conditions'

Menu Item "Simulation Period"

This option allows specification of starting and ending time of the simulation. To aid in this selection, a summary table is given of all the times when pumping or recharge are specified.
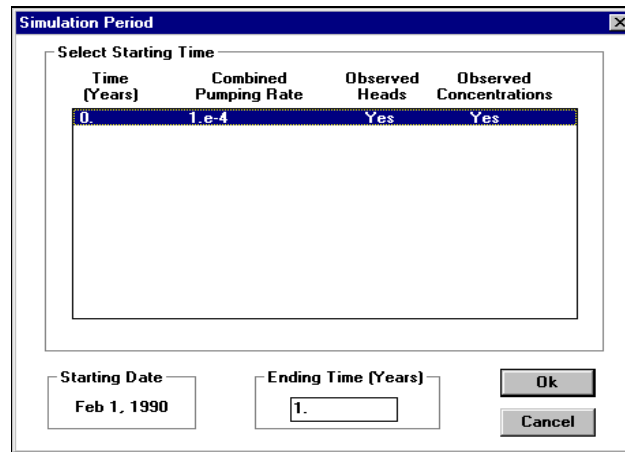
Menu Item "Starting Heads"

The following dialog box allows the selection of starting conditions among the following options: 'Observed values' (earlier entered in menu "Loading"), 'Previously Generated Heads' (from a previous run), 'Constant Heads' and 'Field Filled to Capacity". More information about these options can be found in Section 3, Tutorial.
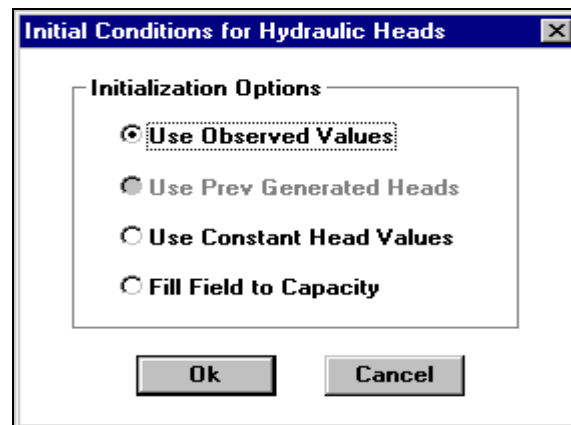
Menu Item "Starting Concentrations"

The following dialog box allows the selection of starting conditions for hydrocarbon and electron acceptors among the following options: 'Observed Values' (entered in menu "Loading"), 'Previously

Generated Concentrations' (from a previous run), and 'Constant Concentrations'. More information about these options can be found in Section 3, Tutorial.
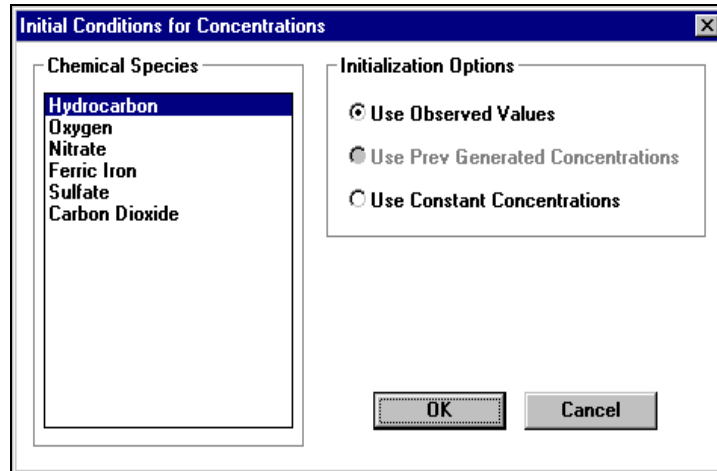
5.4.7   Dialog Boxes Associated with Menu 'Simulator'
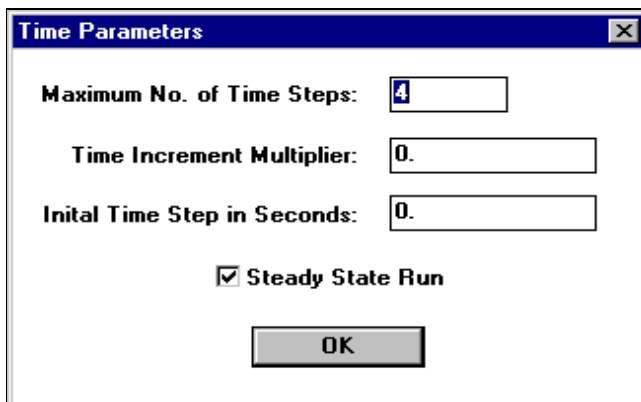
This is the menu that allows activation of the BIOPLUME III run after selection of appropriate runtime options shown below.

Note that the "Bioplume III" button is originally grayed out (not accessible). It becomes accessible only if the starting "Heads" and "Concentrations" are specified in the previous menu.
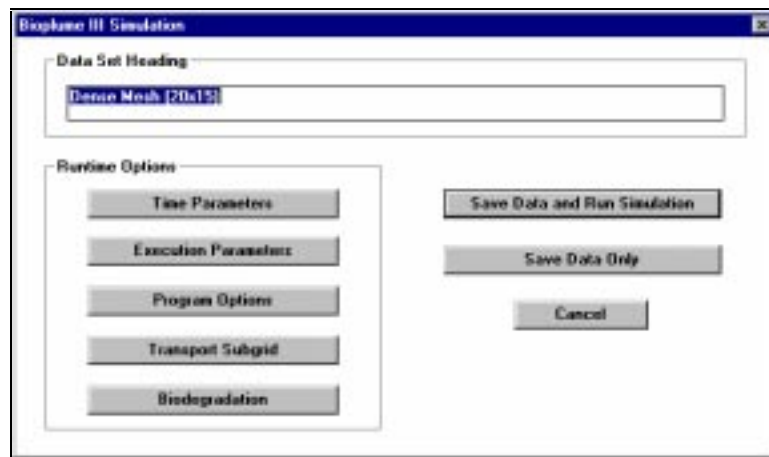
The run time options for BIOPLUME III are the following: Time parameters, Execution parameters, Program options, Transport Subgrid, Biodegradation. These options are discussed below.
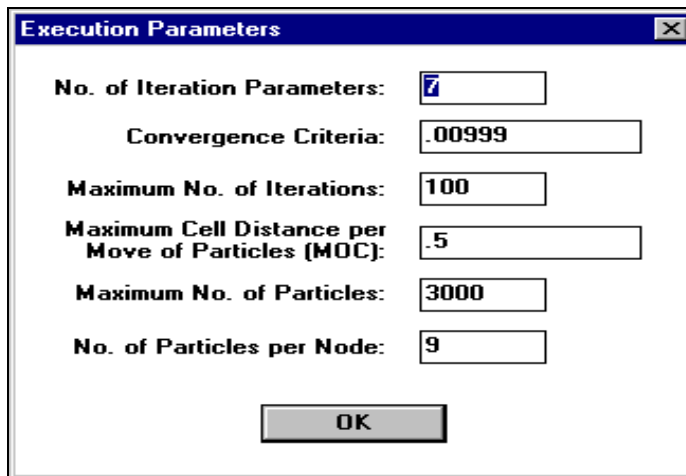
Time Parameters

The time parameters allow the selection of the number of time steps for a particular run. Note that for BIOPLUME III the initial time step should be given in seconds.
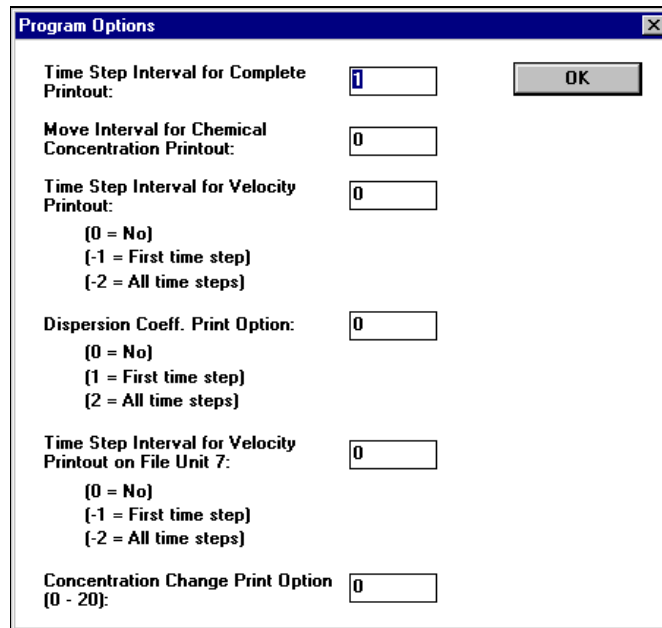
Execution Parameters

These are Standard MOC program runtime parameters. For details, see Section 4, BIOPLUME III Theoretical Development.

Program Options
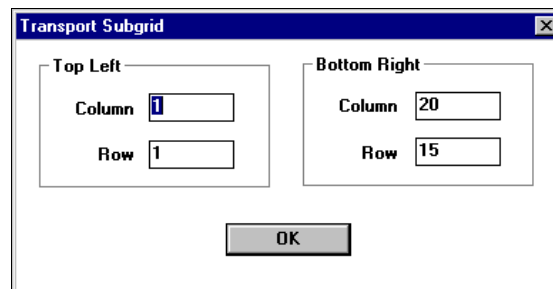
Program Options ☒

Time Step Interval for Complete Printout:	1	OK
Move Interval for Chemical Concentration Printout:	0	
Time Step Interval for Velocity Printout:	0	

(0 = No)
(-1 = First time step)
(-2 = All time steps)

Dispersion Coeff. Print Option: 0

(0 = No)
(1 = First time step)
(2 = All time steps)

Time Step Interval for Velocity Printout on File Unit 7: 0

(0 = No)
(-1 = First time step)
(-2 = All time steps)

Concentration Change Print Option (0 - 20): 0

These are again Standard MOC program parameters. For details, see Section 4, BIOPLUME III Theoretical Development.

Transport Subgrid

Transport Subgrid ☒

Top Left
Column 1
Row 1

Bottom Right
Column 20
Row 15

OK

This is also sub-gridding option of the MOC program. Specify the top left cell (column and row number) and the bottom right cell which defines a sub-region over which the transport simulation will be performed. The flow simulation is performed over the entire grid. This option is less useful with faster and more powerful PC computers.

Biodegradation

This is the Platform biodegradation option selection table. It allows to activate/deactivate electron acceptors, and to select interaction mechanisms (Instantaneous Reaction, Zero Order Reaction and Monod Kinetics).

Now you are finally ready to run the simulation. Press the button "Save Data and Run Simulation" to activate sequentially three executables as follows: an executable to generate BIOPLUME III input stream from the graphics files, an executable that runs the BIOPLUME III algorithm, and an executable to create output graphics. For more details on the proper sequence with which these executables are run see also Section 3, Tutorial.

5.4.8   Dialog Boxes Associated with Menu 'Results'

This menu offers a variety of graphics to display the simulation results. Graphics include: computed Hydraulic Heads, computed Concentrations and Computed Velocities.

Menu Item "Hydraulic Heads"

This option produces the following secondary screen displaying the end of simulation period results.
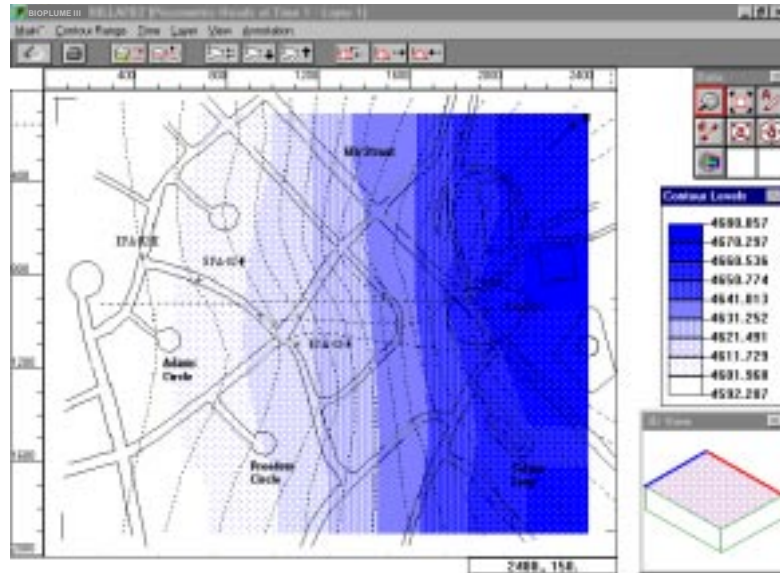
Menu Item "Concentrations

For the Hydrocarbon the following graphics is displayed.
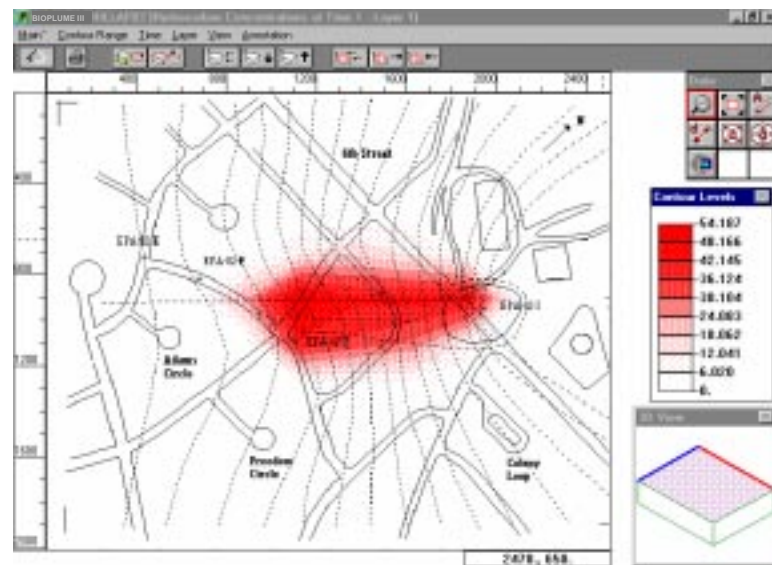
For the Oxygen the following results are displayed at the end of a one year simulation.
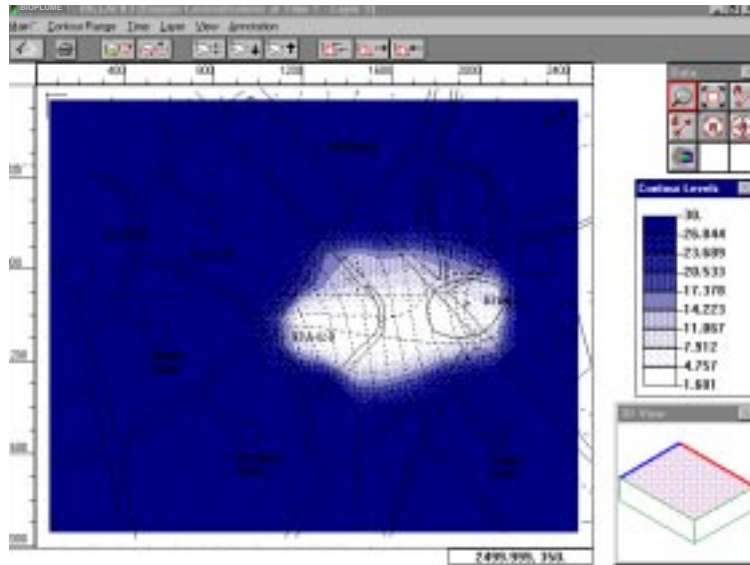
For the Nitrate the following results are displayed at the end of a one year simulation.
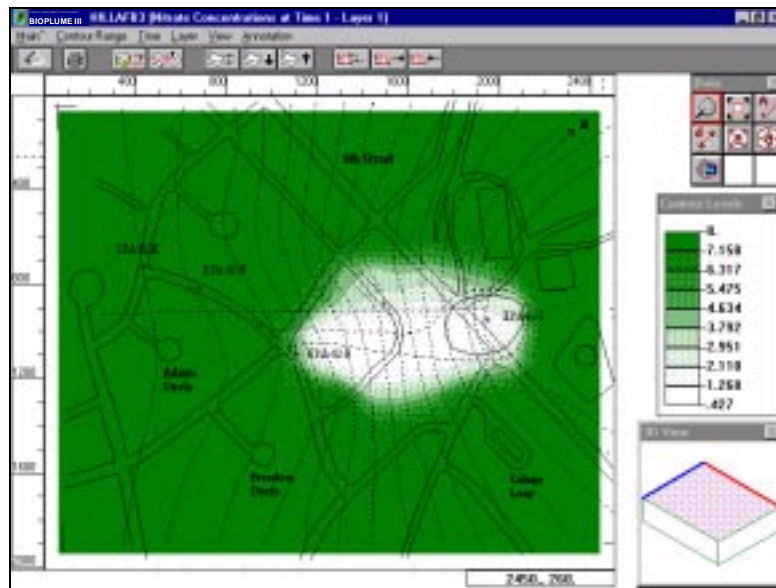
Menu Item "Head Prediction Deviations"

This option produces the distribution of the errors between observations and model predictions of the Hydraulic Heads. Error contours are only displayed at observation times that match the computed times.

Menu Item "Concentration Prediction Deviations"

This option produces the distribution of the errors between observations and model predictions of the Concentrations of various constituents.
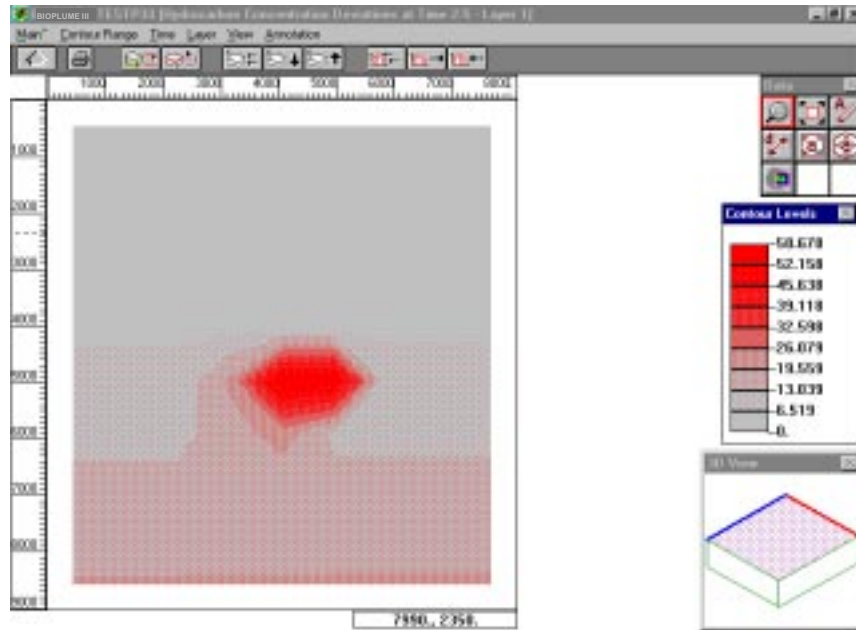
Menu Item "Velocities"

This menu option displays the velocities as shown below.
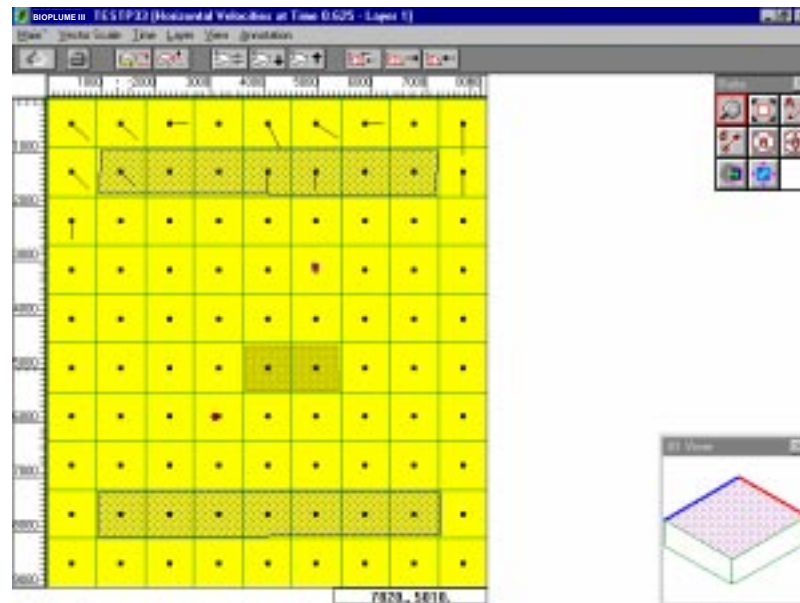
Menu Item "Observation Wells"

This option displays the computed time series of selected concentrations at specified observation points.
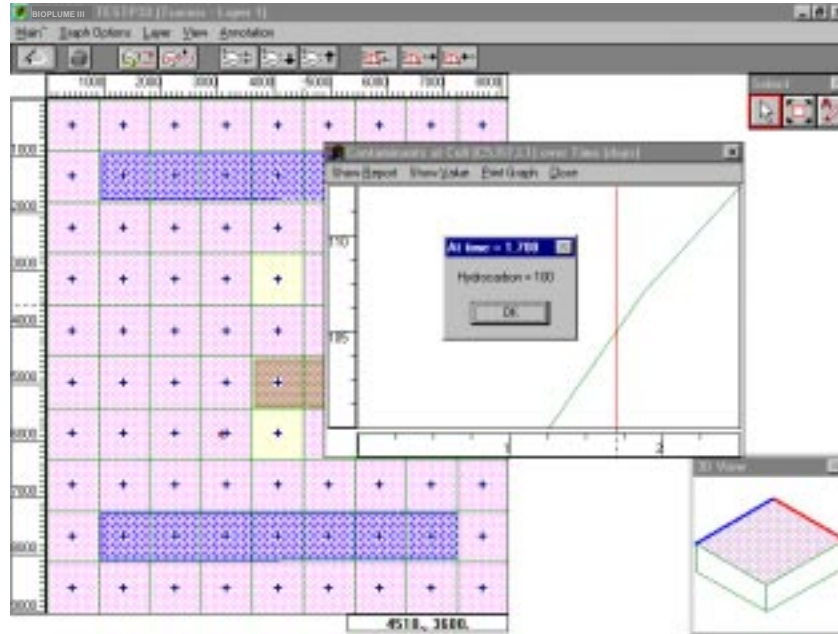
Menu Item "Engineering Graphs"

This option allows the user to display in a secondary screen the results using an engineering format. The depth (z-direction) shows the intensity of the computed concentrations.
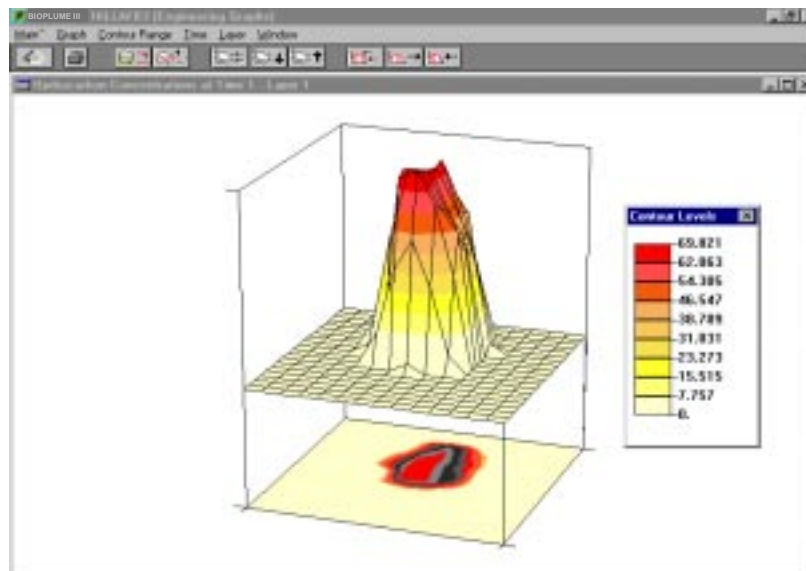
The direct comparison of the computed concentrations of different constituents is also possible by activating option "New" in the secondary menu "Edit".
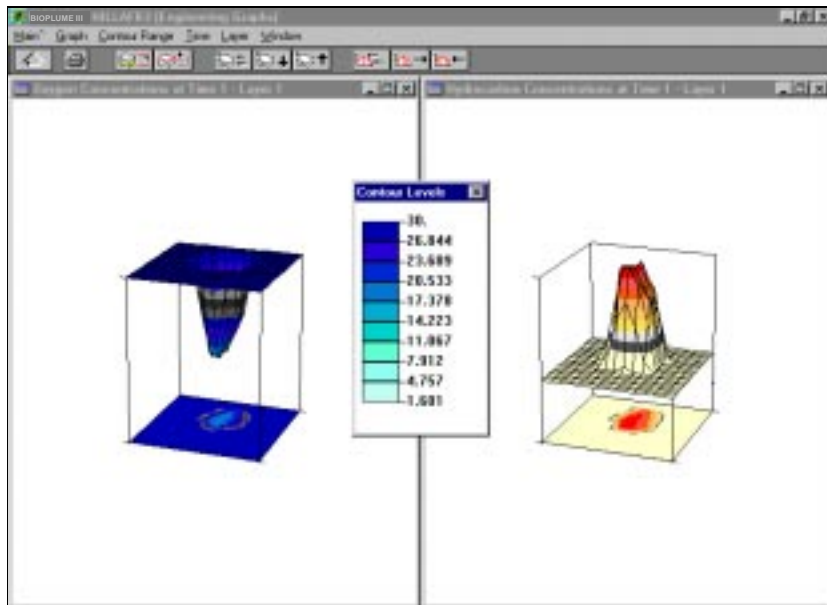
Menu Item "AVI Animation"

Finally, the final option of this menu concerns the video animation (AVI) files. Note that the standard format for Windows digitized video is the Audio-Video Interleaved (AVI) format. An AVI file can be played in Windows with no additional hardware (of course it will be smoother and faster with a video accelerator). Now activate option "AVIanimation". This will invoke the animation module. As it can be seen, a new menu bar appears at the top of the screen. Move to Menu "File" and click on the option "Open AVI". A dialog box appears on the screen with the list of all available video clips (.AVI) files. Select the file **"HILLAFB.AVI"** to obtain the screen shown below. To playback the video clip showing the simulated migration of hydrocarbons, you only have to click on the "Forward" play button that appears at bottom left corner of the AVI window.
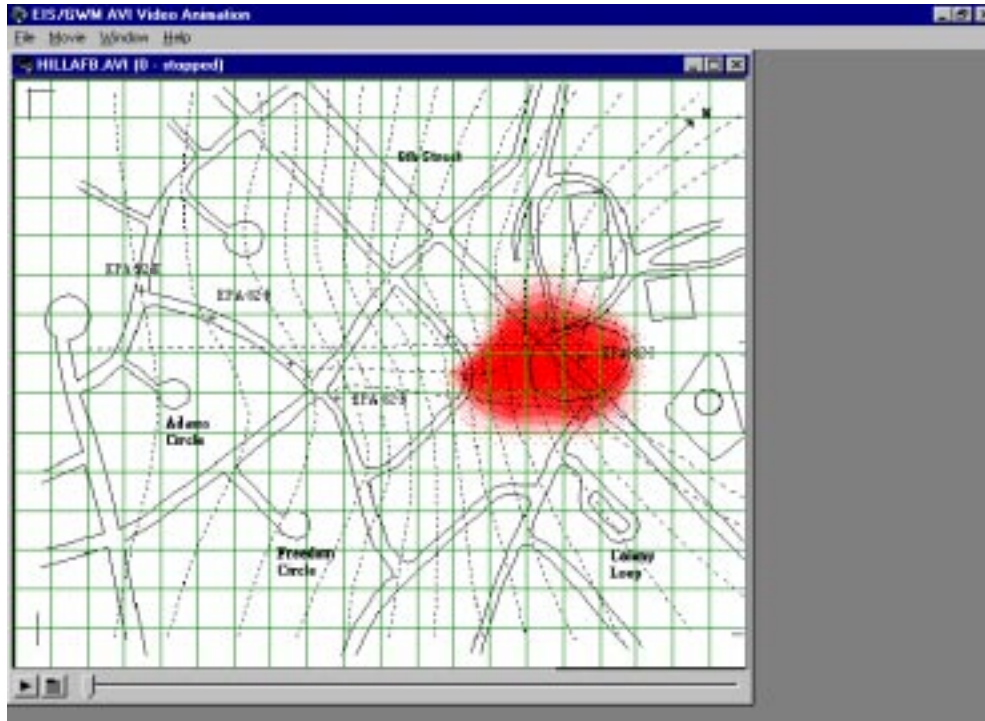
Et voila! The screen comes to life and the video clip stops after a few seconds. The detailed procedure on how to create this AVI file is given in Section 3, Tutorial. All you need to know at this point is that the "HILLAFB.AVI" file was generated from only 4 Bitmap snapshots depicting the simulated plume at 0.25, 0.5 o.75 and 1 year. These bitmaps were selected and created using the grasping tool activated from the available tool box in the secondary menu "Results/Concentrations".

5.4.9   Dialog Boxes Associated with Menu 'View'

This menu provides all the options to change the appearance of the screen. In particular it allows the user to do the following:

Description	Menu Option to Activate
Reduce viewing scale	Zoom In
Enlarge viewing scale	Zoom Out
Zoom to fit the image in the Window of working area	Zoom to Overview
Activate resolution of the cursor movement	Snap Cursor

Show generated grid	Show Grid
Show box with smart-Icons (toolbox)	Show Interaction Tools
Show 3D View window of simulated domain	Show 3D View
Show selected raster image in the background	Show Base Image
Show selected raster image in gray scale	Make Base Image Gray
Printing the Screen/Window	Print

5.4.10 Dialog Boxes Associated with Menu 'Annotation'

One of the nice features of the Platform is the possibility to graphically create annotations. In fact the "Annotation" data network allows the user to write his/her notes (Impressions) at a particular location of the input and output graphics of a particular run. To activate an "Annotation" use the appropriate tool from the toolbox, and with the mouse click at the desired location for the annotation. Then write your remarks in the editing dialog box. Automatically your annotation will be linked to the displayed graphical representation. The options in menu "Annotation" allows you to delete and edit existing Annotations.

5.5 Advanced Topics

5.5.1 Platform Software Architecture

The main objective of the development of the Graphical Platform is to provide the scientist and engineer the means to work in an interactive computer graphics environment where the remediation model under consideration (study) is constantly displayed on the screen. The user navigates through the various modules of the program by means of menus which are always displayed next to the model abstraction. Menu choices are picked and interaction with the model is performed by pointing with a mouse. By pointing to the screen, rather than typing commands, a natural dialogue is developed between the user and the platform.

The key aspect of the Platform protocol is the integration of data management, graphics and algorithmic routines, into a coherent platform which is flexible and simple to use. Integration is achieved by layering the various parts of the program. This layering insulates the high level functional routines from the low level details of data storage and management. This layered approach also promotes program modularity.

The core of all procedures under the Platform is the file data base which stores all data, files, and information pertinent to a particular application. This is the repository of all information used in various parts of the platform (see Figure 5.3). The file data base is only accessible through the data base access routines. The layer above the data base is a collection of routines which implement the computational functionality of the program. These are loosely grouped into several categories. These categories include: Grid editor, Geologic features editor, editor of initial conditions, 2D and 3D graphics routines, Kriging routines, Scientific Engines.

Encircling the functional routines is the user interface with its process scale operator. This is a collection of menu drivers and display routines which allow the analyst to interact with the platform. An important aspect of this part of the platform is that the user need only deal with one interface. There is a reassuring continuity of display and type of interaction as the analyst moves from one part of the program to another.

All parts of the program are coordinated by the process scale operator which automates a great portion of the management chores, and shadows the user's modeling and simulation activities. For the implementation of this software architecture the Platform uses several sub-directories to manage the flow of different software operations.
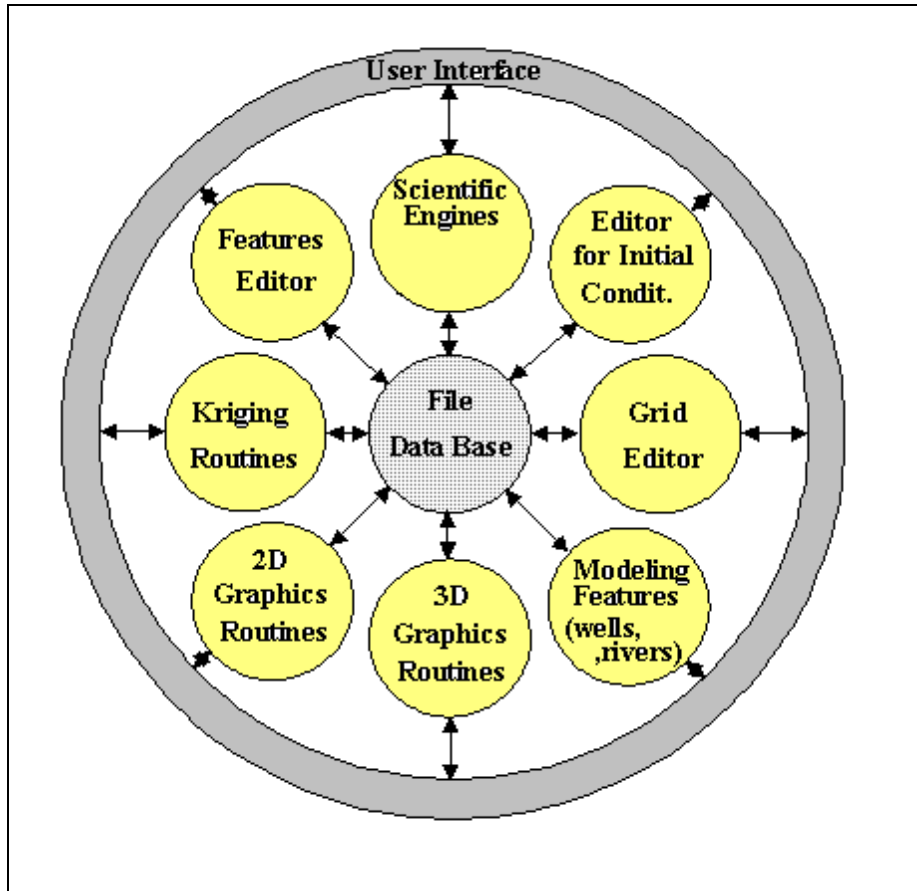
Figure 5.3 Layered Structure of the Graphical Platform Software Architecture.

5.5.2   Platform Input of Natural Attenuation Parameters

The specific data that drive a groundwater contaminant migration simulation model are listed in Table 5.2. They address each and everyone of the mechanisms that the model simulates, namely flow through the porous medium, interaction with surface waters, evapotranspiration losses, drains, other forcing mechanisms such as wells and recharge, multiple dissolved species plumes, chemical reactions, and boundary conditions.

Table 5.2   Input Data Given Per Strata.

Physical Process	Physical Parameter	Function	Link	DefaultValue	Menu
Flow	Horizontal Conductivity	Conveyance		1000.	Domain/Define Strata
	Anisotropy			1.	
	Vertical Conductivity	Conveyance		1000.	
	Storage Coefficient	Transient Computations		0.100	
	Water table Storage factor			0.009	
	Effective Porosity	Intersticial Velocity		0.200	
Dispersion	Longitudinal Dispersivity			0.	Domain/Define Strata
	Transverse Dispers. ratio			1.	
	Vertical Dispers. ratio			1.	
	Effective Mol. Diffusion			0.	
	Bulk Density of Medium			0.	
Sorption	**Linear Isotherm**				Domain/ Chemical Species
	Distribution Coef.			0.	
	Freundlich Isotherm				
	Equilibrium Constant			0.	
	Freundlich Exponent			1.	
	Langmuir Isotherm				
	Equilibrium Constant			0.	
	Total Concentration			0.	
SurfaceWater	Bed Elevation	Gradients with Aquifer	Link with Aquifer		
	Bed Conductivity	Link with Aquifer		1,000	
	Surface Elevation	Gradients with Aquifer			

Physical Process	Physical Parameter	Function	Link	Default Value	Menu
Decay	**Radioactive Decay**				Domain/ Chemical Species
	Half Life (T)			100	
	Rate Constant (1/T)			.006	
	Biodegradation Decay				
	First order rate for dissolved phase			0.	
	Fist order rate for sorbed phase			0.	
IonExchange	Monovalent Exchange				Domain/ Chemical Species
	Ion-exchange selectivity coefficient			0.	
	Ion-exchange capacity			0	
	Divalent exchange				
	Monovalent-Divalent				
	Divalent-Monovalent				
Wells/Drain	Drain Elevation	Gradients with Aquifer	Link with Aquifer		
	Bed Conductivity	Link with Aquifer		1,000	
Slurry Walls	Wall Elevation/Thickness	Gradients with Aquifer	Link with Aquifer		
	Wall Conductivity	Link with Aquifer		1,000	
Discontinuity Fault	Fault Elevation/Thickness	Gradients with Aquifer	Link with Aquifer		
	Fault Conductivity	Link with Aquifer		1,000	

Physical Process	Physical Parameter	Function	Link	Default Value	Menu
Recharge/E.T.	Time Schedule of rate	Aquifer Source			
	Aquifer Layer				
Evapotranspiration	Time Schedule of rate	Aquifer Drain			
	Aquifer Layer				
Boundary Conditions	Constant Head	Fix Head			
	No Flux Boundary	Control Flux			
	General Head Boundary	Impose Flux via conductivity			
	Constant Concentrations	Fix Concentrations			
Initial Conditions	Initial Head	Fix Head			
	Initial Concentrations	Fix Concentrations			
Chemical Reactions	Soil Bulk Density				

5.5.3   Sensitivity of Input Parameters

The model input parameters should be subjected to sensitivity analyses to test model response to the potential range of key parameters. These analyses permit evaluation of the effects on model output (Concentrations) of varying: hydraulic, hydrologic, hydrogeologic properties, dispersivities, source loading rates and other parameters within conceivable ranges quantified by the available "Kriging" procedure.

Each remediation site has its own idiosyncrasies. However, to properly perform a calibration analysis, there is a need to know the relative effects of these input parameters. Figure 5.4 below provides a rough estimate of the importance of these parameters in evaluating the contaminant migration concentration. These estimates allow a quick determination of the parameters needing readjustment

during the calibration process. Clearly the parameters with a high influence on the estimated concentrations must be calibrated first.
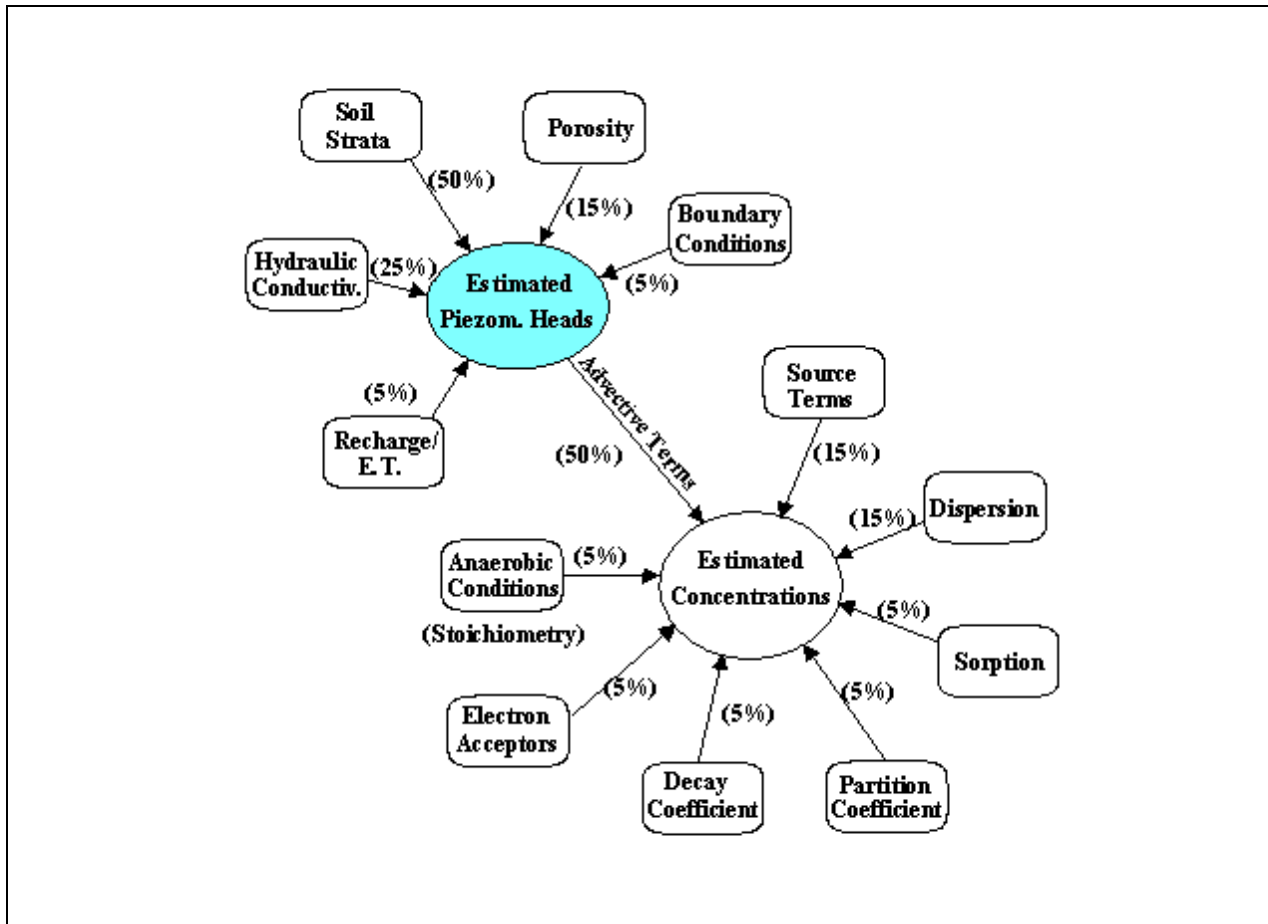
Figure 5.4 Estimates of Sensitivity Analysis.

5.5.4   Concluding Remarks

This concludes the formal presentation of the Platform and the input parameters that are needed to set up a groundwater remediation investigation. However, for a more thorough understanding of the Platform and its use you must also consult the following Sections:

1. Section 3, Tutorial

2. Section 4, Theoretical Development, and

3. Appendix B, Intrinsic Remediation Implementation Protocol

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APPENDIX I.   INPUT DATA

The BIOPLUME III input data are listed in detail in Table I.1. The key variables and concepts used in the model will be described more thoroughly in this section. A number of examples will be given throughout the section to better illustrate some of the variable definitions.

I.1   Discretization of Space

The first step in applying the BIOPLUME III model to a field site involves selecting the size of the model grid and the number of cells contained within the grid. Four variables are used to define the selected grid: **NX, NY, XDEL and YDEL** (Figure I.1). The number of grid cells in the x- and y- directions are defined in NX and NY, respectively and the size of the individual cells are defined in XDEL and YDEL, respectively (see Figure I.1).

Since the model requires that no-flow boundaries be specified around the site, "extra" cells need to be incorporated into the grid design. In other words, if an "active" domain of 12 x 12 cells is needed, a 14 x 14 grid is specified in order to allow for the outer rows and columns to serve as no-flow boundaries.

There are a number of conventions used in the model which are useful to note. First, flow is generally along the y-direction. The origin is designated at the upper left-hand corner of the grid (this means that flow is essentially "down the page"). The x-cells are then counted starting with 1 at the origin and through NX moving to the right of the origin. Similarly, the y-cells are counted starting with 1 at the origin and through NY moving downwards from the origin (see Figure I.1). These conventions may be changed but caution needs to be exercised in entering the input data and analyzing the resulting output to avoid confusion.

I.2   Discretization of Time

BIOPLUME III uses three variables to define simulation time in the model**: NTIM, PINT and NPMP**. The relationship between these variables is illustrated in Figure I.2.

NTIM - is defined as the number of times in a given simulation period that the user may receive model results.

PINT - is defined as the length of time in a given simulation period.

NPMP - defines the number of pumping periods to be simulated. A pumping period is defined as a specified length of time during which the hydrologic conditions at the site remain unchanged.

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
1	TITLE	Alphanumeric	Short description of dataset	
2	NTIM	Integer	Maximum number of time steps in a pumping period	1 ... 100
	NPMP*	Integer	Number of pumping periods	
	NX	Integer	Number of nodes in x direction	3 ... 35
	NY	Integer	Number of nodes in y direction	3 ... 35
	NPMAX	Integer	Maximum number of particles	NX*NY*NPTPND
	NPNT	Integer	Time step interval for printing	
	NITP	Integer	Number of iteration parameters	4 ... 7
	NUMOBS	Integer	Number of observation points	0 ... 5
	ITMAX	Integer	Maximum allowable number of iterations	100... 200
	NREC	Integer	Number of pumping or injection wells	0 ... 50
	NPTPND	Integer	Initial number of particles per node	4, 5, 8, 9 or 16
	NCODES	Integer	Number of node identification code	1 ... 9
	NPNTMV	Integer	Particle move interval for printing chemical output data (Specify 0 to print at end of time step)	
	NPNTVL	Integer	Option for printing computed velocities (0 = do not print; 1 = print for first time step; 2 = print for all time steps)	0, 1 or 2
	NPNTD	Integer	Option for printing computed dispersion equation coefficients (0 = do not print; 1 = print for first time step; 2 = print for all time steps)	0, 1 or 2
	NPDELC	Integer	Option for printing computed changes in concentration 0 = do not print; 1 = print)	0 or 1
	NPNCHV	Integer	Not used	
	IREACT	Integer	Reaction type specifier for contaminant	-1 or 0 ... 7
3	PINT	Real	Pumping period in **years**	
	TOL	Real	Convergence criteria for flow equation	£ 0.01
	POROS	Real	Effective porosity	0.01 ... 1
	BETA	Real	Longitudinal dispersivity in **ft**	
	S	Real	Storage coefficient (S=0 for steady-state flow)	
	TIMX	Real	Time increment multiplier for transient flow (disregarded if $S = 0$)	
	TINIT	Real	Size of initial time step in **seconds** for transient flow (disregarded if $S = 0$)	
	XDEL	Real	Width of cell in x direction in **ft**	
	YDEL	Real	Width of cell in y direction in **ft**	
	DLTRAT	Real	Ratio of transverse to longitudinal dispersivity	
	CELDIS	Real	Maximum cell distance per particle move	0 ... 1
	ANFCTR	Real	Ratio of Tyy to Txx	

180

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
4				
One of the following possibilities depending on the value of IREACT			All data in this series are for contaminant	
IREACT = -1	THALF	Real	Decay half-life for a radioactive compound in **seconds**	
IREACT = 0	no line 4			
IREACT = 1	DK, RHOB, THALF	Real	DK - linear sorption distribution coefficient (**volume/mass**), RHOB - aquifer bulk density (**mass/volume**). These two parameters need to have consistent units, for example DK in cc/g and RHOB in g/cc	
IREACT = 2	RHOB, EKF, XNF, THALF	Real	EKF - Freundlich sorption coefficient, XNF - Freundlich sorption exponent (**dimensionless**)	
IREACT = 3	RHOB, EKL, CEC, THALF	Real	EKL - Langmuir sorption coefficient (**volume/mass, for example, ml/g**), CEC - Maximum sorption capacity or ion-exchange capacity (**mass/mass, for example, ng/g**)	
IREACT = 4	RHOB, EK, CEC, CTOT, THALF	Real	EK - Ion exchange selectivity coefficient (**units depend on stoichiometry**), CTOT - total solution concentration of two exchanging ions (**equivalents/volume**)	
IREACT = 5	RHOB, EK, CEC, CTOT, THALF	Real	Variables defined previously	
IREACT = 6	RHOB, EK, CEC, CTOT, THALF	Real	Variables defined previously	
IREACT = 7	RHOB, EK, CEC, CTOT, THALF	Real	Variables defined previously	
5	THALFS	Real	Source decay half-life in **seconds**	
6	DEC1	Real	Lumped decay coefficient for aerobic and anaerobic biodegradation (**1/seconds**)	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
7	IRECO	Integer	Biodegradation type specifier for oxygen	
8				
One of the following possibilities depending on the value of IRECO				
IRECO = 0	no line 8			
IRECO = 1	DCO, FO, DOMIN	Real	First-order decay rate for aerobic biodegradation (**1/day**), stoichiometric ratio of oxygen required to degrade contaminant, threshold concentration of oxygen below which biodegradation does not occur (**concentration units, mass/volume, for example, mg/l**)	
IRECO = 2	FO, DOMIN	Real	Variables defined previously	
IRECO = 3	FO, DOMIN, CMSO, RMO, RKHO, RKMAXO, RKO	Real	Start w. CMSO - conc. of microorganisms (**mass/volume**), retardation factor for microorganisms, half-saturation constant for contaminant (**mass/volume**), maximum utilization factor for contaminant (1/days), half-saturation constant for oxygen (**mass/volume**)	
9	IRECN	Integer	Biodegradation type specifier for nitrate	
10				
One of the following possibilities depending on the value of IRECN				
IRECN = 0	no line 10			
IRECN = 1	DCN, FN, NMIN	Real	Variables similar to those defined for oxygen	
IRECN = 2	FN, NMIN	Real	Variables similar to those defined for oxygen	
IRECN = 3	FN, NMIN, CMSN, RMN, RKHN, RKMAXN, RKN	Real	Variables similar to those defined for oxygen	
11	IRECF	Integer	Biodegradation type specifier for iron	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
12				
One of the following possibilities depending on the value of IRECF				
IRECF = 0	no line 12			
IRECF = 1	DCF, FF,FMIN	Real	Variables similar to those defined for oxygen	
IRECF = 2	FF,FMIN	Real	Variables similar to those defined for oxygen	
IRECF = 3	FF, FMIN, CMSF, RMF, RKHF, RKMAXF, RKF	Real	Variables similar to those defined for oxygen	
13	IRECS	Integer	Biodegradation type specifier for sulfate	
14				
One of the following possibilities depending on the value of IRECS				
IRECS = 0	no line 14			
IRECS = 1	DCS, FS, SMIN	Real	Variables similar to those defined for oxygen	
IRECS = 2	FS, SMIN	Real	Variables similar to those defined for oxygen	
IRECS = 3	FS, SMIN, CMSS, RMS, RKHS, RKMAXS, RKS	Real	Variables similar to those defined for oxygen	
15	IRECC	Integer	Biodegradation type specifier for carbon dioxide	
16				
One of the following possibilities depending on the value of IRECC				
IRECC = 0	no line 16			
IRECC = 1	DCC, FC, CMIN	Real	Variables similar to those defined for oxygen	
IRECC = 2	FC, CMIN	Real	Variables similar to those defined for oxygen	
IRECC = 3	FC, CMIN, CMSC, RMC, RKHC, RKMAXC, RKC	Real	Variables similar to those defined for oxygen	
Data Set 1	IXOBS	Integer	x coordinate for observation points	
# of lines = NUMOBS	IYOBS	Integer	y coordinate for observation points	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
Data Set 2	IX	Integer	x coordinate of pumping or injection wells	
# of lines = NREC	IY	Integer	y coordinate of pumping or injection wells	
	REC	Real	Pumping (+) or injection (-) rate in **cfs**	
	CNREC	Real	Concentration of injected contaminated water (**mass/volume**)	
	CNREC1	Real	Concentration of injected oxygenated water (**mass/volume**)	
	CNREC2	Real	Concentration of injected nitrate water (**mass/volume**)	
	CNREC3	Real	Concentration of injection iron water (**mass/volume**)	
	CNREC4	Real	Concentration of injected sulfate water (**mass/volume**)	
	CNREC5	Real	Concentration of injected carbon dioxide water (**mass/volume**)	
Data Set 3	INPUT	Integer	Parameter card for transmissivity. If 0 then a constant transmissivity is specified in FCTR. If 1 then transmissivity is read from an array	0 or 1
# of lines = 1 or NY	FCTR	Real	Constant transmissivity value in **sq ft/sec** OR factor to multiply transmissivity array	
	VPRM	Real	Array of transmissivity data in **sq ft per sec**	
Data Set 4	INPUT	Integer	Parameter card for thickness. If 0 then a constant thickness is specified in FCTR. If 1 then thickness is read from an array	0 or 1
# of lines = 1 or NY	FCTR	Real	Constant thickness value in **ft** OR factor to multiply thickness array	
	THCK	Real	Array of thickness data in **ft**	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
Data Set 5	INPUT	Integer	Parameter card for recharge. If 0 then a constant recharge is specified in FCTR. If 1 then recharge is read from an array	0 or 1
# of lines = 1 or NY	FCTR	Real	Constant recharge (-) or discharge (+) value in **ft/sec** OR factor to multiply recharge array	
	RECH	Real	Array of recharge (-) or discharge (+) data in **ft per sec**	
Data Set 6	INPUT	Integer	Parameter card for node identification. If 0 all nodes are identified by FCTR. If 1 then node identification is read from an array	0 or 1
# of lines = 1 or NY	FCTR	Real	Node identification OR factor to multiply node identification array	
	NODEID	Integer	Array of node identification data	
Data Set 7	ICODE	Integer	Instructions for using the NODEID array. When NODEID = ICODE, then the following factors are set	
# of lines = NCODES	FCTR1	Real	Leakance	
	FCTR2	Real	Concentration of contaminated water	
	FCTR2O	Real	Concentration of oxygenated water	
	FCTR2N	Real	Concentration of nitrate water	
	FCTR2F	Real	Concentration of iron water	
	FCTR2S	Real	Concentration of sulfate water	
	FCTR2C	Real	Concentration of carbon dioxide water	
	FCTR3	Real	Recharge (-) or discharge (+)	
	OVERRD	Integer	If OVERRD=0m then the value of RECH is not changed. If OVERRD is nonzero, then the value of RECH is set to FCTR3	
Data Set 8	INPUT		Parameter card for water table. If 0 then a constant water table is specified in FCTR. If 1 then water table is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant water table value in **ft** OR factor to multiply water table array	
	WT		Array of water table data in **ft**	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
Data Set 9	INPUT		Parameter card for initial contaminant concentration. If 0 then a constant initial concentration is specified in FCTR. If 1 then initial contaminant concentration is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant initial contaminant concentration value (**mass/volume**) OR factor to multiply initial contaminant concentration array	
	CONC		Array of initial contaminant concentration data (**mass/volume**)	
Data Set 10	INPUT		Parameter card for initial oxygen concentration. If 0 then a constant initial concentration is specified in FCTR. If 1 then initial oxygen concentration is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant initial oxygen concentration value (**mass/volume**) OR factor to multiply initial oxygen concentration array	
	CONC1		Array of initial oxygen concentration data (**mass/volume**)	
Data Set 11	INPUT		Parameter card for initial nitrate concentration. If 0 then a constant initial concentration is specified in FCTR. If 1 then initial nitrate concentration is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant initial nitrate concentration value (**mass/volume**) OR factor to multiply initial nitrate concentration array	
	CONC2		Array of initial nitrate concentration data (**mass/volume**)	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
Data Set 12	INPUT		Parameter card for initial ferrous iron concentration. If 0 then a constant initial iron concentration is specified in FCTR. If 1 then initial ferrous iron concentration is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant initial ferrous iron concentration value (**mass/volume**) OR factor to multiply initial ferrous iron concentration array	
	CONC3		Array of initial ferrous iron concentration data (**mass/volume**)	
Data Set 13	INPUT		Parameter card for initial ferric iron concentration. If 0 then a constant initial ferric iron concentration is specified in FCTR. If 1 then initial ferric iron concentration is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant initial ferric iron concentration value (**mass/volume**) OR factor to multiply initial ferric iron concentration array	
	CONC3A		Array of initial ferric iron concentration data (**mass/volume**)	
Data Set 14	INPUT		Parameter card for initial sulfate concentration. If 0 then a constant initial concentration is specified in FCTR. If 1 then initial sulfate concentration is read from an array	0 or 1
# of lines = 1 or NY	FCTR		Constant initial sulfate concentration value (**mass/volume**) OR factor to multiply initial sulfate concentration array	
	CONC4		Array of initial sulfate concentration data (**mass/volume**)	
Data Set 15	INPUT		Parameter card for initial carbon dioxide concentration. If 0 then a constant initial concentration is specified in FCTR. If 1 then initial carbon dioxide concentration is read from an array	
# of lines = 1 or NY	FCTR		Constant initial carbon dioxide concentration value (**mass/volume**) OR factor to multiply initial carbon dioxide concentration array	
	CONC5		Array of initial carbon dioxide concentration data (**mass/volume**)	

Table I.1. Input Data for BIOPLUME III

Line #	Parameter	Type	Definition	Range
Data Set 16				
# of lines = 1	ICHK		Parameter to check whether data will be revised for subsequent pumping periods (1 means data will be revised, and remainder of data are specified; 0 means no revisions will be made and data from previous pumping period are used)	
# of lines = 1	NTIM NPNT NITP ITMAX NREC NPNTMV NPNTVL NPNTD NPDELC NPNCHV PINT TIMX TINIT		Previously defined variables (see lines 1 and 3)	
# of lines = NREC	IX IY REC CNREC CNREC1 CNREC2 CNREC3 CNREC4 CNREC5		Previously defined variables (see dataset 2)	

Notes:

* - If NPMP > 1, then data set 16 must be completed
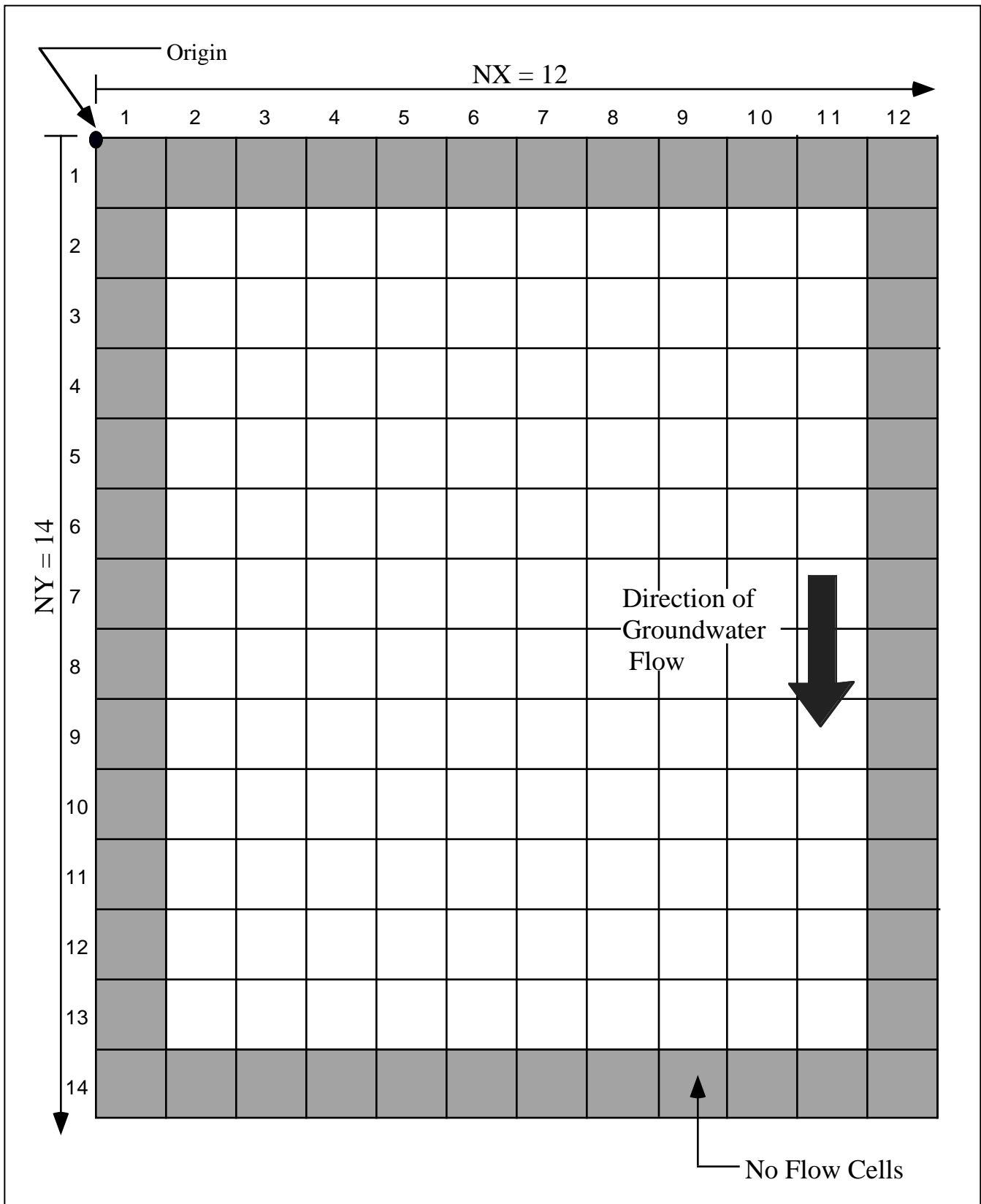
Figure I.1. Grid Discretization in Bioplume III

Real Time

```
|———————————————————————————|—|—|———|———————————|
1970                              1985  1987  1990
2000
Tank                         Contamination  Tank    Pump-and-
installed                    identified   removed   treat system
                                                    installed
```

Model Definitions

```
1st pumping period                    2nd pumping    3rd pumping
                                      period         period
|————————————————————————————————————|—|—|—|—|—|—|—|—|—|—|—|—|
    PINT = 1-17 years                 PINT = 3 years     PINT = 10 years
    NTIM = 1                          NTIM = 3      NTIM = 10

                        [NPMP = 3]
```
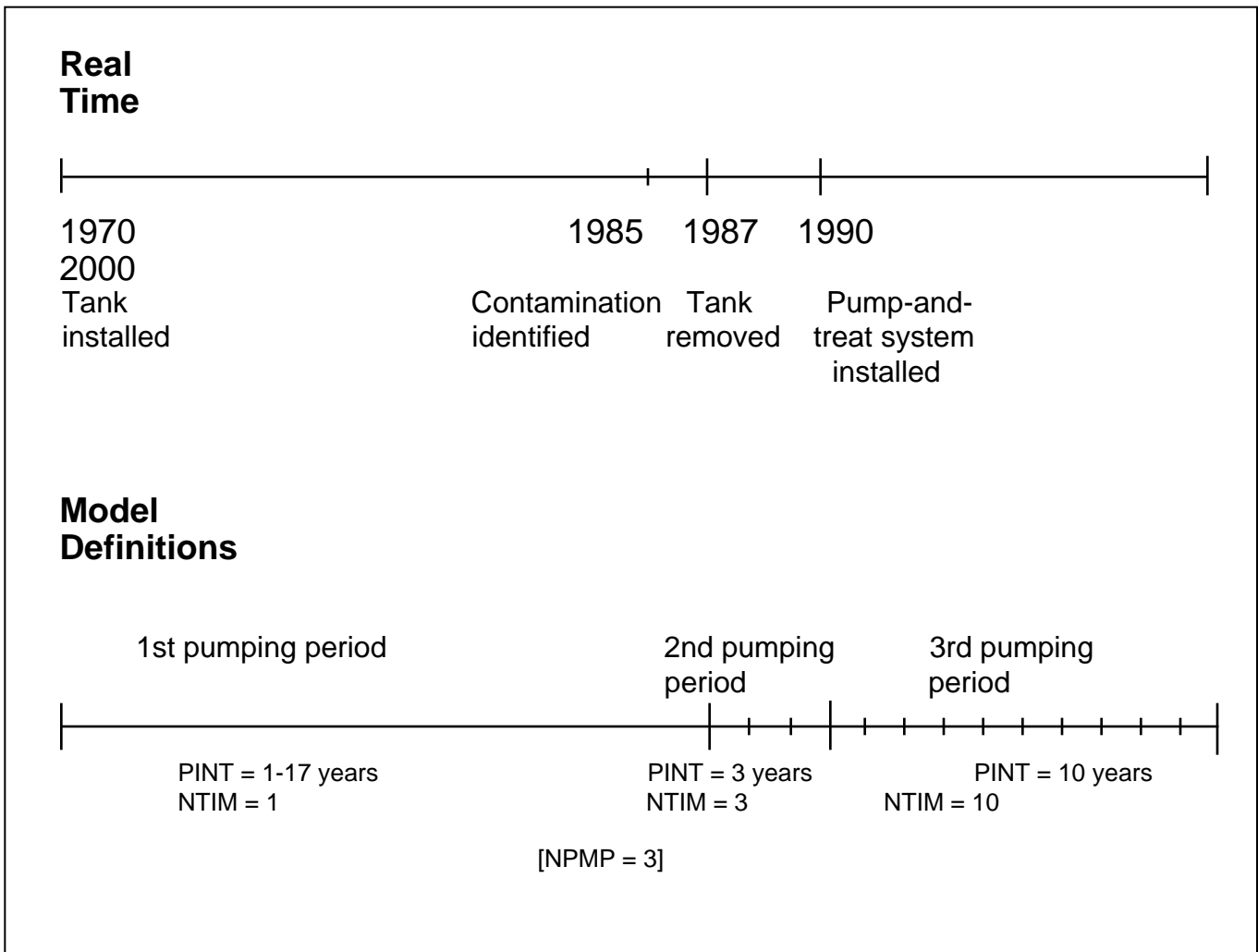
Figure I.2. Discretization of Time in BIOPLUME III

Example I.1:
An underground storage tank was installed at Site A in 1970. A ground water contamination problem was subsequently discovered in 1985. The underground storage tank was removed in 1987 and a pump-and-treat remediation system was installed at the site in 1990 (see Figure I.1). Ground water monitoring was undertaken quarterly throughout the period from 1985 to present day. The modeling objective for this site is to determine the status of the ground water plume in the year 2000.

In order to simulate the period from 1970 to 2000 (total of 30 years), three distinct pumping periods (NPMP = 3) should be used:

1st Pumping Period: 1970 - 1987. This period is characterized by the leaking event which may have taken place any time after the tank was installed (in general, tank failure occurs within a period of 7 - 10 years after installation). The simulation time for this period (PINT) may be anywhere from 1 to 17 years depending on when it is assumed that the tank began leaking. The number of time steps (NTIM) will be one because data were only collected in the last three years of the period (1985 to 1987).

2nd Pumping Period: 1987 through 1990. This period is characterized by the removal of the leaking tank and therefore "cutting off" the source of ground water contamination. The simulation time (PINT) is equal to 3 years and NTIM can be anywhere from 1 to 12 (since ground water data are collected every three months in the three year period). In general, however, it is not efficient to run the model on a quarterly basis because of the possibly long run times, large amounts of data for analysis, and the lack of necessity for that much resolution in model results. An NTIM of 1 or 3 is suggested in this case.

3rd Pumping Period: 1990 through 2000. This period is characterized by the installation of the pump-and-treat system. The simulation time (PINT) is equal to 10 years and an NTIM of 1 or 10 is suggested (this allows viewing of the model results in the year 2000 or annually, respectively).

Note: The BIOPLUME III model internally calculates a "computational time step" to minimize the transport mass balance errors. The "computational time step" can be manipulated by the user to improve the mass balance error or to shorten run times (see Sections I.9, A.3 and A.7).

I.3   Hydrogeologic Characteristics of the Aquifer

A number of variables are used in BIOPLUME III to identify the hydrogeologic characteristics of the aquifer. These include: porosity (**POROS**), longitudinal dispersivity (**BETA**), storativity (**S**), ratio of transverse to longitudinal dispersivity (**DLTRAT**), ratio of longitudinal transmissivity to transverse transmissivity (**ANFCTR**), transmissivity (**VPRM**), recharge (**RECH**) and thickness of the aquifer (**THCK**).

POROS - (effective porosity) is the dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer solids. The porosity is obtained from site specific measurements or from literature values (see Table I.2).

BETA - (longitudinal dispersivity) defines the longitudinal spreading of a plume in the direction of flow. Selection of dispersivity values is difficult because of the impracticability of measuring dispersion in the field. Values for BETA may be obtained using:

Table I.2. Effective Porosity Estimates

Media	Porosity
Gravel, fine	.25 - .38
Sand, coarse	.31 - .46
Sand, fine	.26 - .53
Silt	.34 - .61
Clay	.34 - .60
Sandstone	.005 - .10
Limestone	.001 - .05

Source: Domenico and Schwartz, 1990.

- Data compiled from 50 sites by Gelhar et al. (1985) shown in Figure I.3;
- Data from recent field studies as shown in Table I.3, or;
- Using the relationship suggested by Pickens and Grisak (1981):

BETA = 0.1 Lp, where Lp is the plume length (see Figure I.4) or distance to measurement point in ft.

S - (storativity) is the product of the specific storage and the thickness of the aquifer, where the specific storage is defined as the volume of water that a unit volume of aquifer releases from storage when the pressure head in the unit volume changes a unit amount. Storativity is only used for transient flow analyses and is estimated from pump tests conducted at the site.

DLTRAT - is the ratio of transverse to longitudinal dispersivity. Much like the longitudinal dispersivity, this variable is difficult to estimate. The data in Table I.3 or one of the following relationships may be used:

DLTRAT = 0.33 (Gelhar et al., 1992)
DLTRAT = 0.1 (U. S. Environmental Protection Agency, 1986)

ANFCTR - (ratio of longitundinal transmissivity to transverse transmissivity) is rarely characterized at field sites and is mostly set to 1.

VPRM - (transmissivity) is the product of the hydraulic conductivity and the thickness of the aquifer. VPRM can be obtained from slug tests or pump tests at the site or from published literature values for the hydraulic conductivity (Figure I.5).

RECH - (recharge) is generally obtained from rainfall data and soil infiltration characteristics. This variable is rarely, if ever, measured at field sites. It is usually estimated from local or regional data published by the USGS and the Soil Conservation Service or calibrated.

THCK - (aquifer thickness) is generally obtained from well logs, soil borings and other geologic characterization efforts at the site.

Note: The last three parameters: VPRM, RECH and THCK, may be specified as a constant for the whole site or as a spatially variable parameter such that a different value is entered for each cell in the model grid.

I.4 Boundary Conditions

In order to simulate a field site with the BIOPLUME III model, it is necessary to identify the hydrogeologic conditions that prevail around the site. These hydrogeologic conditions are referred to as *boundary conditions*. The two types of boundary conditions that can be simulated with BIOPLUME III include*: constant head* and *constant flux*.
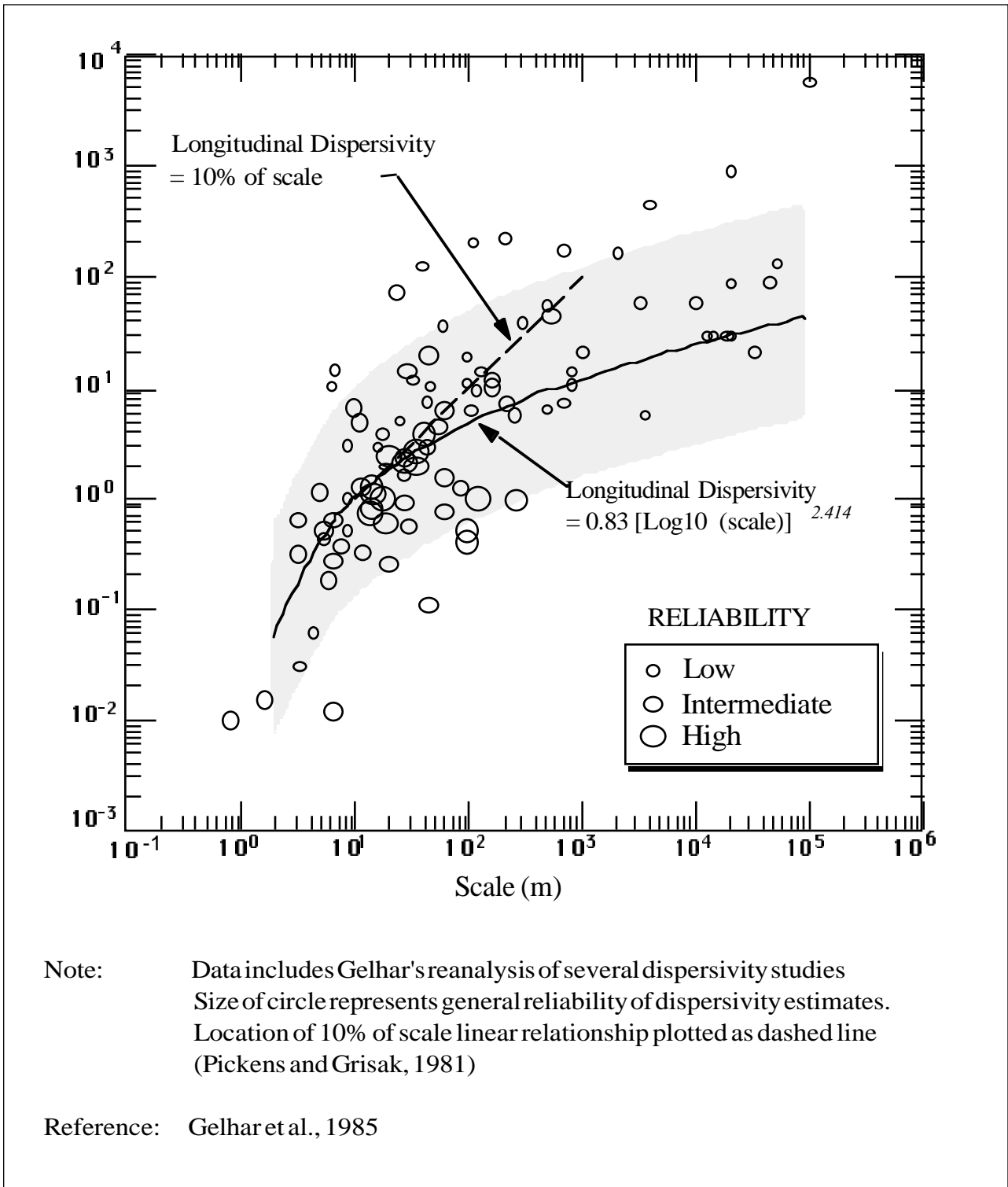
Figure I.3. Longitudinal Dispersivity Chart

The chart contains the following labels and annotations:

Longitudinal Dispersivity = 10% of scale

Longitudinal Dispersivity = 0.83 [Log10 (scale)]$^{2.414}$

RELIABILITY
- ○ Low
- ○ Intermediate
- ○ High

Y-axis values: 10^4, 10^3, 10^2, 10^1, 10^0, 10^{-1}, 10^{-2}, 10^{-3}

X-axis (Scale (m)): 10^{-1}, 10^0, 10^1, 10^2, 10^3, 10^4, 10^5, 10^6

Note: Data includes Gelhar's reanalysis of several dispersivity studies
          Size of circle represents general reliability of dispersivity estimates.
          Location of 10% of scale linear relationship plotted as dashed line
          (Pickens and Grisak, 1981)

Reference: Gelhar et al., 1985

Table I.3. Dispersivity Estimates from Field Experiments

Site	Longitudinal dispersivity (m)	Transverse dispersivity (m)	Vertical dispersivity (m)
Canada Base, Borden, Ontario	.49	.039	.023
MADE Site, Columbus, Mississippi	9.5	2.2	NE
Cape Cod, Massachusetts	.96	.018	.0015

NE = Not Estimated

Sources: Boggs, et. al., 1992
             LeBlanc, Garabedian, et al., 1991
             Garabedian, Gelhar, et al., 1991
             Freyberg, 1986
             Mackay, et. al., 1986
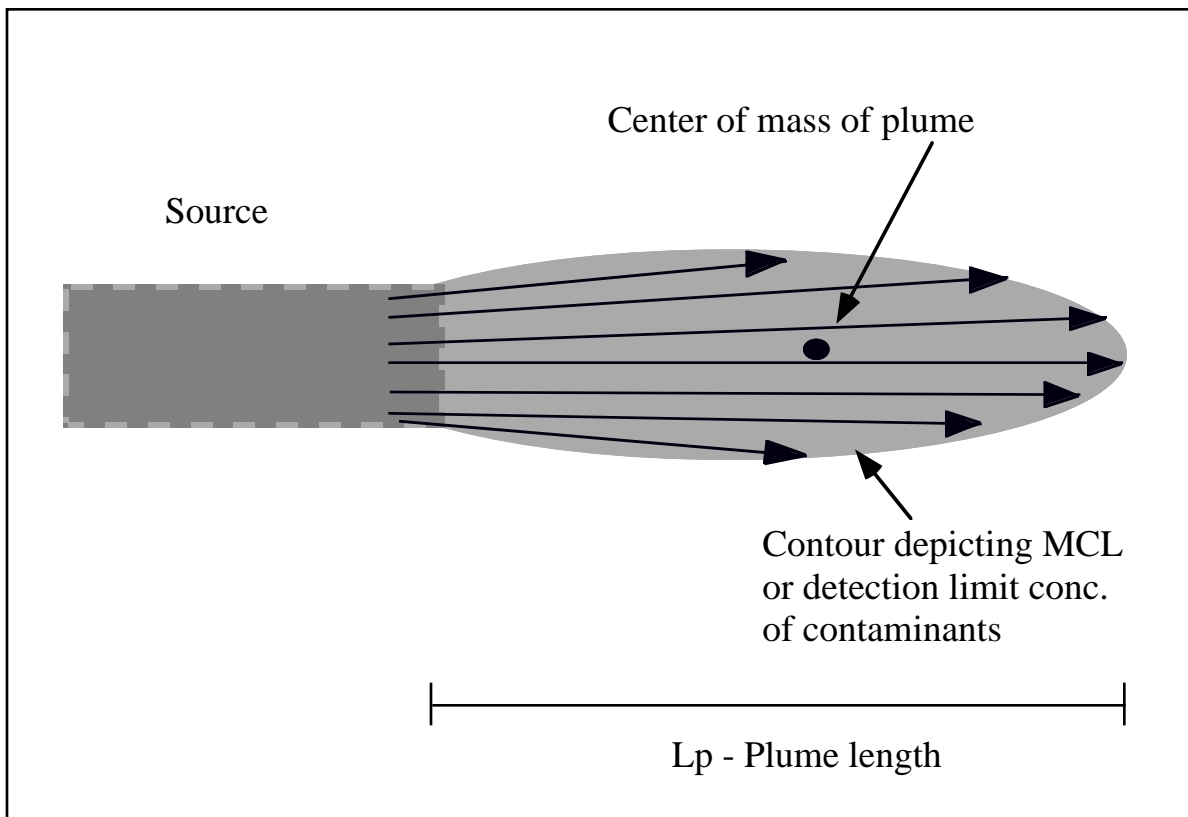
Figure I.4. Illustration of Plume Length for Estimating
Longitudinal Dispersivity
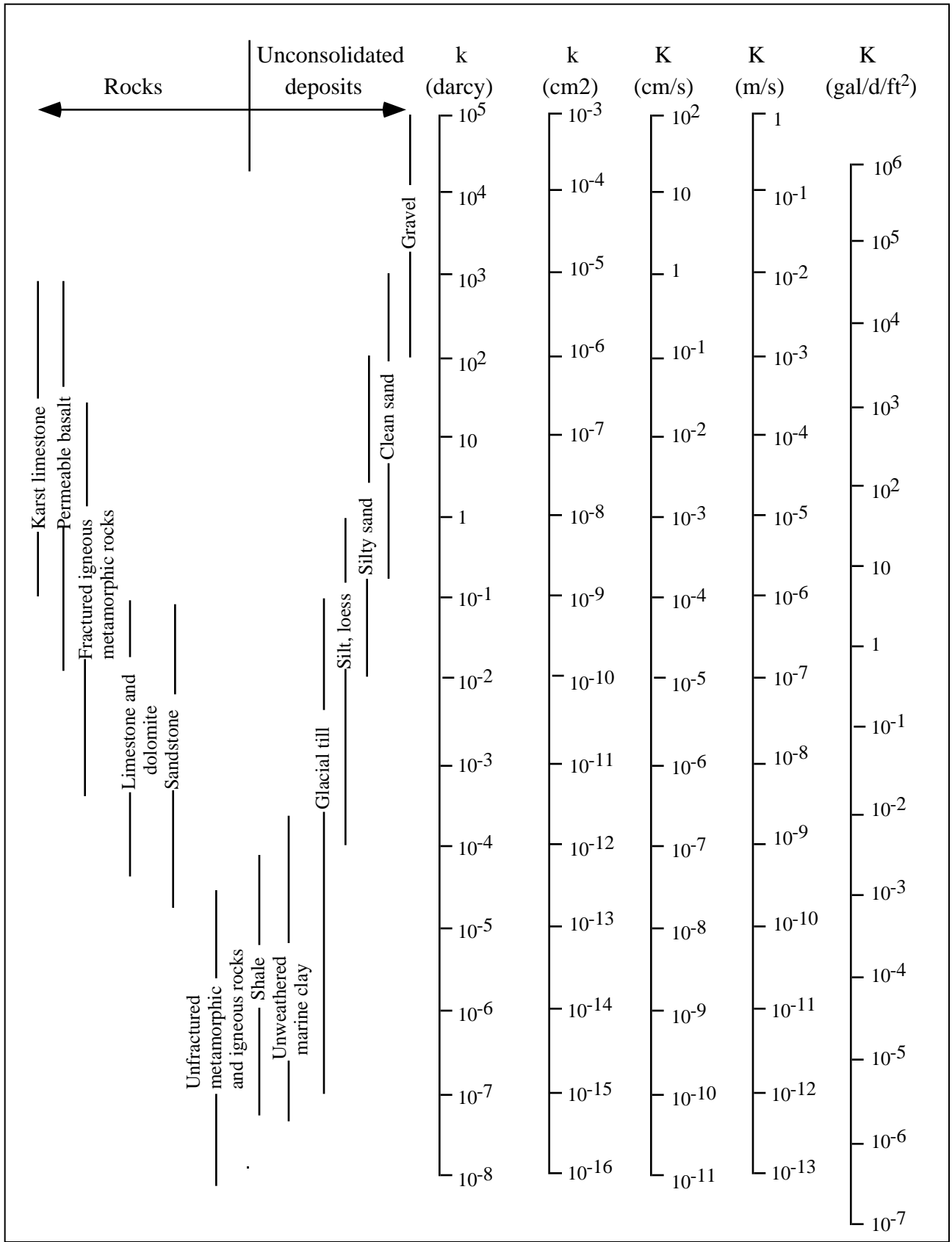
Source: Freeze and Cherry, 1979

Figure I.5. Hydraulic Conductivity for Different Types of Soils

Constant head boundaries refer to cells where the water level is constant throughout the simulation. The head or water level value is specified by the user at the constant head boundaries.

Constant flux boundaries, on the other hand, refer to cells that allow water (and possibly contaminants and electron acceptors) to flow through. In this case, the user specifies the rate of water flow (or flux of water) through the cell and specifies whether the cell is also a source of contamination or electron acceptor(s).

A number of variables in BIOPLUME III allow the user to specify the boundary conditions for the site. These include: NCODES, the NODEID matrix, and the parameters ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD.

The NCODES variable is used to define the number of boundary condition types to be used in the model. For example, if constant head boundary conditions without chemical concentration inflow are to be used for the site, then the NCODES variable is set to one. If, on the other hand, constant head boundaries without chemical concentration inflow are to be used in one portion of the site and constant head boundaries with chemical concentrations inflow are to be used in another portion of the site, then the NCODES variable is set to two.

The NODEID matrix is used to specify the cells at which the boundary conditions will be designated. The NODEID matrix can be thought of as an ON/OFF switch designator. If BIOPLUME III encounters a number between 1 to 9 at any of the cells, the model interprets that as "an ON switch" for additional boundary condition information. BIOPLUME III anticipates that more data would be provided for those cells. The data include the variables ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD. Additionally, if constant head boundaries are used at any of the cells, the water table or WT variable needs to be specified for those cells.

Example I.2:
Figures I.6 and I.7 illustrate two different hydrogeologic scenarios at given field sites. What types of boundary conditions can be used to simulate these conditions?

Site A - The water level conditions at this site are best represented using constant head nodes. The background electron acceptors are specified as input through the boundaries and the contaminant concentrations are specified as input through some of the cells in the upgradient boundary. The measured water levels at the boundaries are used as input water table elevations (WT). The resulting parameter set-up is as follows:

    NCODE = 2

    NODEID Matrix:
    00000000000000
    01111222211110
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    00000000000000
    01111111111110
    00000000000000

    ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD
    1, 1, 0, 8, 10, 0, 20, 18, 0, 0
    2, 1, 100, 8, 10, 0, 20, 18, 0, 0

    WT Matrix
    1 1

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	100	100	100	100	100	100	100	100	100	100	100	100	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	94	94	94	94	94	94	94	94	94	94	94	94	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure I.6. Hydrogeologic Conditions for Site A
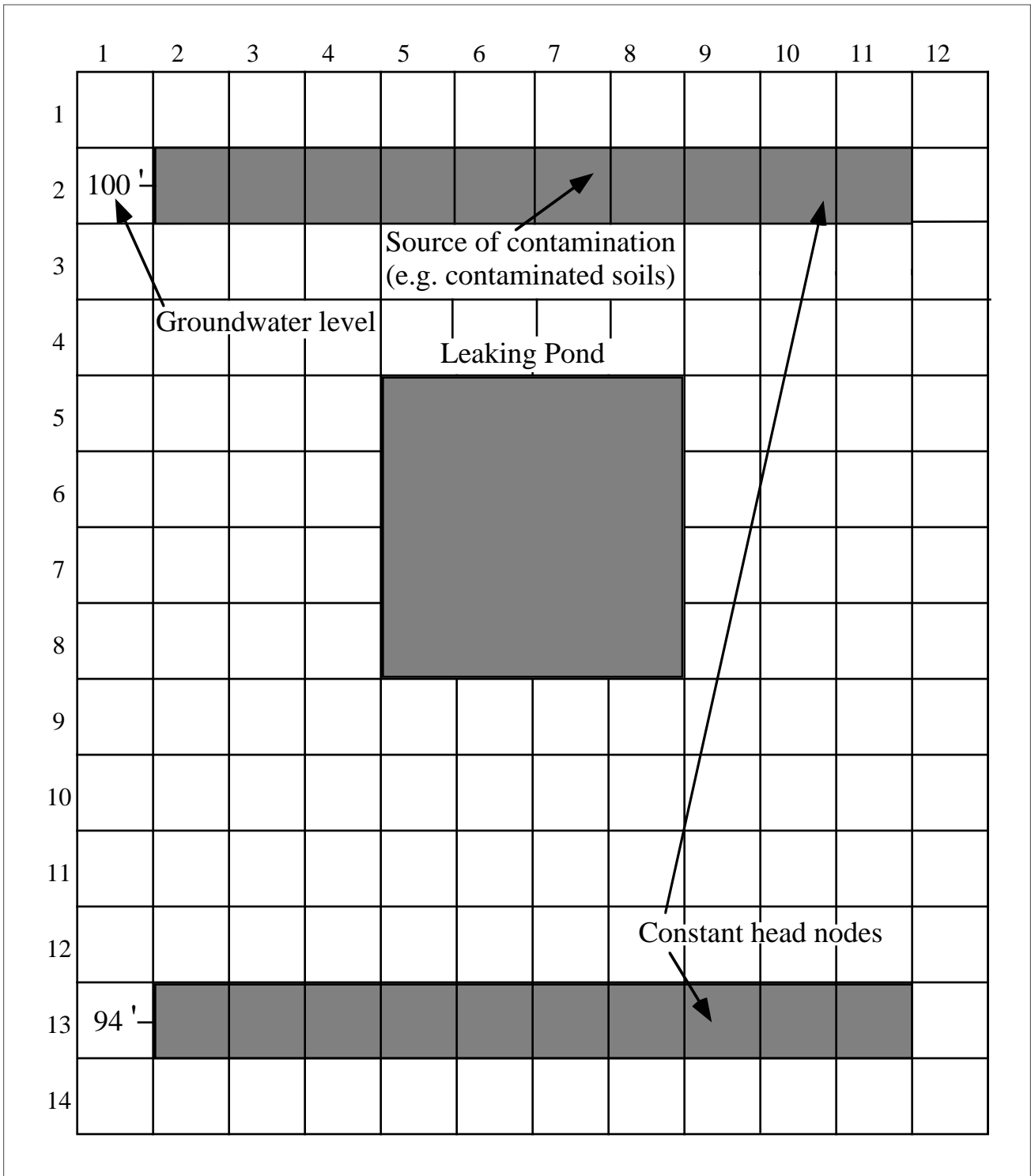
Figure I.7. Hydrogeologic Conditions for Site B

Site B - The water levels at this site are also represented with constant head boundaries. The pond in the middle of the site can be represented using three options: (1) constant head nodes with the corresponding water level in the lake being specified for the appropriate cells; (2) recharge nodes in the NODEID matrix; or leakance cells in the NODEID matrix.

    <u>Option 1 - Constant Head Nodes for Pond</u>
    NCODE = 2

    NODEID Matrix:
    00000000000000
    01111111111110
    00000000000000
    00000000000000
    00000000000000
    00000222200000
    00000222200000
    00000222200000
    00000222200000
    00000000000000
    00000000000000
    00000000000000
    01111111111110
    00000000000000

    ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD
    1, 1, 0, 8, 10, 0, 20, 18, 0, 0
    2, 1, 0, 0, 0, 0, 0, 0, 0, 0

    WT Matrix
    1 1

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	100	100	100	100	100	100	100	100	100	100	100	100	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	101	101	101	101	0	0	0	0	0
0	0	0	0	0	101	101	101	101	0	0	0	0	0
0	0	0	0	0	101	101	101	101	0	0	0	0	0
0	0	0	0	0	101	101	101	101	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	94	94	94	94	94	94	94	94	94	94	94	94	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

Option 2 - Recharge Cells for Pond

NCODE = 2

NODEID Matrix:
00000000000000
01111111111110
00000000000000
00000000000000
00000000000000
00000222200000
00000222200000
00000222200000
00000222200000
00000000000000
00000000000000
00000000000000
01111111111110
00000000000000

ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD
1, 1, 0, 8, 10, 0, 20, 18, 0, 0
2, 1, 0, 0, 0, 0, 0, 0, -1.0e-7, 1

WT Matrix
1 1

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	100	100	100	100	100	100	100	100	100	100	100	100	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	94	94	94	94	94	94	94	94	94	94	94	94	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

```
Option 3 - Leakance Cells for Pond

NCODE = 2

NODEID  Matrix:
00000000000000
01111111111110
00000000000000
00000000000000
00000000000000
00000222200000
00000222200000
00000222200000
00000222200000
00000000000000
00000000000000
00000000000000
01111111111110
00000000000000

ICODE, FCTR1, FCTR2, FCTR2O, FCTR2N, FCTR2F, FCTR2S, FCTR2C, FCTR3, and OVERRD
1, 1, 0, 8, 10, 0, 20, 18, 0, 0
2, -1.0e-9, 0, 0, 0, 0, 0, 0,0, 0

WT  Matrix
1 1
```
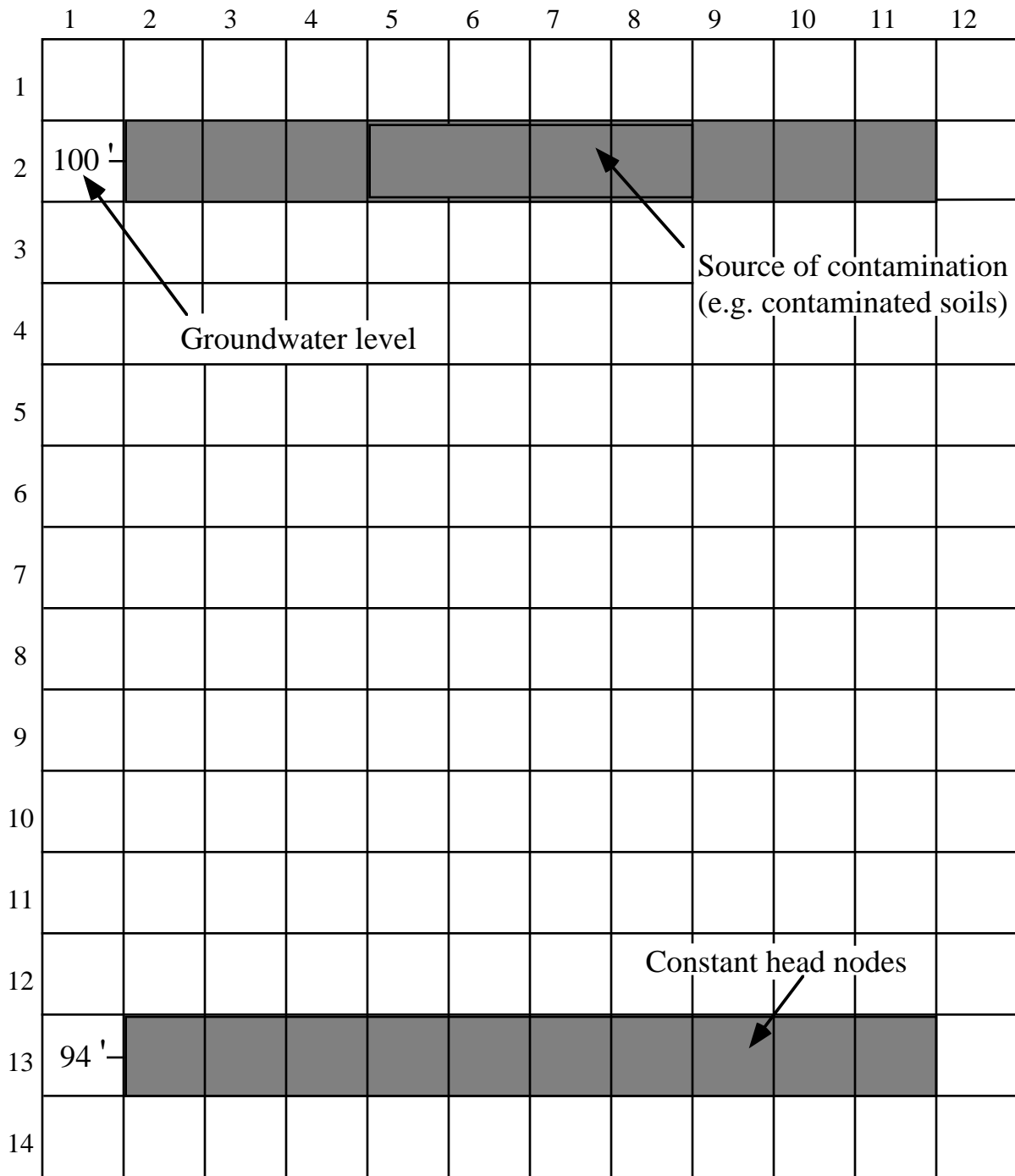
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	100	100	100	100	100	100	100	100	100	100	100	100	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	94	94	94	94	94	94	94	94	94	94	94	94	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

Note that if the lake was leaking contaminants, the lake can additionally be represented using injection wells.

Note:
A related variable to boundary conditions is the hydraulic gradient measured at the site. The BIOPLUME III model generates water level information throughout the site that should "mimic" the measured water levels. Therefore, hydraulic gradients observed at the site should be similar to those generated by the model.

I.5   Initial Conditions

The head and concentrations at the start of the simulation period need to be specified in the BIOPLUME III input. The specific variables include: initial water table (WT), initial concentration of contaminants (CONC), oxygen (CONC1), nitrate (CONC2), ferrous iron (CONC3), ferric iron (CONC3A), sulfate (CONC4), and carbon dioxide (CONC5).

The initial water table (WT) may be developed by contouring water level data measurements and entering the resulting values into each cell in the model grid. This is however, time consuming and not entirely necessary since the model will recompute the water table anyway. The user can enter "0" for the initial water table elevation everywhere except where constant head nodes have been specified (the actual water level is entered for those).

The initial concentration of contaminants (CONC) and the initial concentrations for all the electron acceptors (CONC1 through CONC5) are determined from monitoring well data.

Note: The BIOPLUME III model does not require specific units for concentration. The user may select between mg/L and **m**g/L. The model doesrequire that the user use a consistent set of units for all the concentration input. Therefore, if **m**g/Lfor example are to be used, then all the concentration data need to be entered in that systems of units. The output concentrations generated by the model will also reflect the same units as the input.

I.6   Sources and Sinks

The introduction of water or release of water from the aquifer (including contaminants and electron acceptors) is referred to as sources and sinks. These can be simulated using injection/pumping wells, recharge/discharge cells or constant head cells. The use of recharge and constant head nodes to represent sources and sinks has been illustrated in the previous section. This section will focus on the use of injection wells to represent sources and/or pumping and injection scenarios. The model parameters for injection/pumping wells include: NREC, REC, CNRECH, CNRECO, CNRECN, CNRECF, CNRECS, and CNRECC.

NREC - defines the number of injection or pumping wells that will be used in the model input.

REC - specifies the injection (-ve) or pumping rate (+ve) for each of the wells.

CNRECH - specifies the concentration of contaminant in injected water (parameter set to 0 for pumping wells).

CNRECO - specifies the concentration of oxygen in injected water (parameter set to 0 for pumping wells).

CNRECN - specifies the concentration of nitrate in injected water (parameter set to 0 for pumping wells).

CNRECF - specifies the concentration of ferrous iron in injected water (parameter set to 0 for pumping wells).

CNRECS - specifies the concentration of sulfate in injected water (parameter set to 0 for pumping wells).

CNRECC - specifies the concentration of carbon dioxide in injected water (parameter set to 0 for pumping wells).

I.7 Sorption, Source Decay, Radioactive Decay and Ion-Exchange Variables

A number of variables are used in the model to represent source decay, radioactive decay, sorption and ion-exchange reactions. The parameter IREACT is used to designate which of these reactions are to be used in the current simulation:

IREACT	REACTION	PARAMETERS TO BE SPECIFIED
-1	decay only	THALF
0	no reaction	None
1	linear sorption	DK, RHOB, THALF
2	Freundlich sorption	RHOB, EKF, XNF, THALF
3	Langmuir sorption	RHOB, EKL, CEC, THALF
4	monovalent exchange	RHOB, EK, CEC, CTOT, THALF
5	divalent exchange	RHOB, EK, CEC, CTOT, THALF
6	mono-divalent exchange	RHOB, EK, CEC, CTOT, THALF
7	di-monovalent exchange	RHOB, EK, CEC, CTOT, THALF

THALF is the decay half-life used for radioactive compounds. This half-life is applied both to the specified source concentration and to the dissolved concentrations in the model.

RHOB - is the aquifer bulk density. Typical values are included in Table I.4.

DK - is the linear sorption distribution coefficient more typically referred to as K_d. The distribution coefficient is generally computed using the following relationship:

> K_d = $K_{oc} \bullet f_{oc}$ where K_{oc} is the normalized distribution coefficient (see Table I.5 for typical values) and f_{oc} is the fraction of organic carbon found in uncontaminated soils at the site. The variable f_{oc} can be determined from laboratory analyses of the soils at the site or using the typical values listed in Table I.4.

EKF - is the Freundlich sorption coefficient.

XNF - is the Freundlich sorption exponent.

EKL - is the Langmuir sorption coefficient.

Table I.4. Typical Bulk Densities and f_{oc} Values (part 1 of 2)

Representative Values of Dry Bulk Density for Common Aquifer Matrix Materials

Aquifer Matrix	Dry Bulk Density (gm/cm3)
Clay	1.00 - 2.40
Glacial Sediments	1.15 - 2.10
Loess	0.75 - 1.60
Fine Sand	1.37 - 1.81
Medium Sand	1.37 - 1.81
Coarse Sand	1.37 - 1.81
Gravely Sand	1.37 - 1.81
Fine Gravel	1.36 - 2.19
Medium Gravel	1.36 - 2.19
Coarse Gravel	1.36 - 2.19
Sandstone	1.60 - 2.68
Shale	1.54 - 3.17
Limestone	1.74 - 2.79
Granite	2.24 - 2.46
Basalt	2.00 - 2.70

Sources: Walton, 1988
          Domenico and Schwartz, 1990

Table I.4. Typical Bulk Densities and f_{oc} Values (part 2 of 2)

Representative Values of Total Organic Carbon for Common Sediments

Texture	Depositional Environment	Fraction Organic Carbon	Site Name
medium sand	fluvial-deltaic	0.00053 - 0.0012	Hill AFB, Utah [c]
fine sand		0.0006 - 0.0015	Bolling AFB, D.C. [c]
fine to coarse sand	back-barrier (marine)	0.00026 - 0.007	Patrick AFB, Florida [c]
organic silt and peat	glacial (lacustrine)	0.10 - 0.25	Elmendorf AFB, Alaska [c]
silty sand	glaciofluvial	0.0007 - 0.008	Elmendorf AFB, Alaska [c]
silt with sand, gravel and clay (glacial till)	glacial moraine	0.0017 - 0.0019	Elmendorf AFB, Alaska [c]
medium sand to gravel	glaciofluvial	0.00125	Elmendorf AFB, Alaska [c]
loess (silt)	eolian	0.00058 - 0.0016	Offutt AFB, Nebraska [c]
fine - medium sand	glaciofluvial or glaciolacustrine	< 0.0006 - 0.0061	Truax Field, Madison, Wisconsin [c]
fine to medium sand	glaciofluvial	0.00021 - 0.019	King Salmon AFB, Fire Training Area, Alaska [c] Dover AFB, Delaware [c]
fine to coarse sand	glaciofluvial	0.00029 - 0.073	Battle Creek ANGB, Michigan [c]
sand	fluvial	0.0057	Oconee River, Georgia [a]
coarse silt	fluvial	0.029	Oconee River, Georgia [a]
medium silt	fluvial	0.020	Oconee River, Georgia [a]
fine silt	fluvial	0.0226	Oconee River, Georgia [a]
silt	lacustrine	0.0011	Wildwood, Ontario [b]
fine sand	glaciofluvial	0.00023 - 0.0012	Various sites in Ontario [b]
medium sand to gravel	glaciofluvial	0.00017 - 0.00065	Various sites in Ontario [b]

a/ Karickhoff, 1981
b/ Domenico and Schwartz, 1990
c/ Wiedemeier et al., 1995b

Table I.5. Typical Distribution Coefficients

Compound	K_{oc} (cm^3/g)
Benzene	83
Toluene	300
Ethylbenzene	1100
Xylene	240

Source: Texas Natural Resource Conservation
Commission, 1994.

CEC - is the maximum sorption capacity or ion exchange capacity.

EK - is the Ion-exchange selectivity coefficient.

CTOT - is the total solution concentration of two exchanging ions.

THALFS - represents the source decay rate.

I.8   Biodegradation Variables

A number of variables are used in BIOPLUME III to simulate the aerobic and anaerobic biodegradation of contaminants. An overall first-order decay biodegradation rate (DEC1) can be designated to simulate the lumped effect of aerobic and anaerobic processes. Alternatively, detailed information about the electron acceptors may be provided to simulate their individual impacts. A biodegradation type specifier for each of the electron acceptors (IRECO, IRECN, IRECF, IRECS, IRECC) is used to select between the first-order, instantaneous, and Monod kinetic models. The electron acceptor data for oxygen, for example, depends on the selected kinetic model:

    First-Order Decay Simulations:
    DCO - is the first-order decay rate for oxygen.
    FO - is the concentration of available oxygen in the ground water. This value is needed to allow the model to decay hydrocarbons as long as oxygen is present in the aquifer. If oxygen concentrations reach their specified threshold concentrations (DOMIN), the biodegradation reaction is terminated. This ensures that the first-order decay model does not overestimate the amount of biodegradation that is likely to occur in the aquifer.
    DOMIN - is the threshold oxygen concentration.

    Instantaneous Reaction Simulations:
    The variables **FO** and **DOMIN** (defined previously) are required.

    Monod Kinetic Simulations:
    In addition to **FO** and **DOMIN** (as in the case of the first-order model, these parameters are provided to ensure this model does not overestimate the amount of biodegradation that is likely to occur in the aquifer), the following parameters are required:

    CMSO - is the concentration of microorganisms in the aquifer.
    RMO - is the microbial retardation coefficient.
    RKHO - is the half-saturation constant for the contaminant.
    RKMAXO - is the maximum growth rate for the contaminant.
    RKO - is the half-saturation constant for oxygen.

    Similar variables are defined for all the electron acceptors.

I.9 Numerical Parameters

A number of variables used in BIOPLUME III define "numerical parameters" needed in the solution method used by the model. These include: **NPTPND**, **NPMAX**, **CELDIS**, **NITP**, **ITMAX**, **TOL**, **TIMX**, and **TINIT**.

NPTPND is the number of particles to be used in each cell in the model. The number of particles used in each cell will impact the runtime required for the model. A smaller number of particles will allow the model to run in a shorter period of time but may increase the mass balance errors in the simulation. In general, 9 particles provide adequate model accuracy without causing excessively long runtimes.

NPMAX is the maximum number of particles for the whole grid. In general, NPMAX should be set to a number greater than NX•NY•NPTPND.

CELDIS defines the maximum allowable distance within the cell that a particle is allowed to move in a time step. A CELDIS of 0.5 implies that a particle is not allowed to move more than half a cell length during the time step. This variable is needed in order to control the movement of the particles and the mass balance errors in the model (see Section A.3 in Appendix A). A smaller CELDIS causes lower numerical mass balance errors but may increase runtimes. In general, a CELDIS of 0.5 is recommended.

NITP is the number of iteration parameters used in solving the flow equation. A value of 7 is recommended for this variable.

ITMAX is the maximum number of iterations to be used in solving the flow equation. A value of 200 (the maximum) is recommended for this variable. If the model is unable to arrive at a solution of the flow equation using this value, an error message will be generated and the model run will be terminated. In this case it is recommended that the user review the input data for possible errors.

TOL is the convergence criterion that is used to iteratively solve the flow equation. A value $\pounds$ 0.001 is recommended.

TIMX and **TINIT** define the time steps for transient simulations. TINIT is the size of the initial time step, and TIMX is the multiplier that will be used to generate subsequent time steps from TINIT. For example, if TINIT is set to 1000 seconds and TIMX is set to 10, the second time step will be 10 x 1000 = 10,000 seconds, the third time step will be 10,000 x 10 = 100,000 seconds, and so on.

I.10 Output Control Parameters

A number of variables in BIOPLUME III can be used to control the amount of output that is generated by the model. These include: **NPNT**, **NPNTMV**, **NPNTVL**, **NPNTD**, **NPDELC**, and **NPNCHV**. The majority of these parameters, except for **NPNT**, are typically set to "0. **NPNT** is usually set to "1" to allow viewing of the output at the end of the time step.

Other variables are used to control the type of output that can be generated by the model. These include variables that designate the number and location of observation points: **NUMOBS**, **IXOBS** and **IYOBS**.

NUMOBS is the number of observation or monitoring wells to be specified. A maximum of 5 is allowed.

IXOBS and **IYOBS** define the locations of the specified number of monitoring wells.

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APPENDIX II. INTERPRETATION OF OUTPUT

II.1   Standard Output File (SOF)

The BIOPLUME III model generates a Standard Output File (SOF) that lists the results from a specific model run. It is often very useful to review this file for two purposes: (1) to ensure the accuracy of the input data since the SOF contains a summary of this data; and (2) to verify that the model run was completed without significant errors or warnings during execution. The SOF file first lists the input data for the run followed by computed head and concentration maps. Additionally, the SOF contains mass balance data for the hydraulic and transport calculations from the model run. Finally, the SOF file contains data at observation wells if they had been specified by the user.

II.2   Graphical Output File (GOF)

A companion output file to the standard file discussed above is the Graphical Output File (GOF). The GOF contains all the significant output data from a model run that can be used to generate graphical output such as contour maps for heads and concentrations. The data in the GOF can be extracted and used in conjunction with a graphics generation software program to generate mapped results from the model.

II.3   Resulting Heads

Typically, the SOF and GOF contain the computed heads for the site based on the input data provided by the user. The head data are listed in three different but associated formats as follows:

```
1st Format - computed head matrix in decimal format
N =   1
 NUMBER OF ITERATIONS =   20
1HEAD  DISTRIBUTION - ROW
 NUMBER OF TIME STEPS =    1
     TIME(SECONDS) = 0.78894E+08
     TIME(DAYS)   = 0.91312E+03
     TIME(YEARS)  = 0.25000E+01
```

.0000000	.0000000	.0000000	.000000	.0000000	.0000000	.0000000	.0000000	.0000000
.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	.0000000
.0000000	99.9510147	99.9506046	99.9518232	99.9567243	99.9632506	99.9688484	99.9719650	.0000000
.0000000	99.9024628	99.8996127	99.8999880	99.9118469	99.9274539	99.9402101	99.9470698	.0000000
.0000000	99.8567306	99.8453541	99.8366370	99.8631898	99.8944758	99.9174271	99.9290041	.0000000
.0000000	99.8223890	99.7884550	99.7380312	99.8098146	99.8698476	99.9060372	99.9225293	.0000000
.0000000	99.8219954	99.7480648	99.5172336	99.7682048	99.8690780	99.9143640	99.9325607	.0000000
.0000000	99.8955020	99.8645340	99.8146013	99.8766615	99.9238635	99.9497385	99.9607587	.0000000
.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	.0000000
.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000	.0000000

2nd Format - computed head matrix in integer format
1HEAD DISTRIBUTION - ROW
 NUMBER OF TIME STEPS =   1
     TIME(SECONDS) = 0.78894E+08
     TIME(DAYS)   = 0.91312E+03
     TIME(YEARS) = 0.25000E+01

0 0   0   0   0   0   0   0   0 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0 100 100 100 100 100 100 100 0
0 0   0   0   0   0   0   0   0 0

3rd format - computed drawdown in integer format
1DRAWDOWN
   0   0   0   0   0   0   0   0 0
   0   0   0   0   0   0   0   0 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0 -100 -100 -100 -100 -100 -100 -100 0
   0   0   0   0   0   0   0   0 0
   0   0   0   0   0   0   0   0 0

II.4   Resulting Concentrations

Typical output from BIOPLUME III lists the resulting concentrations for the contaminant and
the electron acceptors at the site. The concentration matrices are listed in the SOF in integer
format, while they are listed in decimal format in the GOF. For example, the concentration
matrix for hydrocarbon in the SOF might be:

   0 0   0   0   0   0   0   0   0 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0 98 98 98 98 98 98 98 0
   0 0   0   0   0   0   0   0   0 0

The equivalent matrix in the GOF would be:

```
.000000  .000000  .000000  .000000  .000000  .000000  .000000  .000000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  97.5000  .000000
.000000  .000000  .000000  .000000  .000000  .000000  .000000  .000000  .000000
```

II.5   Mass Balance Results

Two types of mass balances are reported in the BIOPLUME III output: (1) the hydraulic mass balance; and (2) the transport mass balance. The hydraulic mass balance is reported in general following the water table calculations. Typically, the information includes the following:

CUMULATIVE MASS BALANCE -- (IN FT**3)

```
RECHARGE AND INJECTION             =       0.00000E+00
PUMPAGE AND E-T WITHDRAWAL          =       0.00000E+00
CUMULATIVE NET PUMPAGE             =       0.00000E+00
WATER RELEASE FROM STORAGE          =       0.00000E+00
LEAKAGE INTO AQUIFER                =       0.00000E+00
LEAKAGE OUT OF AQUIFER              =        0.00000E+00
CUMULATIVE NET LEAKAGE             =       0.00000E+00
  MASS BALANCE RESIDUAL             =       0
   ERROR (AS PERCENT)               =       0.00000E+00
```

RATE MASS BALANCE -- (IN C.F.S.)

```
LEAKAGE INTO AQUIFER                =       0.00000E+00
LEAKAGE OUT OF AQUIFER              =        0.00000E+00
NET LEAKAGE   (QNET)                =       0.00000E+00
RECHARGE AND INJECTION             =       0.00000E+00
PUMPAGE AND E-T WITHDRAWAL          =       0.00000E+00
NET WITHDRAWAL  (TPUM)              =       0.00000E+00
```

The majority of the output is self-explanatory. The first part lists the total volumes of water into and out of the aquifer in ft^3 and the second part lists the data in terms of rate in cu. ft/sec. The last variable in the first part of the data is the hydraulic mass balance error for the flow. The hydraulic mass balance error should be relatively low (less than 1%).

The transport mass balance is provided for the contaminant and for the electron acceptors. The data provided for the contaminant, for example, includes:

CHEMICAL MASS BALANCE

```
MASS IN BOUNDARIES    =  0.00000E+00
MASS OUT BOUNDARIES   =  0.00000E+00
MASS PUMPED IN        = -0.00000E+00
MASS PUMPED OUT       = -0.00000E+00
MASS LOST W. O2 BIODEG.  =  0.00000E+00
MASS LOST W. NO3 BIODEG.  =  0.00000E+00
MASS LOST W. Fe  BIODEG.  =  0.00000E+00
MASS LOST W. SO4 BIODEG.  =  0.00000E+00
MASS LOST W. CO2 BIODEG.  =  0.00000E+00
MASS LOST BY DECAY    =  0.00000E+00
MASS ADSORBED ON SOLIDS=  0.00000E+00
INITIAL MASS ADSORBED  =  0.00000E+00
INFLOW MINUS OUTFLOW   = -0.00000E+00
INITIAL MASS DISSOLVED =  0.00000E+00
PRESENT MASS DISSOLVED =  0.00000E+00
CHANGE MASS DISSOLVED  = -0.00000E+00
CHANGE TOTL.MASS STORED=  0.68039E+09
COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
MASS BALANCE RESIDUAL  = -0.00000E+00
ERROR  (AS PERCENT)    = -0.00000E+00
COMPARE INITIAL MASS STORED WITH CHANGE IN MASS STORED:
ERROR  (AS PERCENT)    =  0.00000E+00
```

Mass in/out Boundaries estimates the amount of mass that enters or leaves the boundaries of the specified grid. Mass pumped in/out estimates the mass entering or leaving the model grid through injection and pumping wells. Losses due to biodegradation and first-order decay mechanisms are listed individually in the matrix. Similarly adsorbed mass (initial and current) is also listed. Present Mass Dissolved represents the mass currently remaining in the aquifer. The remainder of the mass balance data illustrate the various steps in the mass balance calculations to estimate the resulting error. The user is referred to Section A.5 for further details.

Note: The units used in the mass balance calculations depend on the concentration units specified by the user. For example, if the user specified all the input concentration data using mg/L, then the mass balance information would have units of mg/L•ft^3. In order to obtain the mass in mg, the user needs to multiply the numbers in the mass balance matrix by 28.03 to convert the L to ft^3.

APPENDIX III.   QUESTIONS MOST ASKED

III.1   Can I use the model for an unconfined aquifer?

The model, while designed for a confined aquifer, may certainly be used for simulating an unconfined aquifer. The only condition placed on the model would involve injection and pumping activities. As a general rule of thumb, any change in head due to injection and pumping should not exceed 10 - 15% of the specified saturated thickness of the aquifer. If this condition is violated and heads are allowed to vary outside this range (due to pumping/injection), the accuracy of the hydraulic solution would decline thus potentially causing errors in the transport solution. This is mainly because the specific difference between a confined and unconfined aquifer has to do with the saturated thickness being constant in one and variable in the other as water is removed from or added to the aquifer.

III.2   I need to model a larger grid.

The model grid, in principle, can be as large as needed. In practice, however, there is a limitation based on the amount of memory available in the particular computer platform being used. Consult your particular platform implementation version to determine the maximum grid size that can be accommodated. If a larger grid size is still desired, you can modify and recompile the code.

III.3   Should I assume steady-state or transient hydraulics?

The majority of hydraulic conditions at sites, unless a pump test or a specific transient scenario is being simulated, can be adequately modeled assuming steady-state hydraulics. This is particularly true if a long period of time is being simulated (on the order of years). While most sites experience seasonal variations, it is not practical to simulate these events individually over a long period of time. A common approach involves establishing "an average" hydraulic condition for the site and using it for the model simulations.

III.4   I have large mass balance errors ...

Mass balance errors are influenced by a number of model parameters. Pumping or injecting significant amounts of water into or out of the aquifer generates relatively high velocities around the pumping/injection zones and might cause large mass balance errors. Two model parameters: NPTPND and CELDIS, directly affect mass balance errors. A larger number of particles per cell generates less error but requires longer runtimes. The relationship between CELDIS and mass balance errors is not as direct. Decreasing CELDIS might improve the mass balance error or cause it to oscillate in different time periods. Again, a smaller CELDIS causes longer runtimes.

III.5   My model runs forever ...

Model runtime is determined by the number of particle moves that the program has to complete. The number of particle moves required is determined internally by the model based on one of four criteria (see Section A.3 in Appendix A).

In order to reduce runtimes, you need to determine which criterion is being used for the run in question and change the parameter that influences the internal calculation of the number of particle moves required. To determine the criterion being used, you need to terminate the computer run in question (by using an "escape" sequence of keys and not by rebooting computer) and examine the output file generated from the run by searching for the words STABILITY CRITERIA.

III.6   My model is generating particles. Is there something wrong?

In some situations, a cell may become void of particles. In order to ensure numerical accuracy, the model limits the number of cells that can be void of particles to a small percentage of the total number of cells that represent the aquifer. If the limit is exceeded, the numerical solution of the transport equation is terminated at the end of the time increment and the concentrations are saved. Then the model regenerates the initial particle distribution throughout the grid and assigns the "final" concentrations at the time of termination as the new "initial" particle concentrations. The solution is then continued in time.

III.7   My plume is running off the page. Is this OK?

This is one of the most common mistakes made in using BIOPLUME III. The grid used is basically too small and the plume migrates beyond the edge of the model grid. The resulting model may not accurately represent site conditions. You need to re-examine your grid design and lengthen your grid as necessary to allow the plume to be contained within the model grid.

III.8   I'm setting up all my cells as constant-head nodes to fix the ground water elevations at the cells. Will it work?

This is not a particularly useful approach. A significant step of modeling the site involved calibrating the hydraulics. If you were to fix the water table, you would not be able to judge the effectiveness of the model in predicting the site conditions.

III.9   What happens to particles that migrate off the grid?

Neither water or dissolved chemicals are allowed to cross a no-flow boundary in the model. Under certain conditions it might be possible for a particle to be advected across the boundary during a time increment. The model responds to this situation by relocating the particle within the aquifer by reflection across the boundary.

APPENDIX A.   BACKGROUND INFORMATION ON THE USGS MOC MODEL

A.1   Introduction

The USGS Method of Characteristics (MOC) Model was developed by L. F. Konikow and J. D. Bredehoeft in 1978 (Konikow and Bredehoeft, 1978). The model has been revised numerous times since its development. The latest modification completed in 1989 incorporated into the model decay and equilibrium-controlled sorption or ion exchange (Goode and Konikow, 1989). The 1989 version of MOC was used to develop BIOPLUME III.

The MOC model simulates solute transport in flowing ground water. The model is flexible in that it can be applied to a wide range of problem types. It is applicable to one- or two-dimensional problems involving steady-state or transient flow. The model computes changes in concentration over time caused by the process of advection, hydrodynamic dispersion, and mixing or dilution from fluid sources. In its 1978 version, the model assumed that the solute is non-reactive and that gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.   The 1989 version of the model simulates exponential decay such as radioactive decay; reversible equilibrium-controlled sorption with Linear, Freundlich, or Langmuir isotherms; and reversible equilibrium-controlled ion exchange for monovalent and divalent ions. The aquifer may be heterogeneous and/or anisotropic.

The MOC model couples the ground water flow equation with the solute transport equation. The computer code uses an alternating-direction implicit procedure to solve a finite-difference approximation to the ground water flow equation, and it uses the method of characteristics to solve the solute transport equation. The latter uses a particle tracking procedure to represent advective transport and a two-step explicit procedure to simulate hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. The explicit procedure used in the MOC model has several stability criteria which are used internally to address time-step limitations.

A.2   Theoretical Background

A.2.1   Flow Equation

The equation solved in MOC describing the transient two-dimensional flow of homogeneous compressible fluid through a nonhomogeneous anistropic aquifer is given by:

$$\frac{\partial}{\partial x_i}\left(T_{ij}\,\frac{\partial h}{\partial x_j}\right) \;=\; S\,\frac{\partial h}{\partial t} + W \qquad i,j \;=\; 1,2 \qquad\qquad (A.1)$$

where

T_{ij} is the transmissivity tensor, L^2/T;

h	is the hydraulic head, L;
S	is the storage coefficient, (dimensionless);
t	is the time, T;
$W = W(x,y,t)$	is the volume flux per unit area (positive sign for outflow and negative for inflow), L/T; and
x_i and x_j	are the Cartesian coordinates, L.

The fluxes considered in MOC include direct withdrawal or recharge, such as well pumpage, injection, or evapotranspiration, and steady leakage into or out of the aquifer through a confining layer, streambed, or lakebed:

$$W(x,y,t) \quad = \quad Q(x,y,t) - \frac{K_z}{m}(H_e - h) \tag{A.2}$$

where

Q	is the rate of withdrawal (positive sign) or recharge (negative sign), L/T;
K_z	is the vertical hydraulic conductivity of the confining layer, streambed or, lakebed, L/T;
m	is the thickness of the confining layer, streambed or, lakebed, L; and
H_e	is the hydraulic head in the source bed, stream, or lake, L.

The average seepage velocity of ground water is derived from Darcy's law:

$$V_i \quad = \quad -\frac{K_{ij}}{n}\frac{\partial h}{\partial x_j} \tag{A.3}$$

where

V_i	is the seepage velocity in the direction of x_i , L/T;
K_{ij}	is the hydraulic conductivity tensor, L/T; and
n	is the effective porosity of the aquifer, (dimensionless).

A.2.2   Transport Equation

The transport equation solved in MOC is given by:

$$\frac{\partial(Cb)}{\partial t} \quad = \quad \frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(bCV_i) - \frac{C'W}{n} \quad i,j=1,2 \tag{A.4}$$

where

| C | is the concentration of the dissolved chemical species, M/L^3 ; |
| D_{ij} | is the coefficient of hydrodynamic dispersion (a second-order tensor), L^2 /T; |

b   is the saturated thickness of the aquifer, L; and

C'   is the concentration of the dissolved chemical in a source or sink fluid, M/L^3 .

The first term on the right side of the equation represents the change in concentration due to hydrodynamic dispersion. The second term describes advection while the third term describes a fluid source or sink.

A.2.3   MOC Assumptions

The main assumptions in MOC include:

1.   Darcy's law is valid and hydraulic-head gradients are the only driving mechanism for flow.

2.   The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.

3.   Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.

4.   No chemical reactions occur that affect the fluid properties, or the aquifer properties.

5.   Ionic and molecular diffusion are negligible contributors to the total dispersive flux.

6.   Vertical variations in head and concentration are negligible.

7.   The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

A.2.4.   Numerical Methods

A.2.4.1 Flow Equation. The flow equation (Equation A.1) is approximated with an implicit finite difference equation. The resulting finite difference equation is solved using an iterative alternating-direction implicit (ADI) procedure. After the head distribution has been computed for a given time step, the velocity of ground water flow is computed at each node using an explicit finite-difference form of Equation (A.3).

A.2.4.2 Transport Equation - The Method of Characteristics. The Method of Characteristics is used to solve the transport equation in this model. The approach taken by MOC is not to solve Equation (A.4) directly, but rather to solve an equivalent system of ordinary differential equations. Representative fluid particles are advected with the flowing ground water and changes in their chemical concentrations are observed as they move (see Figure A.1).

The first step in MOC involves placing a number of traceable particles in each cell of the finite-difference grid. These particles are distributed in a uniform geometric pattern throughout the grid
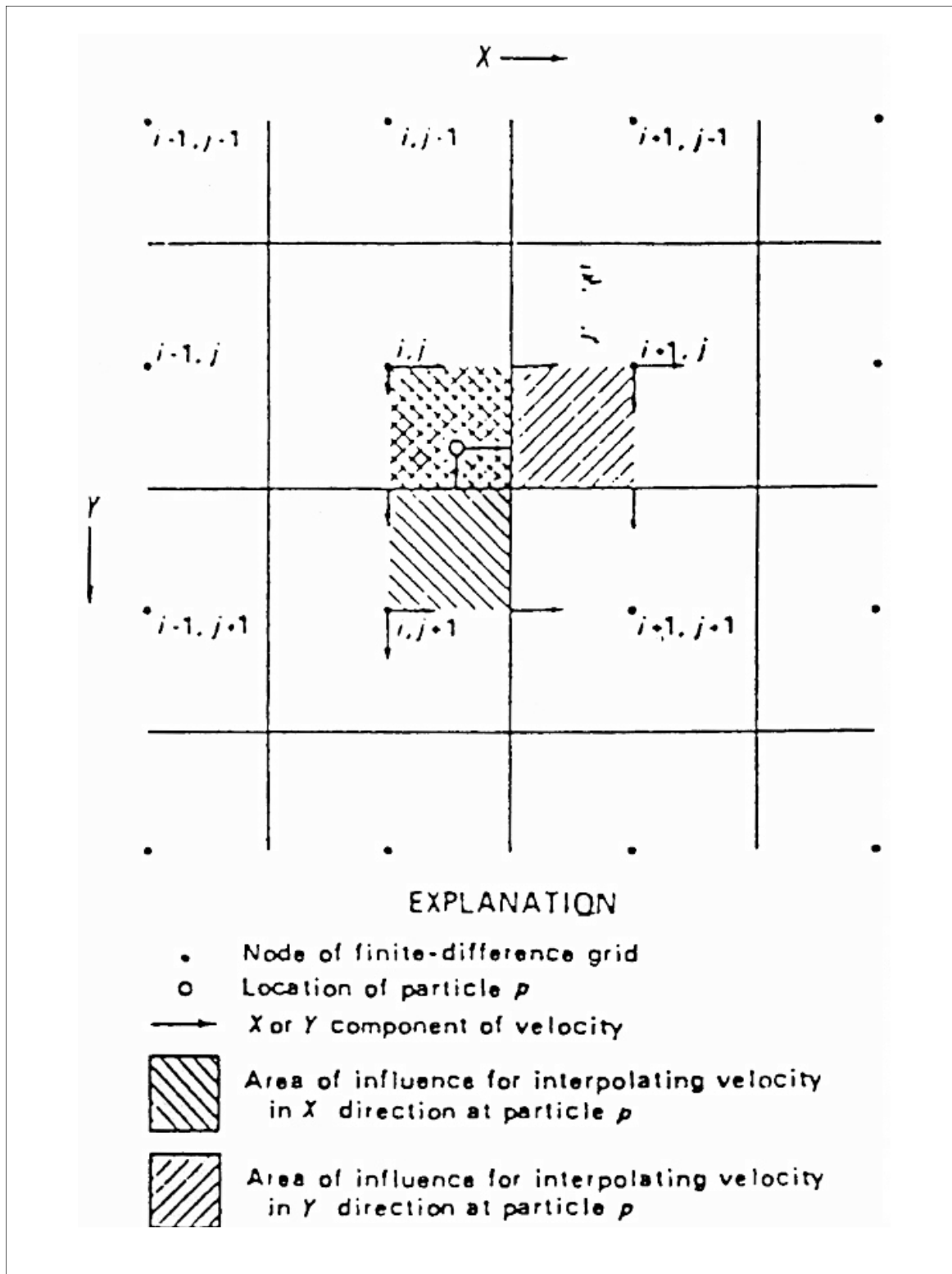
Source: Konikow and Bredehoeft, 1978

Figure A.1 Relation of Flow Field to Movement of Particles

(four, five, eight, nine or sixteen particles are allowed per cell in MOC). The location of each particle is specified by its x- and y- coordinates. The initial concentration assigned to each point is the initial concentration associated with the node of the cell containing the particle.

For each time step every particle is moved a distance proportional to the length of the time increment and the velocity at the location of the particle. After all particles have been moved, the concentration at each node is temporarily assigned the average of the concentrations of all particles then located within the area of that cell. The moving particles thus simulate advective transport because the concentrations at each node of the grid will change with each time step as different particles having different concentrations enter and leave the area of that cell.

The changes in concentration caused by hydrodynamic dispersion and fluid sources are then computed at each node of the grid rather than directly at the location of each particle because of the difficulty in computing concentration gradients at a large number of moving points.

A.3   Stability Criteria

The explicit numerical solution of the solute-transport equation has a number of stability criteria associated with it. These may require that the flow time step be subdivided into a number of smaller time increments to accurately solve the transport equation. There are four stability criteria that drive the transport time-step determination: dispersion, mixing and advection in the x- and y- directions.

Dispersion Citerion: $\Delta t \leq \text{Min over grid} \left(\dfrac{0.5}{\dfrac{D_{xx}}{\Delta x^2} + \dfrac{D_{yy}}{\Delta y^2}} \right)$ (A.5)

Mixing Criterion: $\Delta t \leq \text{Min over grid} \left(\dfrac{nb_{ijk}}{W_{ijk}} \right)$ (A.6)

Velocity Criteria: $\Delta t \leq \dfrac{\gamma \Delta x}{Vx_{max}}$ (A.7)

$\Delta t \leq \dfrac{\gamma \Delta y}{Vy_{max}}$ (A.8)

where γ is the fraction of the grid dimension that particles will be allowed to move (CELDIS in the input stream).

If the time step used in the flow computations exceeds the smallest of the time steps computed using equations (A.5 through A.8), then the time step will be subdivided into the appropriate number of smaller time increments required for solving the solute transport equation.

These criteria determine to a large degree the length of runtimes for a model simulation. Therefore to decrease runtimes (with the possible outcome of increasing numerical errors), one has to determine which of the stability criteria influences the time step calculation and modify the parameters involved accordingly.

A.4   Boundary and Initial Conditions

To obtain a solution to the equations that describe ground water flow and solute transport, it is necessary to specify boundary and initial conditions for the domain of the problem. Two types of boundary conditions are incorporated into MOC: constant-flux and constant-head boundary conditions. These can be used to represent artificial boundaries for the model as well as to represent the real boundaries of the aquifer.

A constant-flux boundary can be used to represent aquifer underflow, well withdrawals, or well injection. A finite flux is designated by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is necessary around the area of interest for MOC. No-flow boundaries can also be located elsewhere in the grid to simulate natural limits or barriers to ground water flow. No flow boundaries are designated by setting the transmissivity equal to zero at appropriate nodes, thereby precluding the flow of water or dissolved chemicals across the boundaries of the cell containing that node.

A constant-head boundary is used to represent parts of the aquifer where the head will not change with time, such as recharge boundaries or areas beyond the influence of hydraulic stresses. In MOC, constant head boundaries are simulated by adjusting the leakage term at the appropriate nodes. This is accomplished by setting the leakage to a sufficiently high value (such as 1.0 s^{-1}) to allow the head in the aquifer at a node to be implicitly computed as a value that is essentially equal to the value of H_e, which would be specified as the described constant-head altitude.

A.5   Mass Balance

Mass balance calculations are performed after specified time intervals to help check the numerical accuracy and precision of the solution. The principle of conservation of mass requires that the total mass inflows and outflows (or net flux) must equal the accumulation of mass (or change in mass stored):

$$\Sigma\text{Inflows} - \Sigma\text{Outflows} \quad = \quad \Delta\text{Mass Stored} \tag{A.9}$$

The difference between the net flux and the mass accumulation is the mass residual (R_m):

$$R_m \quad = \quad \Delta M_s - M_f \tag{A.10}$$

where

ΔM_s is the change in mass stored in aquifer, M; and

M_f is the net mass flux, M.

The change in mass stored is evaluated using the equation:

$$\Delta M_s \quad = \quad \sum_i \sum_j b_{ij} \, n\Delta x\Delta y \, (C_{ijk} - C_{ijo}) \tag{A.11}$$

where C_{ijo} is the initial concentration at node (i,j), M/L^3 ; and

$$M_f \quad = \quad \sum_i \sum_j \sum_k \Delta x\Delta y\Delta t_k \, W_{ijk} \, C'_{ijk} \tag{A.12}$$

The percent error (E) in the mass balance is computed in two different ways. First, the residual is compared with the average of the net flux and the net accumulation:

$$E_1 \quad = \quad \frac{100.0 \, (M_f - \Delta M_s)}{0.5 \, (M_f + \Delta M_s)} \tag{A.13}$$

Equation (A.13) is a good measure of the accuracy of the numerical solution when the flux and the change in mass stored are relatively large. Equation (A.13) does not account for initial mass stored in the aquifer. A second type of error computed by the model accounts for this situation by comparing the residual with the initial mass of solute (M_o) in the aquifer:

$$E_2 \quad = \quad \frac{100.0 \, (M_f - \Delta M_s)}{M_o} \tag{A.14}$$

Equation (A.14) becomes meaningless, however, when M_o is zero or small relative to ΔM_s . In these cases, the model will compute a third type of error measure:

$$E_3 \quad = \quad \frac{100.0 \, (M_f - \Delta M_s)}{M_o - M_f} \tag{A.15}$$

In general, either one or both of E_1 or E_3 is computed by the model.

A.6   Evaluation of MOC - Comparison with Analytical Solutions

The accuracy of the MOC model was evaluated by comparing one-dimensional model simulations to an analytical solution of contaminant transport (steady-state flow through a homogeneous isotropic medium; Konikow and Bredehoeft, 1978).   The analytical solution consisted of the following system of equations:

$$\frac{C(x,t) - C_O}{C_L - C_O} = \frac{1}{2}\, \text{erfc}\left(-\frac{x - qt/n}{\sqrt{4D_L t}}\right) \tag{A.16}$$

Initial Conditions
$$C = C_O \quad \text{for} \quad t \leq 0 \quad \text{and} \quad -\infty < x < 0$$
$$C = C_L \quad \text{for} \quad 0 \leq x < +\infty$$

Boundary Conditions
$$\frac{\partial C}{\partial x} = 0 \qquad \text{for } t > 0 \text{ and } x = \pm\, \infty$$
$$C = C_L \qquad \text{for } x = +\, \infty$$
$$C = C_O \qquad \text{for } x = -\, \infty$$

where

erfc is the complimentary error function, and

$q = nV$ is the specific discharge, LT^{-1}

Figure A.2 presents the results from the comparisons for two different values of dispersivity. As can be seen from Figure A.2, there was exact agreement between modeled results and the analytical solution for higher dispersion. There is a small difference in the modeled results at some nodes for the case of low dispersion. The authors of MOC attribute these differences to the error in computing the concentration at a node as the arithmetic average of the concentrations of all particles located in that cell.

The MOC model was also evaluated by comparing it to the analytical solution for the problem of plane radial flow in which a well continuously injects tracer at a constant rate q_W , and a constant concentration C_O :

$$\frac{C}{C_O} = \frac{1}{2}\, \text{erfc}\left(\frac{r^2/2 - Gt}{\sqrt{4/3\alpha_1 r^{-3}}}\right) \tag{A.17}$$
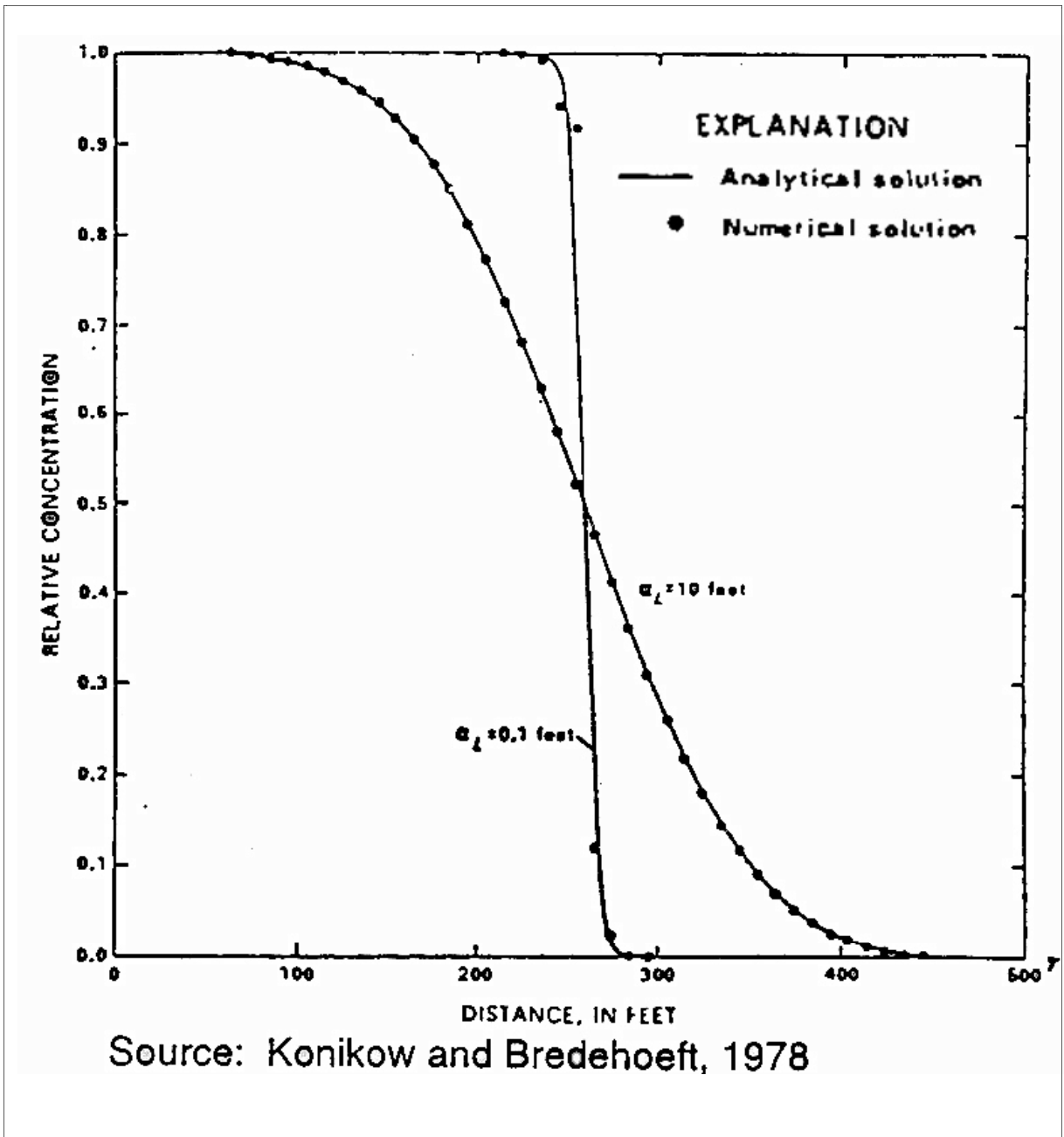
Source: Konikow and Bredehoeft, 1978

Figure A.2   Comparison Between Analytical Model and MOC
for Dispersion in 1-D Steady-State Flow

where

$G \qquad = q_w/2\pi nb = Vr$

r   is the radial distance from the center of the well, L; and

$\bar{r} \qquad = \sqrt{(2Gt)}$ is the average radius of the body of injected water, L.

Figure A.3 presents the results from the comparison. Here again, there is good agreement between the modeled data and the analytical solution. Some numerical dispersion can be seen in the modeled results. The authors attribute this problem to the regeneration of particles in the model.

A.7   Mass Balance Tests

The accuracy and precision of the numerical methods used in MOC were evaluated by computing the mass balance error for three problems: (1) the spread of a tracer slug; (2) the effects of wells; and (3) the effects of user options.

Spreading of a Tracer Slug. This problem illustrates the mass balance errors resulting from advection and dispersion modeling in MOC. A slug of tracer was placed in four cells of a grid whose boundary conditions generated a steady-state flow field that was moderately divergent in some places and moderately convergent in other places (see Figure A.4). The aquifer was assumed to be homogeneous and isotropic. The parameters used in the model run are listed in Table A.1. The slug of known tracer was allowed to move downgradient for 2 years. The model was run for two cases: (1) no dispersion; and (2) a longitudinal dispersivity of 100 ft. Figure A.5 illustrates the resulting mass balance errors for the two cases. As can be seen from Figure A.5, the mass balance errors ranged from -8 to +8%.

Effects of Wells. This problem evaluates the mass balance errors for scenarios where the flow field is influenced by wells. The grid and boundary conditions used for this problem are shown in Figure A.6. The problem simulates one injection well and one pumping well. The parameters for this problem are listed in Table A.2. The aquifer was assumed to be isotropic and homogeneous. The problem was simulated for 2.4 years and assumed steady-state flow. This problem was also simulated for two cases: (1) no dispersion; and (2) a longitudinal dispersivity of 100 ft. Figure A.7 illustrates the resulting mass balance errors for the two cases. As can be seen from Figure A.7, the mass balance errors ranged from -8 to +8%.

Effects of User Options. There are two parameters that are specified by the user that impact the accuracy, precision and efficiency of the model results. These include the initial number of particles per node (NPTPND) and the maximum fraction of the grid dimensions that particles are allowed to move (CELDIS). The set-up for the effects of wells problem was used to evaluate the effect of these two parameters on mass balance results. Figure A.8 illustrates the relationship between the number of particles (NPTPND) and the mass balance error. The errors are smaller for higher numbers of particles. However, it is noted that longer runtimes are also required. Figure A.9 illustrates the relationship between CELDIS and mass balance errors. It can be seen from Figure A.9 that the impact of CELDIS on the error is more complicated. A decrease in
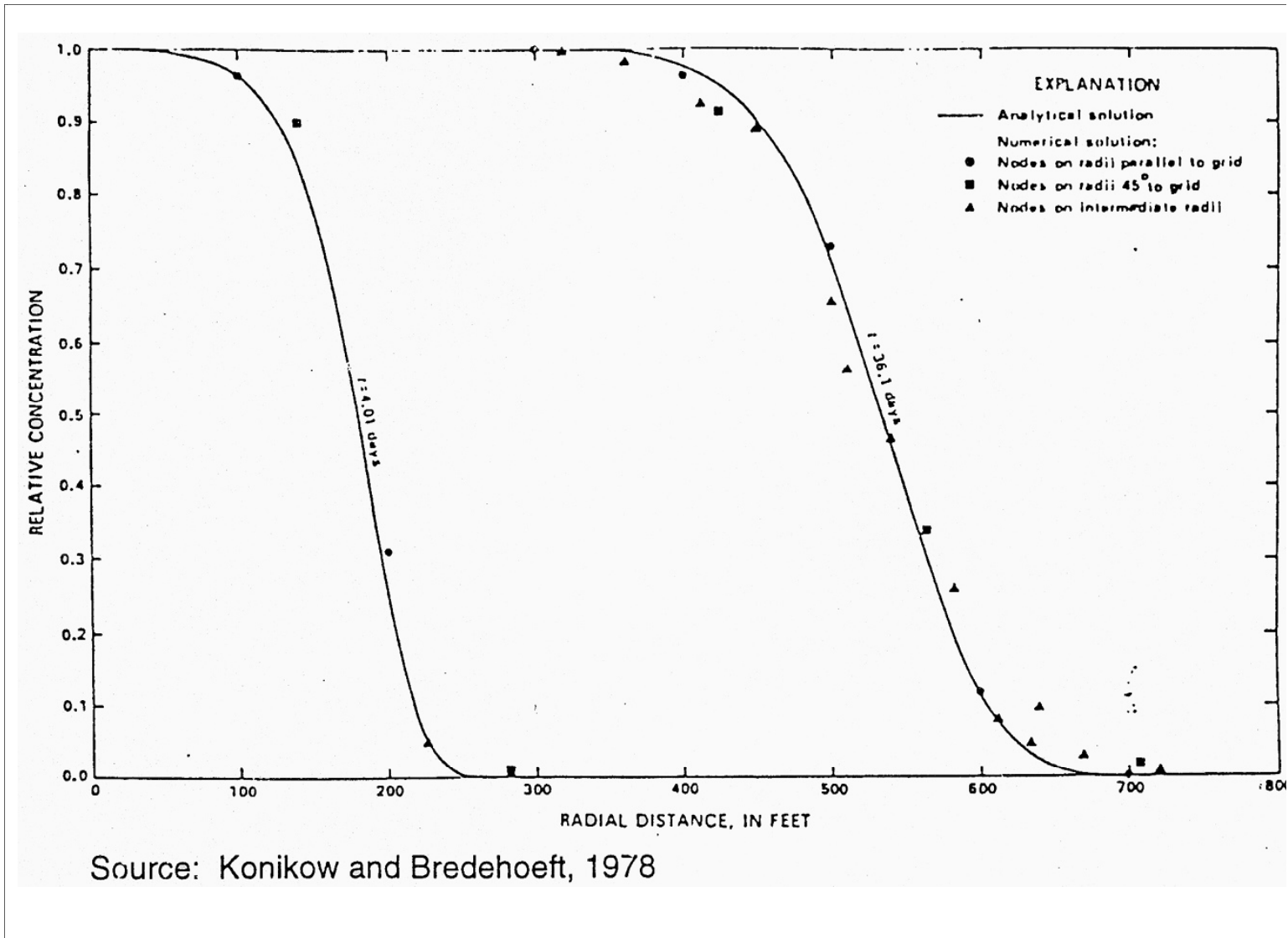
Source: Konikow and Bredehoeft, 1978
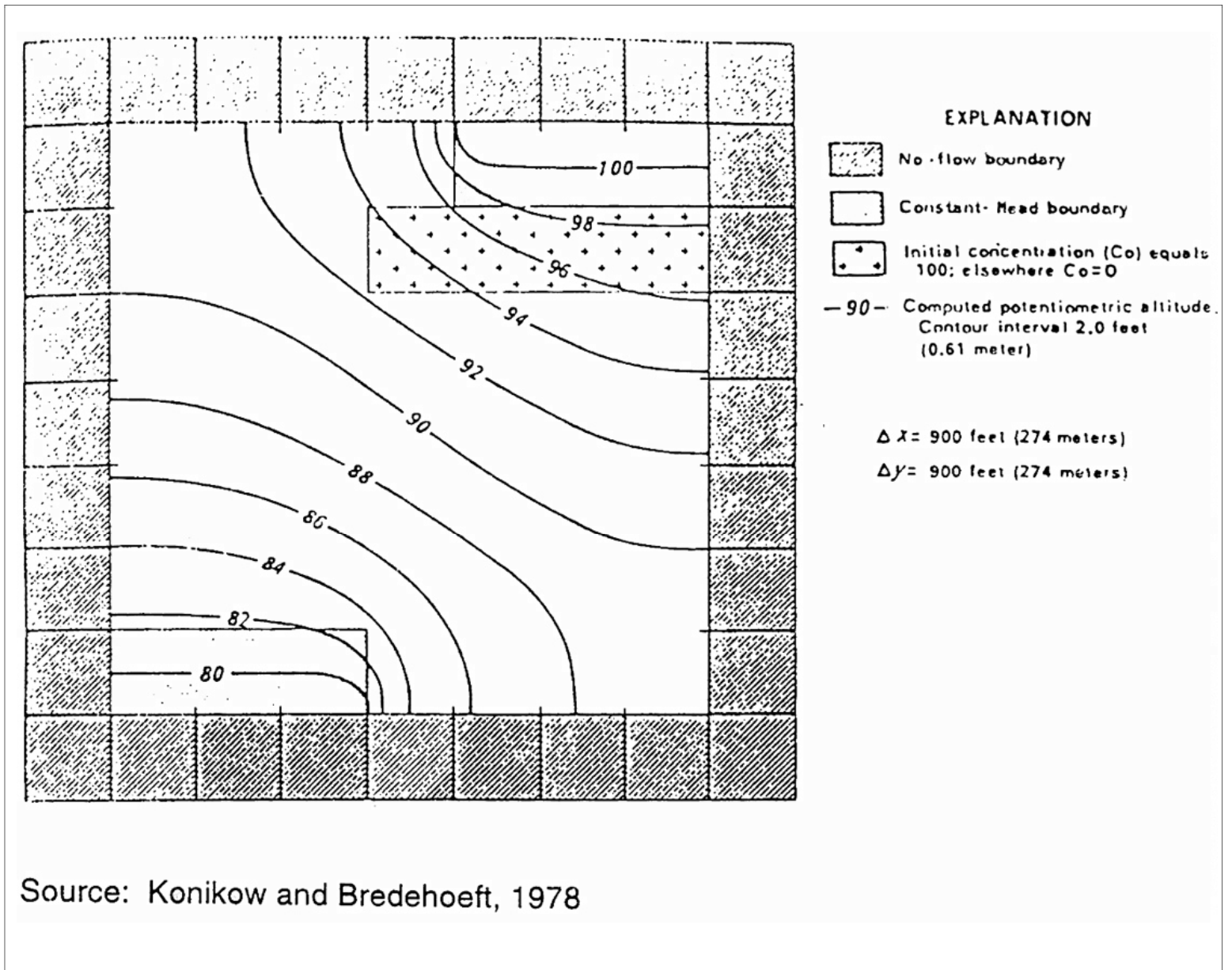
Figure A.3   Comparison Between Analytical Model and MOC for
Dispersion Plane Radial Steady-State Flow

Source: Konikow and Bredehoeft, 1978

Figure A.4   Grid Boundary Conditions and Flow Field
for the Tracer Slug Mass Balance
Test Problem

Table A.1. Model Parameters for the Tracer Slug Mass Balance Test Problem

Aquifer Properties		Numerical Parameters	
K	= 0.005 ft/s. = $(1.5 \times 10^{-3}$ m/s)	ΔX	= 900 ft (274 m)
b	= 20.0 ft = 6.1 m	ΔY	= 900 ft (274 m)
S	= 0.0	CELDIS	= 0.49
n	= 0.30	NPTPND	= 9
α_T/α_L	= .30		

Source: Konikow and Bredehoeft, 1978

Figure A.5   Mass Balance Errors for the
Tracer Slug Mass Balance Problem

EXPLANATION

▨ No-flow boundary

▨ Constant-head boundary

⊖ Injection well

⊕ Withdrawal well

—90— Computed potentiometric altitude
Contour interval 2.0 feet
(0.61 meter)

Δ X = 900 feet (274 meters)
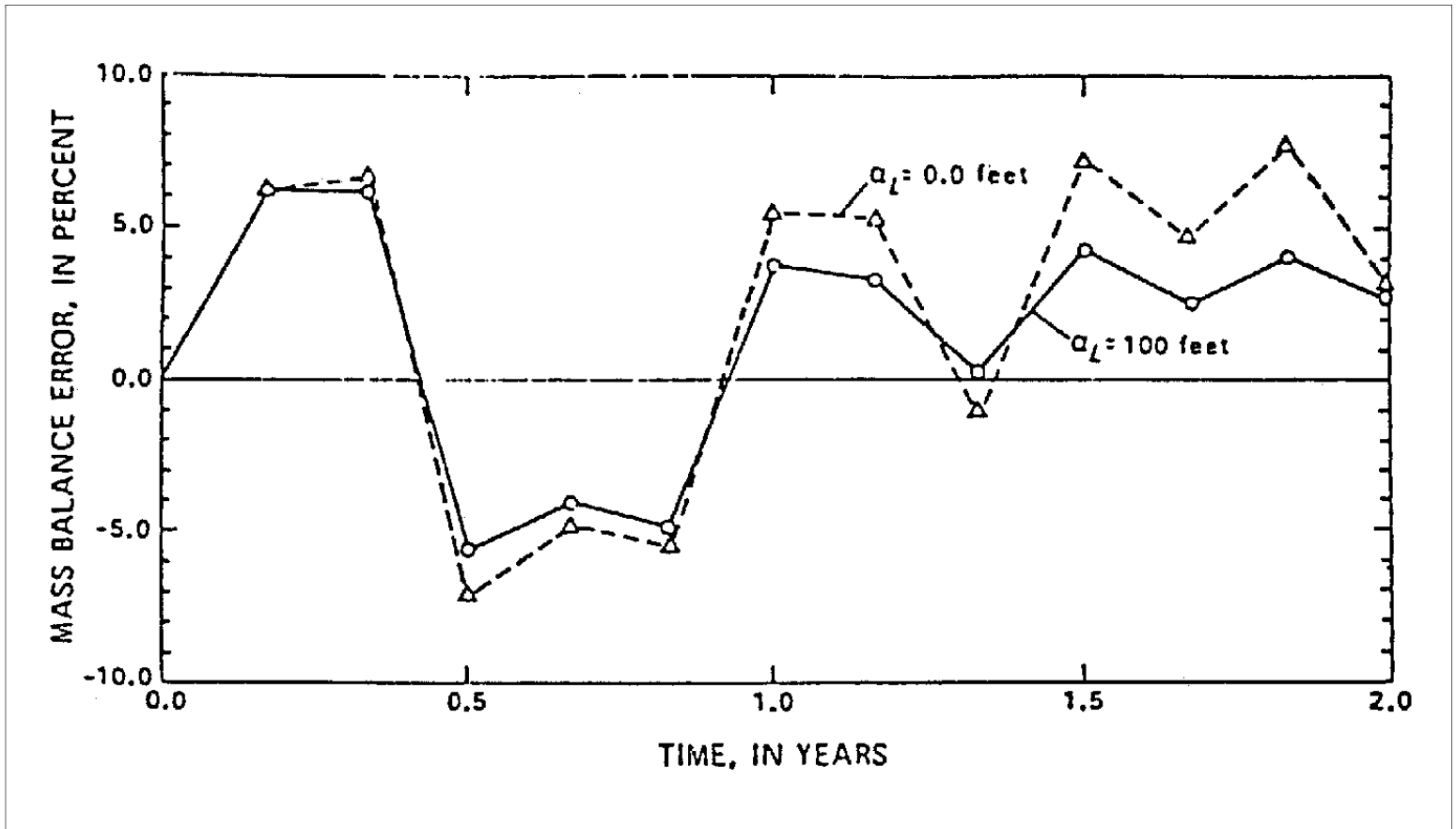
Δ Y = 900 feet (274 meters)
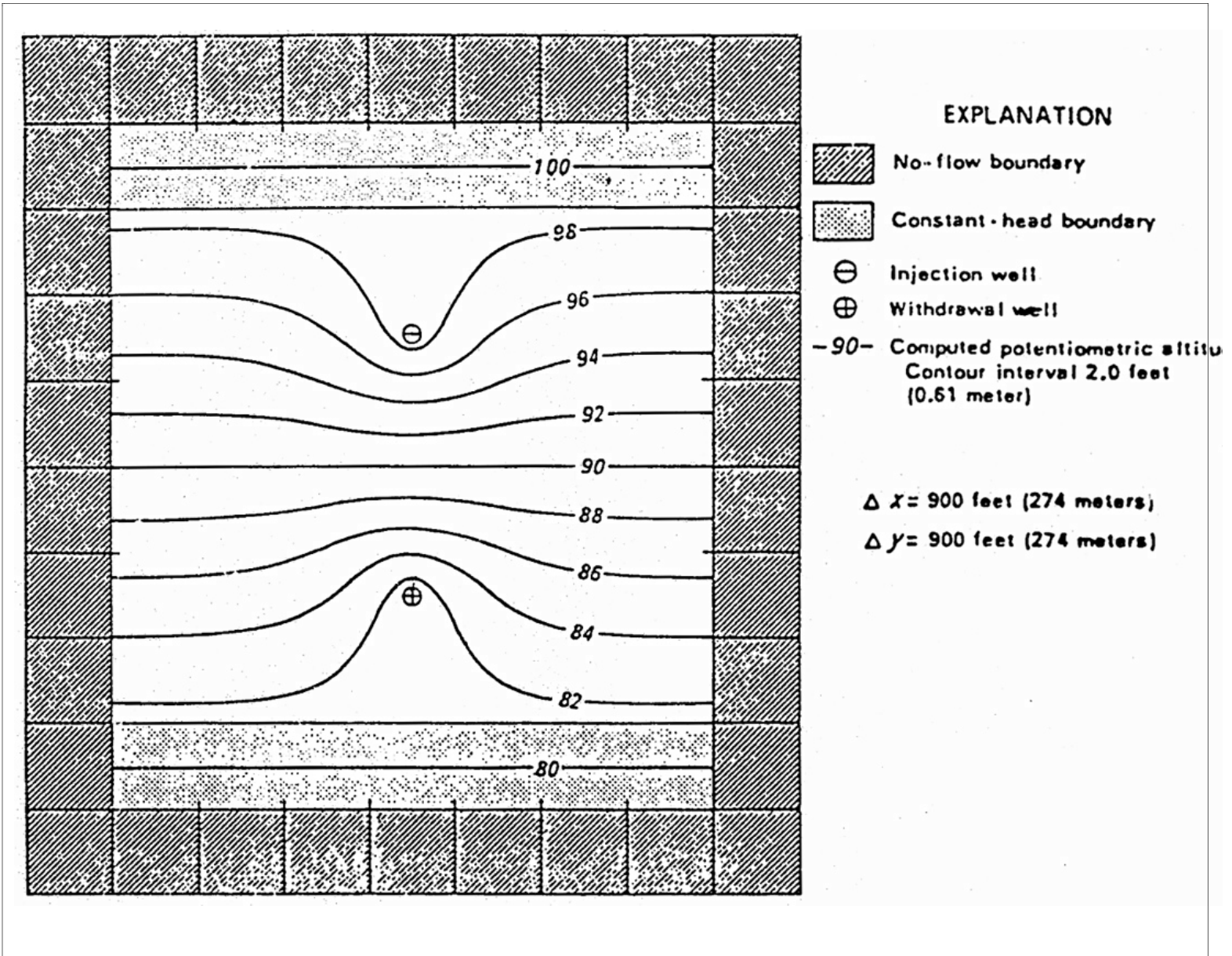
Source: Konikow and Bredehoeft, 1978

Figure A.6   Grid, Boundary Conditions and Flow Field for
Effects of Wells Mass Balance Test Problem

Table A.2. Model Parameters for the Effects of Wells Mass Balance Test Problem

Aquifer Properties		Numerical Parameters	
K	$= 0.005$ ft/s. $= (1.5 \times 10^{-3}$ m/s)	DX	$=$ 900 ft (274 m)
b	$= 20.0$ ft $= (6.1$ m)	DY	$=$ 900 ft (274 m)
S	$= 0.0$	CELDIS	$= 0.49$
n	$= 0.30$	NPTPND	$= 9$
a_T/a_L	$= .30$		
C'	$= 100.0$		
C_O	$= 0.0$		
q_W	$= 1.0$ ft^3 / s $= (0.028$ m^3 / s)		
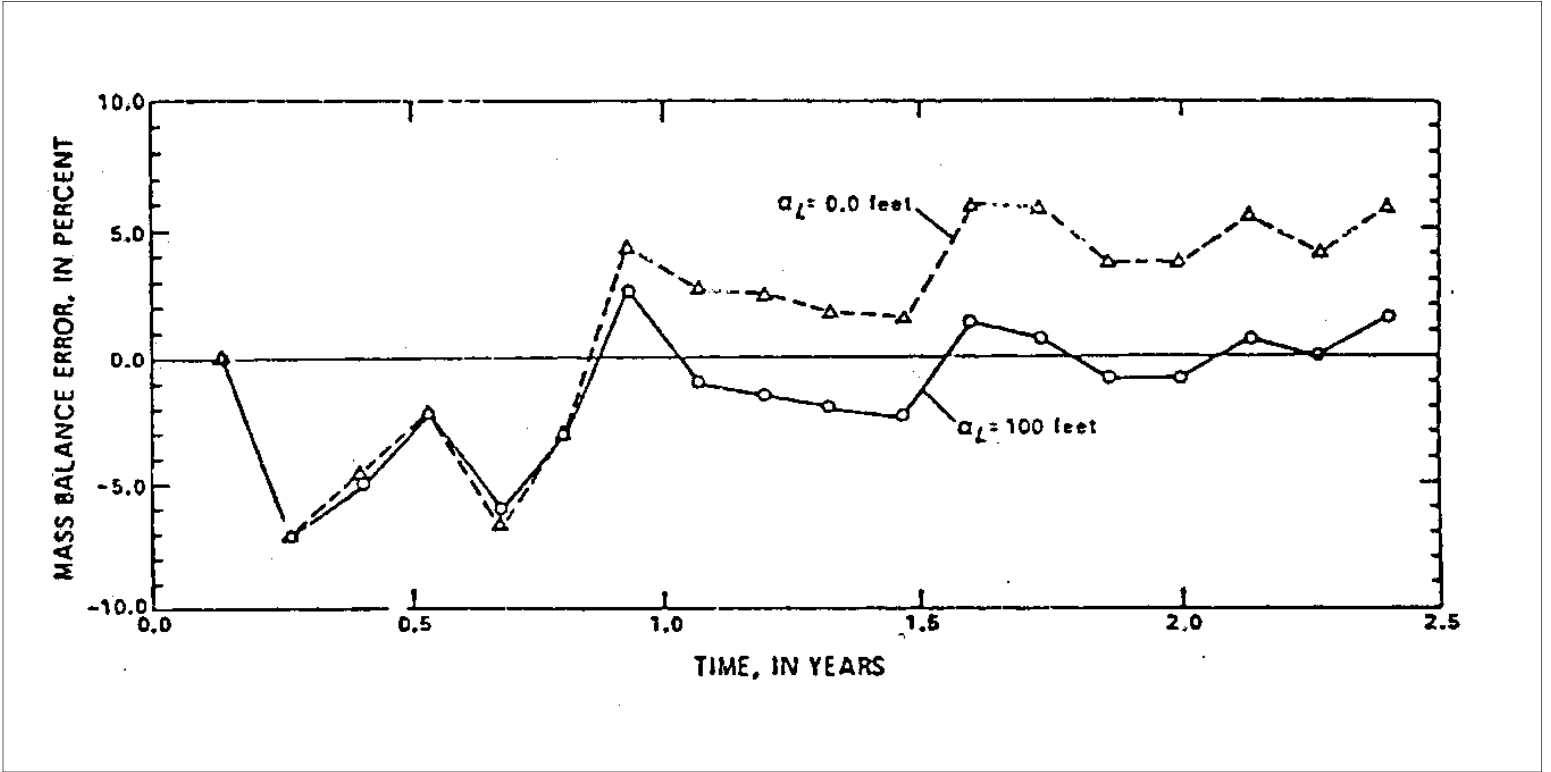
Figure A.7   Mass Balance Errors for the Effects of
Wells Mass Balance Problem
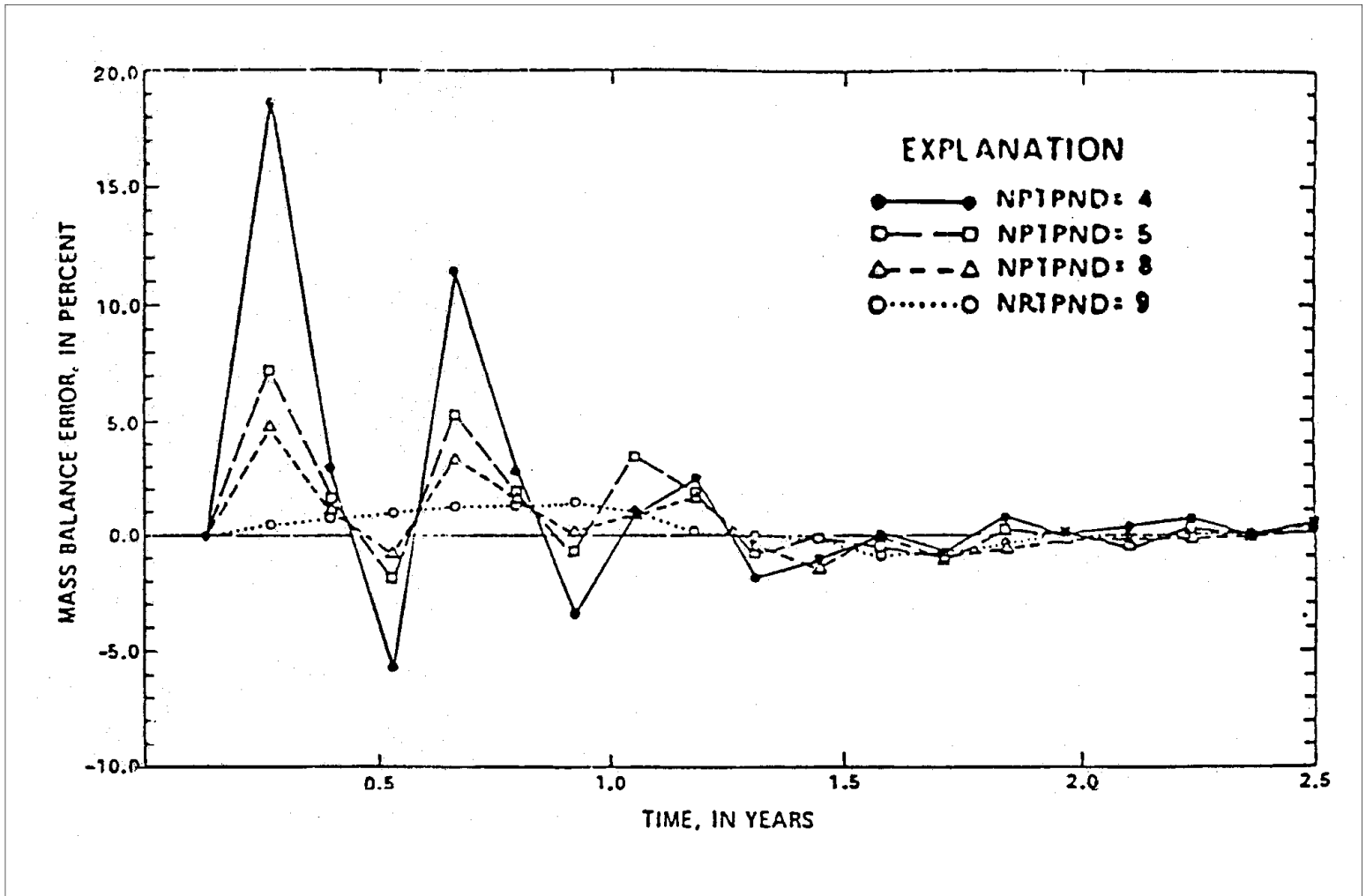
Figure A.8   Effect of Number of Particles
on Mass Balance Error
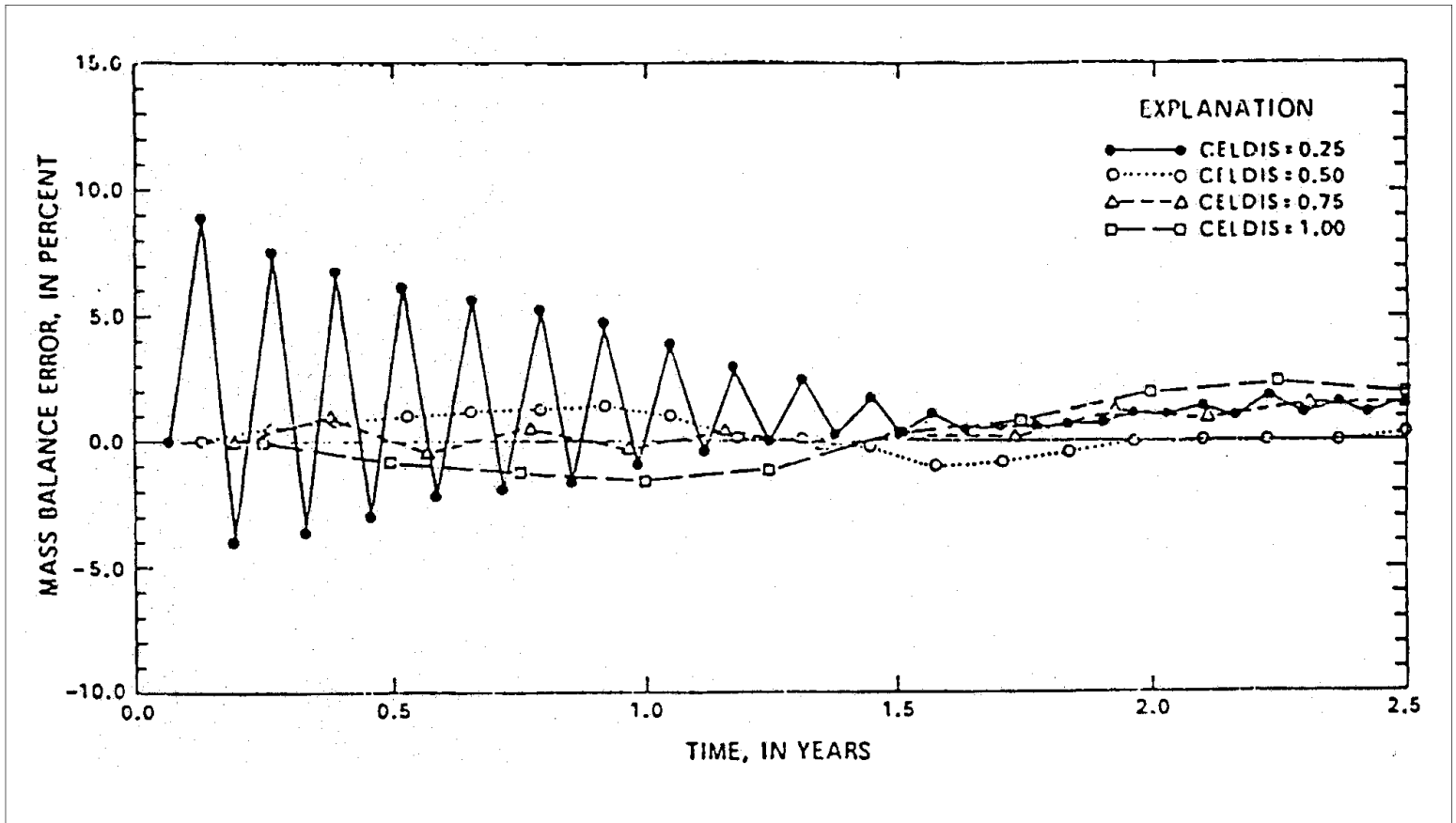
Source: Konikow and Bredehoeft, 1978

Figure A.9   Effect of Maximum Cell Distance
(CELDIS) on Mass Balance Errors

CELDIS from 0.5 to 0.25 caused the mass balance errors to oscillate for the first 1.5 years before the solution converged to a small error. Again, a smaller CELDIS caused longer runtimes.

The effects of NPTPND and CELDIS on the mass balance error are problem dependent. In problems where CELDIS is not the influencing stability criterion, varying CELDIS will not have an effect on mass balance errors. In general, it is recommended that the user specify 9 particles per cell (NPTPND = 9) and a CELDIS of 0.5 for model runs (initial model set-up or calibration runs can be developed using a smaller number of particles (4 or 5) and a higher number for CELDIS (0.75 or 1) as a first-cut).

A.8   References

Goode, D. J. and L. F. Konikow, Modification of a Method of Characteristics Solute Transport Model to Incorporate Decay and Equilibrium-Controlled Sorption or Ion Exchange, USGS, Water Resources Investigation Report 89-4030, Reston, Virginia, 1989.

Konikow, L. F. and J. D. Bredehoeft, Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water, Techniques of Water Resources Investigation of the United States Geological Survey, Book 7, Reston, Virginia, 1989.

APPENDIX B.   IMPLEMENTING THE AIR FORCE INTRINSIC REMEDIATION PROTOCOL USING THE GRAPHICAL PLATFORM

B.1   Context of the Remedial Investigation Using the Platform

Remediation and containment are the enabling technologies for the immediate control of the spread of contamination, and for the long-term management strategy, especially where natural degradation is allowed to play a constructive role. The mechanism for determining the overall best remediation strategy is by implementing comprehensive Remedial Investigation/ Feasibility studies. These two complementary investigations represent respectively, the diagnostic and the prognostic aspects of the remediation process. The Remedial Investigation (diagnosis) is conducted concurrently with the Feasibility Study (prognosis), and emphasizes data collection and site characterization. The data collected during the diagnostic phase of the study are used to evaluate the existing state of the site, and to support the analysis and decision-making activities of the feasibility study, including the formulation of remedial alternatives. Comprehensive geomedia rehabilitation must include both aspects of the solution.

The primary objective of an Intrinsic Remediation (IR) or Natural Attenuation investigation is to show that natural processes cause contaminant degradation and can reduce contaminant concentrations in groundwater to below regulatory standards before exposure pathways reach susceptible populations. This requires that the potential, extent, and concentration of the contaminant plume must be projected in time and space. This projection should be based on historic variations and the current extent of the contaminant plume as well as the measured rates of contaminant attenuation.

It is the responsibility of the proposer to provide sufficient evidence to demonstrate that a selected remediation mechanism will reduce contaminant concentrations to acceptable levels before potential receptors are reached. This requires the use of a model for both the diagnostic and prognostic phase of the remediation study, so that consideration be given to all possible contaminant migration scenarios. In what follows we give more details on how to implement Remedial Investigations and Feasibility Studies using the Graphical User Interface Platform in conjunction with BIOPLUME III.

Quantification of contaminant migration and attenuation rates and successful implementation of a remediation scheme require the following steps:

In the Diagnostic phase
1. Review existing data

2. Develop preliminary conceptual model for the site and assess potential impact of selected remediation [Enter hydrogeologic data in the Platform]

3. Perform site characterization in support of selected remediation [Use kriging results to enhance site boring location]

4. Refine conceptual model based on site characterization data [Calibrate flow and contaminant migration models in the Platform]

In the Prognostic phase
5. Model intinsic bioremediation scenarios using different features of the Platform.

6. Prepare long-term monitoring plan, and

7. Present findings to regulatiual agencies and obtain approval for the selected remediation   plan with long-term monitoring options.

These activities follow the recommendations of the "Technical Protocol for Implementing Intrinsic Remediation with Long-Term Monitoring for Natural Attenuation of Fuel Contamination Dissolved in Ground Water" by Todd H. Wiedemeier, John T. Wilson, Donald H. Kampbell, Ross N. Miller, and Jerry E. Hansen, AFCEE, 1995.

In the present document we elaborate on the implementation of the tasks described in the above referenced Protocol using the Platform. For ease of reference we adopt the same order as the Protocol. In fact, as shown in Figure B.1, the present document provides all the logical connections between the technical protocol on intrinsic remediation and the Graphical Platform.
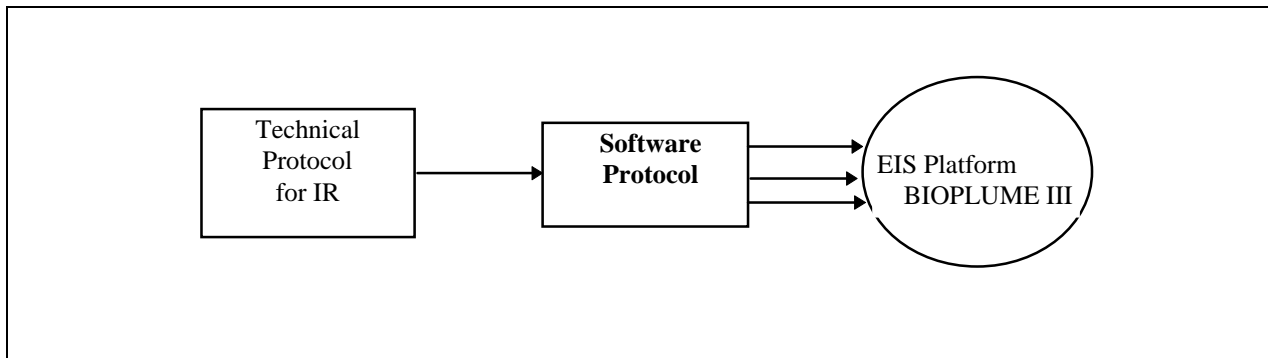
Figure B.1 Logical Connection Between Technical Protocol and the Platform.

B.1.1   Review Existing Site Data

The first step in the remediation investigation is to review existing site-specific data to determine if a selected procedure is a viable remedial option. Critical review of existing data also allows development of a preliminary conceptual model. The preliminary conceptual model is an essential tool for identifying any shortcomings in the data, and in developing a scientifically advantageous and cost-effective plan for additional data collection.

The information that must be obtained during data review includes the following categories:

Soil and ground water quality data:

- Firstly, the three-dimensional distribution of mobile and residual NAPL and dissolved-phase contaminants. The distribution of mobile and residual NAPL will be used to define the dissolved-phase plume source area.

- Ground water and soil geochemical data.

- Historic water quality data showing variations in contaminant concentrations through time.

- Chemical and physical characteristics of the contaminants.

- Potential for biodegradation of the contaminants.

Geologic and hydrogeologic data:

- Lithology and stratigraphy of the geologic medium.

- Grain-size distribution (percent sand, silt, and clay).

- Aquifer hydraulic conductivity.

- Ground water flow gradients and potentiometric or water table surface maps   (over several seasons, if possible).

- Preferential flow paths.

- Interactions between ground water and surface water and rates of infiltration/recharge.

Location of potential receptors:

- Groundwater well locations.

- Ground water discharge points downgradient of site.

If little or no site-specific data are available, then all future site characterization activities should also include collecting the data necessary to support the intrinsic remediation. Use of the Platform can greatly streamline this additional data collection activity which is otherwise necessary for a convincing and successful implementation of the remedial action.

B.1.2   Develop Preliminary Conceptual Model

The existing site characterization data are used to develop a conceptual geohydrologic model of the site and a preliminary assessment of the potential for alternative remediation schemes. The conceptual model is a word description of the three-dimensional representation of the ground water flow and contaminant migration system based on available geological, hydrological, climatological, and analytical data for the site. This type of conceptual model is more detailed than generic descriptions commonly used for risk analysis that consider the location of contaminant sources, transport pathways, exposure points, and receptors only qualitatively. The conceptual model is the most important step in properly developing a site contamination simulation model (diagnostic phase) which will be used to determine optimal placement of additional data collection points as necessary to aid in the remediation investigation.

The Platform offers an ideal framework to build this model in a graphical interactive environment that allows the user to visually inspect all his modeling choices. Figure B.2 shows a typical Platform screen with a background image which is used as a canvas on which to build the appropriate model data at the appropriate locations.

Practically all the site data described in Section B.1 can now be input into the model through the use of logpoints, wells and several dialog boxes. The Platform shadows the user's activity through all steps of the modeling process. Errors, when they occur, will be identified and corrected on the spot considerably reducing the time to validate the model.
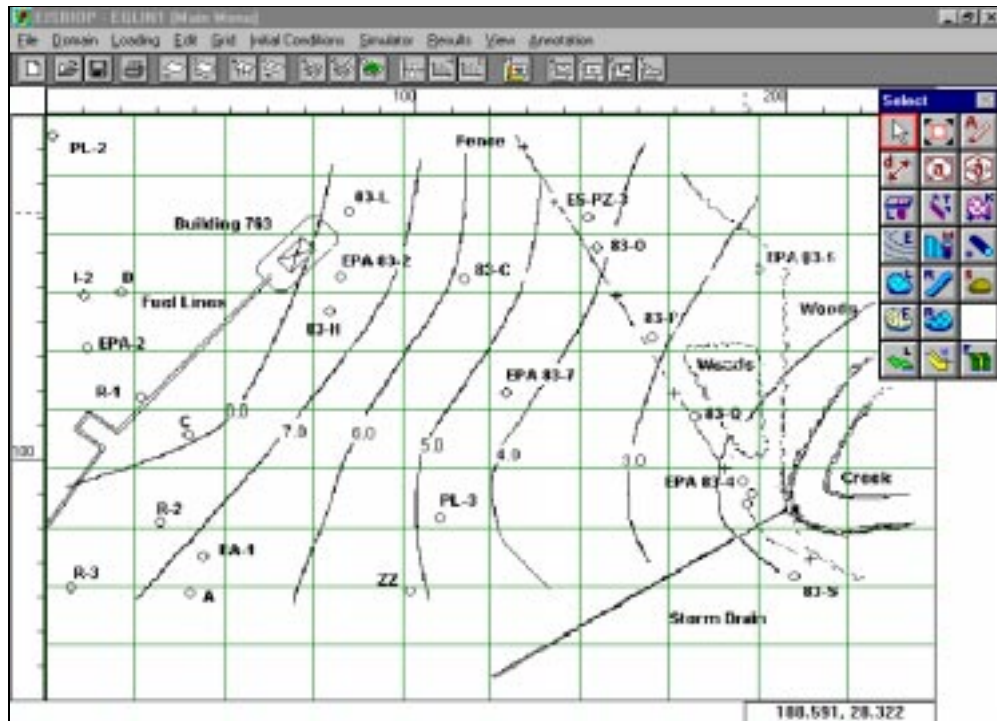

Figure B.2 General Configuration of the Platform.

Successful model development involves the following steps:

- Definition of the problem to be solved (usually the unknown nature and extent of existing and future contamination),

- Integration of all available data in the Platform including:

    - Local geologic and topographic maps,

    - Hydraulic data,

    - Site stratigraphy, and

    - Contaminant concentration and distribution data.

    - Conceptual model development, including extent of the site, boundary conditions, loading conditions, driving mechanisms, assimilative capacity.

- Determination of additional data requirements including:

    - Borehole locations and monitoring well spacing,

    - An approved sampling and analysis plan, and

    - Any data requirements that have not been adequately addressed.

The purpose for developing the conceptual model is to assess the potential for remediation. Existing data can be useful in determining if intrinsic remediation will be sufficient to prevent a dissolved-phase contaminant plume from completing exposure pathways, or from reaching a predetermined point of compliance, in concentrations above applicable regulatory standards. The goal of the remedial investigation is to determine the likelihood of pathway completion by estimating the migration and future extent of the plume based on geologic and contaminant properties, biodegradability, aquifer properties, head gradients, and the location of the plume and contaminant source relative to the potential receptor (i.e., the distance between the leading edge of the plume and the potential receptor).

If the contaminant plume is in its migration phase, then the remediation scheme should be based on containment and on contaminant reduction, and site characterization activities should be designed in support of this remedial option. On the other hand, if exposure pathways have already been completed and contaminants pose an unacceptable risk, then other remedial measures should be considered. However, even in the latter case attention should be given to use to the fullest extent the natural attenuation capacity of the site. In this case, containment of the plume may prevent the further migration of the plume along the exposure pathway while giving it time to self-destruct over the natural or enhanced biodegradation cycle. This combination of containment in favor of biodegradation and treatment of the receptor areas can help reduce the overall cost and duration of the remedial action.

The backbone to all these activities is again the Platform main screen (see Figure B.2), which provides all the necessary tools to build the conceptual model with the data collected during the site investigation.

B.2 Site Characterization in Support of Intrinsic Remediation

Detailed site characterization is necessary to document the potential for remediation at a site. As discussed in Section B.1, review of existing site characterization data is particularly useful before initiating site characterization activities. Such review allows identification of data gaps and in conjunction with the diagnostic model guide the most effective placement of additional data collection points, using the kriging (generalized covariance) scheme supported by the Platform.

The site characterization phase of the remediation investigation provides two important pieces of information about the site: whether natural mechanisms of contaminant attenuation are occurring at rates sufficient to protect human health and the environment; and sufficient site-specific data for diagnostic phase model development to allow prediction of the future extent and concentration of the contaminant plume. Site characterization in support of remediation should include at least the following set of parameters:

- Extent and type of soil and ground water contamination.

- Location and extent of contaminant source areas) (i.e., areas containing mobile or residual NAPL).

- The potential for a continuing source due to leaking tanks or pipelines.

- Ground water geochemical parameters.

- Regional hydrogeology, including:

    - Drinking water aquifers, and

    - Regional confining units.

- Local and site-specific hydrogeology, including:

    - Local drinking water aquifers.

    - Location of industrial, agricultural, and domestic water wells.

    - Patterns of aquifer use.

    - Lithology.

    - Site stratigraphy, including identification of transmissive and non-transmissive units.

    - Grain-size distribution (percent sand, silt, and clay).

    - Aquifer hydraulic conductivity.

    - Ground water hydraulic information.

- Preferential flow paths.

- Location and type of surface water bodies.

- Areas of local ground water recharge and discharge.

- Definition of potential exposure pathways and receptors.

The following sections describe technologies that can be used in collecting site characterization data.

B.2.1 Soil Characterization

In order to adequately define the subsurface hydrogeologic system and to determine the amount and three-dimensional distribution of dissolved hydrocarbons, mobile and residual NAPL and other dissolved organic contaminants that can act as a continuing source of ground water contamination, extensive soil characterization must be completed. Soil characterization is important in determining the source mechanism of a dissolved pollutant plume, but also for direct remedial action if the soil contamination is above soils standards.

Soil Sampling

The purpose of soil sampling is to determine the subsurface distribution of hydrostratigraphic units and the distribution of mobile contaminants. These objectives can be achieved through the use of conventional soil borings or cone penetrometer testing. All soil samples should be collected, described, and analyzed in accordance with EPA standard procedures. Figure B.3 illustrates a typical site investigation using a CPT rig. The data collected at the borehole of each CPT location can be sorted and directly input into the program using the logpoint control from the available toolbox.
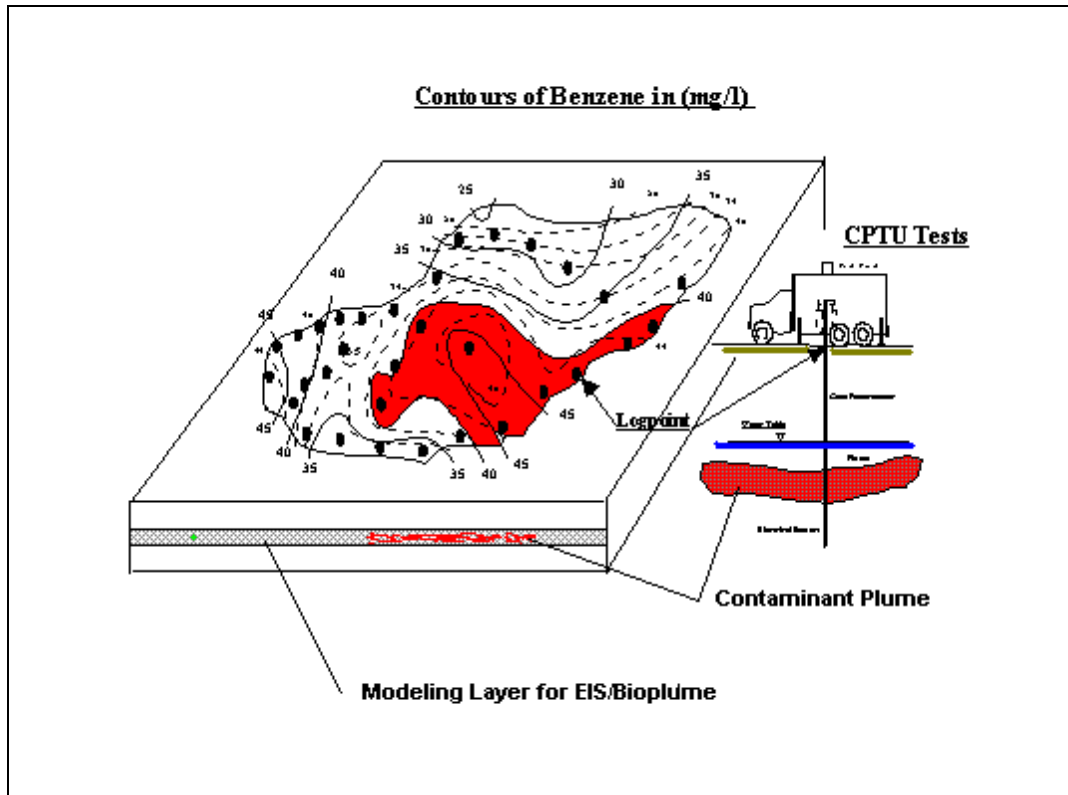
Figure B.3 Soil Sampling Using CPT Technology.

Soil Analytical Protocol

This analytical protocol includes all of the parameters necessary to document remediation of fuel hydrocarbons, including the effects of sorption and biodegradation (aerobic and anaerobic) of fuel hydrocarbons. Some analytes are given as a reference below. These data are usually collected at a logpoint and their distribution given at different depths as a profile. Figure B.4 shows a typical CPTU boring log. These raw data must be interpreted and sorted to determine the proper value that will be entered into the program. A usual approach is to identify the geologic strata where the contamination takes place and average the soil properties though the thickness of this strata as illustrated in Figure B.4.
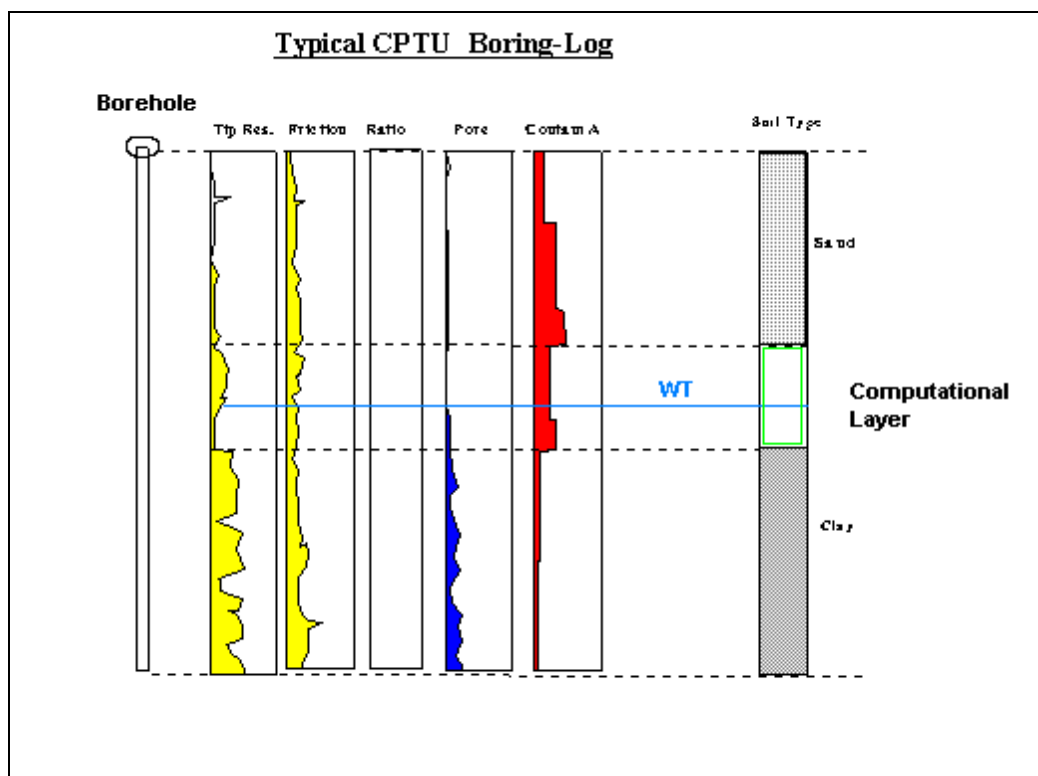
Figure B.4 Typical CPTU Boring Log.

Total Volatile and Extractable Hydrocarbons

Knowledge of the location, distribution, concentration, and total mass of TPH sorbed to soils or present as mobile NAPL is required to calculate contaminant partitioning from these phases into the dissolved phase. The presence or absence of TPH is also used to define the edge of the nonaqueous phase liquid (NAPL) plume. Knowledge of the location of the leading edge of the NAPL plume is important in properly setting up the BIOPLUME III model.

Aromatic Hydrocarbons

Knowledge of the location, distribution, concentration, and total mass of fuel-derived hydrocarbons of regulatory concern (especially BTEX) sorbed to soils or present as mobile NAPL is required to calculate contaminant partitioning from mobile and residual NAPL into the dissolved phase.

Total Organic Carbon

Knowledge of the total organic carbon (TOC) content of the aquifer matrix is important in sorption and solute-retardation calculations. TOC samples should be collected from a background location in the zones where most contaminant migration is expected to occur.

Dehydrogenase Activity

The dehydrogenase test is a qualitative method used to determine if aerobic bacteria are present in an aquifer in quantities capable of biodegrading fuel hydrocarbons. If the test gives a positive result, a sufficient number of microorganisms capable of aerobic metabolism and/or denitrification are present in the aquifer. If the test is negative, the number of aerobic microorganisms capable of aerobic metabolism is insufficient in the aquifer. However, the dehydrogenase test gives no indication of the relative abundance of anaerobic microorganisms capable of utilizing sulfate, iron III, or carbon dioxide for anaerobic biodegradation.

Grain Size Distribution

The grain size distribution of the aquifer matrix is an important indicator of hydraulic conductivity. In addition, clay minerals can be important sites for contaminant adsorption, especially when organic carbon comprises less than about 0.1 percent of the aquifer matrix. Because of this, knowledge of the relative abundance of clay minerals is important in sorption and solute retardation calculations.

Soil Gas Analysis

The concentrations of soil gas oxygen, carbon dioxide, and total combustible hydrocarbons are important in defining the extent of NAPL contamination. This information can be used to define the edge of the free-phase plume and to estimate the potential for natural biodegradation of vadose zone fuel residuals. Depleted oxygen levels and elevated carbon dioxide levels in soil gas are indicative of aerobic biodegradation of fuel hydrocarbons in the unsaturated zone, which may be enhanced if additional oxygen is provided through bioventing.

B.2.2   Ground Water Characterization

Sufficient information must be collected about the ground water system to adequately determine the amount and three-dimensional distribution of dissolved-phase contamination and to document its biochemical evolution. Ground water samples must be collected to show measurable changes in the chemistry of ground water in the affected area which is brought about by biodegradation. By measuring these changes, a case can be made for the presence of intrinsic remediation taking place at the site.

Ground Water Sampling

Ground water samples may be obtained from monitoring wells or point-source sampling devices such as the 'Geoprobe', 'Hydropunch', or the cone penetrometer. All ground water samples should be collected in accordance with EPA standards.

Ground Water Analytical Protocol

The analytical protocol must include all parameters necessary to document the remediation process. For intrinsic remediation of fuel hydrocarbons the analytical protocol should include the effects of sorption and aerobic and anaerobic biodegradation. Data obtained from the analysis of ground water for these analytes will be used to scientifically document intrinsic remediation of fuel hydrocarbons and to model the past behavior of the plume (diagnostic phase) and the long term prediction of its evolution (prognostic phase). The following sections describe the most prevailing ground water analytical parameters used in the Platform. Most of these data are usually entered as distributed or uniform parameters throughout the 2D modeling domain. Appropriate dialog boxes allow the user to input their values as shown in Figure B.5.

Figure B.5 Platform controls to input water quality data.

To enter the values of the measured contaminant, electron acceptors or byproducts, use the well control tool from the toolbox. This operation is presented in Figure B.6, where after properly locating the well in space you enter and input the physical parameters in an editing mode. To enter this editing mode you double click on the well and obtain the dialog box shown in Figure B.6. At this stage you enter or edit the time sequence of the in situ information and enter the values of the variable in the dialog box shown in Figure B.7. This figure shows a typical input stream of the measured oxygen at the site. The Oxygen value at time 0 constitutes the initial condition while the subsequent entries can be used as targets for the model calibration. Note that the Platform automatically distributes the logpoint information to the area covered by the simulation.
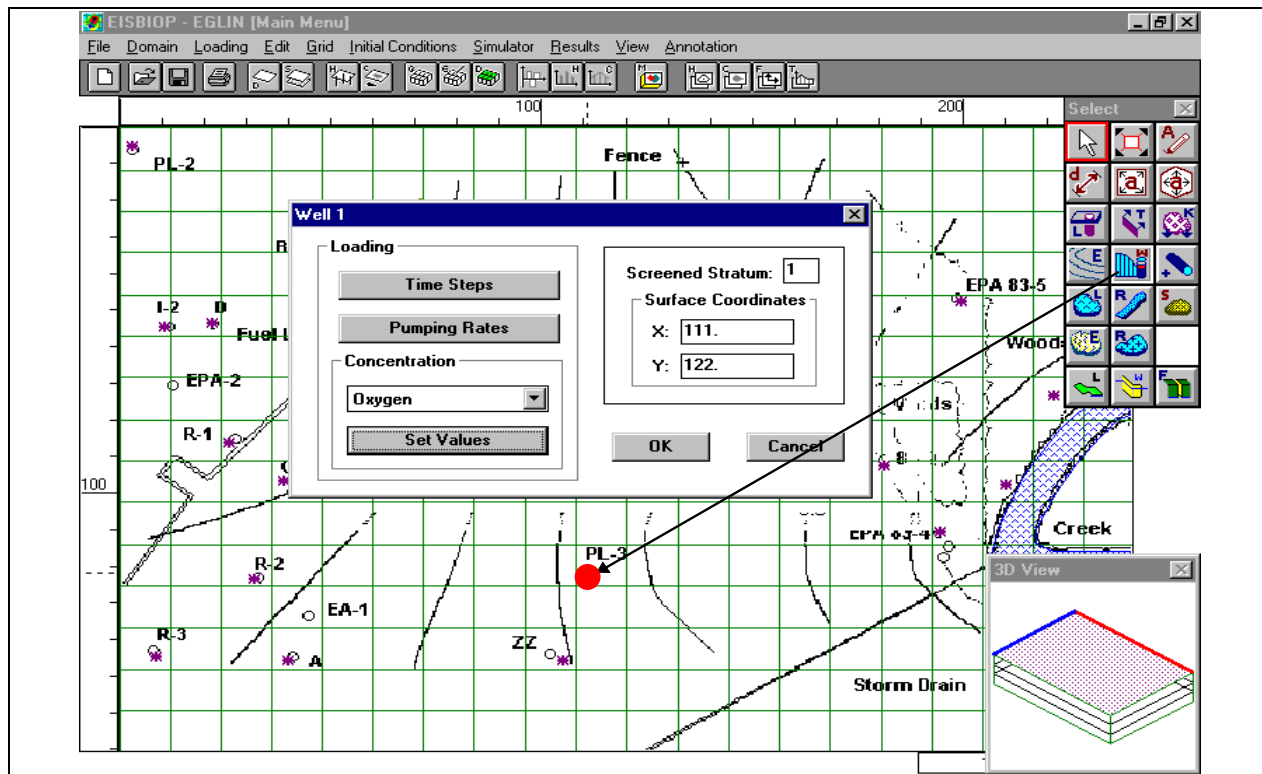
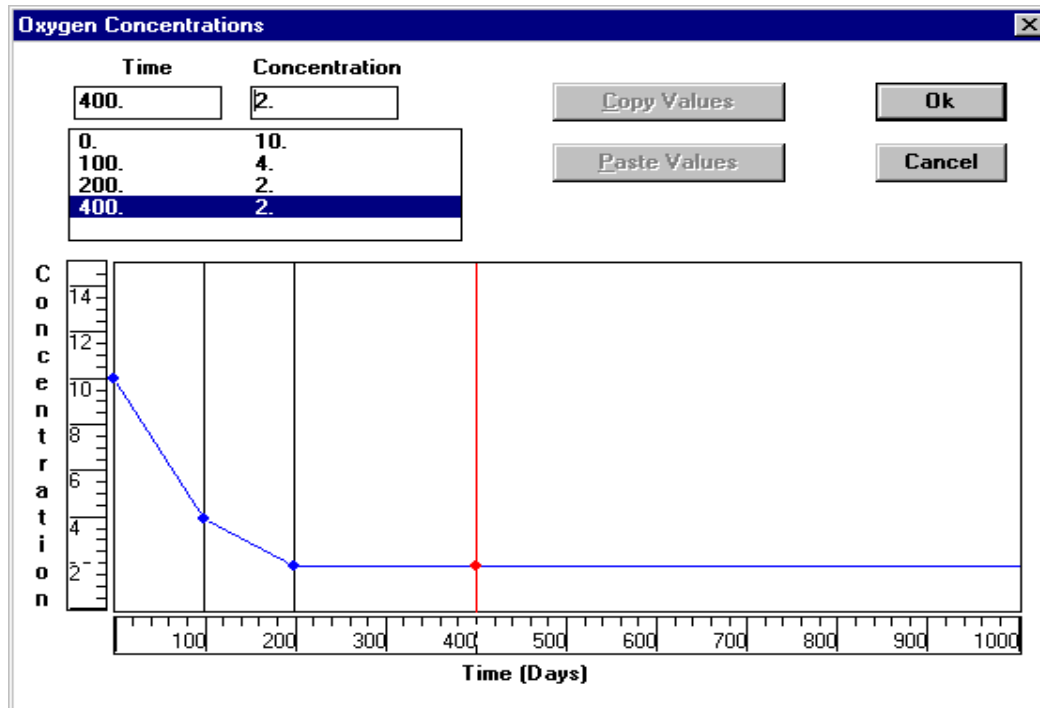Figure B.6 Entering Well Data in the Platform.

Figure B.7 Platform Input of in Situ Measured Oxygen.

The same input procedure is used for most of the components influencing intrinsic remediation described below.

Dissolved Oxygen

Dissolved oxygen is the most thermodynamically favored electron acceptor used in the biodegradation of fuel hydrocarbons. Dissolved oxygen concentrations are used to estimate the mass of contaminant that can be biodegraded by aerobic processes. As a rule, the stoichiometric ratio of dissolved oxygen consumed by microbes to destroyed BTEX compound is 1.0 mg/L of dissolved oxygen consumed to approximately 0.32 mg/L of BTEX compounds destroyed. During aerobic biodegradation, dissolved oxygen levels are reduced as aerobic respiration occurs. Also, anaerobic bacteria (obligate anaerobes) generally cannot function at dissolved oxygen levels greater than about 0.5 mg/L. Therefore, higher values of dissolved oxygen indicate that aerobic biodegradation is likely at work.

Dissolved oxygen measurements should be taken during well purging and immediately before and after sample acquisition using a direct-reading meter. Because most well purging techniques can allow aeration of collected ground water samples, it is important to minimize potential aeration.

Oxidation/Reduction Potential (E_H)

The oxidation/reduction (redox) potential of ground water (EH) is a measure of electron activity and is an indicator of the relative tendency of a solution to accept or transfer electrons. Redox reactions in ground water are usually biologically mediated and therefore, the redox potential of a ground water system depends upon and influences rates of biodegradation. Knowledge of the redox potential of ground water is also important because some biological processes only operate within a prescribed range of redox conditions. Knowledge of the redox potential of ground water can be used as an indicator of certain geochemical activities such as sulfate reduction. The redox potential of ground water generally ranges from -400 millivolts (mV) to 800 mV.

Redox potential can be used to provide real time data on the location of the contaminant plume, especially in areas undergoing anaerobic biodegradation. Mapping the redox potential of the ground water while in the field allows the field scientist to determine the approximate location of the contaminant plume. To map the redox potential of the ground water while in the field it is important to have at least one redox measurement (preferably more) from a well located upgradient of the plume. The redox potential of a ground water sample taken inside the contaminant plume should be somewhat lower than that taken in the upgradient location. Redox potential measurements should be taken during well purging and immediately before and after sample acquisition using a direct-reading meter. Because most well purging techniques can allow aeration of collected ground water samples (which can affect redox potential measurements), it is important to minimize potential aeration.

pH, Temperature, and Conductivity

Because the pH, temperature, and electric conductivity of a ground water sample can change significantly within a short time following sample acquisition, these parameters must be measured in the field in unfiltered, unpreserved, "fresh" water collected by the same technique as the samples taken for laboratory analyses. The measurements should be made in a clean glass container separate from those intended for laboratory analysis and the measured values should be recorded in the ground water sampling record.

The pH of ground water has an effect on the presence and activity of microbial populations in ground water. This is especially true for methanogens which may be active after all aerobic, sulfate reduction, and nitrate reduction degradation has taken place. Microbes capable of degrading petroleum hydrocarbon compounds generally prefer pH values varying from 6 to 8 standard units.

Electric conductivity is a measure of the ability of a solution to conduct electricity. For ground water, conductivity is directly related to the concentration of ions in solution, increasing as ion concentration increases. Like chloride, conductivity is used to ensure that ground water samples collected at a site are representative of the water comprising the saturated zone in which the dissolved-phase contamination is present. If the conductivities of samples taken from different sampling points are radically different, then the waters may be from different hydrogeologic zones.

Ground water temperature directly affects the solubility of oxygen and other geochemical species. The solubility of dissolved oxygen is temperature dependent, being more soluble in cold water than in warm water. Ground water temperature also affects the metabolic activity of bacteria. Rates of hydrocarbon biodegradation roughly double for every 10° C increase in temperature ("Q"$_{10}$ rule) over the temperature range between 5° and 25° C. Ground water temperatures less than about 5° C tend to inhibit biodegradation, and slow rates of biodegradation are generally observed in such waters.

Alkalinity

The total alkalinity of a ground water system is indicative of a water's capacity to neutralize acid. Alkalinity is defined as the net concentration of strong base in excess of strong acid with a pure CO_2-water system as the point of reference (Domenico and Schwartz, 1990). Alkalinity results from the presence of hydroxides, carbonates, and bicarbonates of elements such as calcium, magnesium, sodium, potassium, or ammonia. These species result from the dissolution of rock (especially carbonate rocks), the transfer of CO_2 from the atmosphere, and respiration of microorganisms. Alkalinity is important in the maintenance of ground water pH because it buffers the ground water system against acids generated through both aerobic and anaerobic biodegradation processes.

Nitrate

In the hierarchical order of processes occurring in the microbiological treatment zone, after dissolved oxygen has been depleted, nitrate may be used as an electron acceptor for anaerobic biodegradation. Nitrate concentrations are used to estimate the mass of contaminant that can be biodegraded by denitrification processes. By knowing the volume of contaminated ground water, the background nitrate concentration, and the concentration of nitrate measured in the contaminated area, it is possible to estimate the mass of BTEX lost to biodegradation. Stoichiometrically, each 1.0 mg/L of ionic nitrate consumed by microbes results in the destruction of approximately 0.21 mg/L of BTEX compounds. Nitrate concentrations are a direct input parameter to the Platform.

Sulfate and Sulfide Sulfur

After dissolved oxygen and nitrate have been depleted in the microbiological treatment zone, sulfate may be used as an electron acceptor for anaerobic biodegradation. This process is termed sulfanogenesis and results in the production of sulfide. Sulfate concentrations are used as an indicator of anaerobic degradation of fuel compounds. By knowing the volume of contaminated ground water, the background sulfate concentration, and the concentration of sulfate measured in the contaminated area, it is possible to estimate the mass of BTEX lost to biodegradation through sulfate reduction. Stoichiometrically, each 1.0 mg/L of sulfate consumed by microbes results in the destruction of approximately 0.21 mg/L of BTEX. Sulfate concentrations are a direct input parameter for the Platform.

Ferrous Iron

Ferric iron is also used as an electron acceptor during anaerobic biodegradation of petroleum hydrocarbons after nitrate or sulfate depletion, or some times in conjunction with them. During this process, ferric iron is reduced to the ferrous form which may be soluble in water. Ferrous iron concentrations are used as an indicator of anaerobic degradation of fuel compounds. By knowing the volume of contaminated ground water, the background ferrous iron concentration, and the concentration of ferrous iron measured in the contaminated area, it is possible to estimate the mass of BTEX lost to biodegradation through ferric iron reduction. Stoichiometrically, the degradation of 1 mg/L of BTEX results in the production of approximately 21.8 mg/L of ferrous iron during ferric iron reduction. Iron concentrations are used as a direct input parameter to the Platform. The equivalent amount of Ferric Iron is estimated from the measured Ferrous Iron, which is used as model input. BIOPLUME III simulates the hydrocarbon reduction and the corresponding Ferric Iron depletion.

Carbon Dioxide

Metabolic processes operating during biodegradation of fuel hydrocarbons result in the production of carbon dioxide (CO_2). Accurate measurement of CO_2 produced during biodegradation is difficult because carbonate in ground water (measured as alkalinity) serves as both a source and sink for free CO_2. If the CO_2 produced during metabolism is not removed by

the natural carbonate buffering system of the aquifer, CO_2 levels higher than background may be observed. Comparison of empirical data to stoichiometric calculations can provide estimates of the degree of microbiological activity and the occurrence of in situ mineralization of contaminants.

Methane

During methanogenesis (an anaerobic biodegradation process), carbon dioxide (or acetate) is used as an electron acceptor, and methane is produced. Methanogenesis generally occurs after oxygen, nitrate, and sulfate have been depleted in the treatment zone. The presence of methane in ground water is indicative of strongly reducing conditions. Because methane is not present in fuel, the presence of methane in ground water above background concentrations in contact with fuels is indicative of microbial degradation of fuel hydrocarbons. Methane concentrations can be used to estimate the amount of BTEX destroyed in an aquifer. By knowing the volume of contaminated ground water, the background methane concentration, and the concentration of methane measured in the contaminated area, it is possible to estimate the mass of BTEX lost to biodegradation through methanogenesis reduction. The degradation of 1 mg/L of BTEX results in the production of approximately 0.78 mg/L of methane during methanogenesis. **Methane concentrations are used as an indirect input parameter to the Platform. The equivalent amount of CO_2 is estimated from the measured methane, which is used as model input. BIOPLUME III simulates the hydrocarbon reduction and the corresponding CO_2 depletion**.

Chloride

Chloride is used to ensure that ground water samples collected at a site are representative of the water comprising the saturated zone in which the dissolved-phase contamination is present (i.e. to ensure that all samples are from the same ground water flow system). If the chloride concentrations of samples taken from different sampling points are radically different, then the waters may be from different hydrogeologic zones.

Total Petroleum Hydrocarbons and Aromatic Hydrocarbons

These analytes are used to determine the type, concentration, and distribution of fuel hydrocarbon in the aquifer. Of the compounds present in most gasolines and jet fuels, the BTEX compounds generally represent the regulatory contaminants of concern. For this reason, these compounds are generally of significant interest in the fate and transport analysis. At a minimum, the aromatic hydrocarbon analysis (Method SW8020) must include the BTEX compounds and the trimethylbenzene and tetramethylbenzene isomers. The combined dissolved-phase concentrations of BTEX, trimethylbenzene, and tetramethylbenzene should not be greater than about 30 mg/L for a JP4 spill. If these compounds are found in concentrations greater than 30 mg/L then sampling errors such as emulsification of NAPL in the ground water sample have likely occurred and should be investigated.

B.2.3   Aquifer Parameter Estimation

Hydraulic Conductivity

Hydraulic conductivity is a measure of an aquifer's ability to transmit water and is perhaps the most important aquifer parameter governing fluid flow in the subsurface. The velocity of ground water and dissolved-phase contamination is directly related to the hydraulic conductivity of the saturated zone. In addition, subsurface variations in hydraulic conductivity directly influence contaminant fate and transport by providing preferential paths for contaminant migration. Estimates of hydraulic conductivity are used to determine residence times for contaminants and tracers and to determine the seepage velocity of ground water.

The most common methods used to measure hydraulic conductivity in the subsurface are aquifer pumping tests and slug tests. One drawback to these methods is that they average hydraulic properties over the screened interval of the well. To help alleviate this potential problem, the screened interval of the well should be selected after consideration is given to subsurface stratigraphy. Information about subsurface stratigraphy should come from geologic boring logs completed on continuous cores. An alternate method to delineate zones with high hydraulic conductivity is to use pressure dissipation data from CPT logs.

Pumping Tests

Pumping tests generally give the most reliable information on hydraulic conductivity but are difficult to conduct in contaminated areas because the water produced during the test generally must be contained and treated. In addition, a minimum 4-inch-diameter well is generally required to complete pumping tests in highly transmissive aquifers because the 2-inch submersible pumps available today are not capable of producing a flow rate large enough for meaningful pumping tests.   In areas with fairly uniform aquifer materials, pumping tests can be completed in uncontaminated areas and the results used to estimate hydraulic conductivity in the contaminated area. Pumping tests should be conducted in narrowly screened wells that are screened in the most transmissive zones in the aquifer.

Slug Tests

Slug tests are a commonly used alternative to pumping tests. They are relatively easy to conduct and, in general, produce reliable information. One commonly cited drawback to slug testing is that this method generally gives hydraulic conductivity information only for the area immediately surrounding the monitoring well. Slug tests do, however, have two distinct advantages over pumping tests; they can be conducted in 2-inch monitoring wells, and they produce no water. If slug tests are going to be relied upon to provide information on the three-dimensional distribution of hydraulic conductivity in an aquifer, multiple slug tests must be performed. It is not advisable to rely on data from one slug test in one monitoring well. Because of this, slug tests should be

conducted at several monitoring wells at the site. Like pumping tests, slug tests should be conducted in wells that are narrowly screened in the most transmissive zones in the aquifer.

Hydraulic Gradient

The hydraulic gradient is the change in hydraulic head between two points over the distance between these points. Hydraulic gradients are most easily visualized if all known (measured) heads are portrayed on a contoured map. This is done automatically with the Platform using one of the kriging options. A static representation of the hydraulic head map is not sufficient because seasonal variations in ground water flow direction can have a profound influence on contaminant transport. Sites in upland areas are less likely to be affected by seasonal variations in ground water flow direction than those sites situated near surface water bodies such as rivers and lakes. In situ measured gradients are the most commonly used variables for the calibration of the groundwater flow model (advective part of the contaminant migration problem).

To determine the effect of seasonal variations in ground water flow direction on contaminant migration, quarterly ground water level measurements should be taken over a period of at least 1 year. For many sites, historic data to that effect already exist.

Processes Causing an Apparent Reduction in Total Contaminant Mass

Several processes cause a reduction in contaminant concentrations and an apparent reduction in the total mass of contaminant in a system. Processes causing an apparent reduction in contaminant mass include dilution, sorption, and hydrodynamic dispersion. In order to determine the mass of contaminant removed from the system it is necessary to correct observed concentrations for the effects of these processes. The following sections give a brief overview of these processes and their evaluation with the Platform.

To estimate the degree of biodegradation, it is important to adjust measured BTEX concentrations for those processes that cause a concentration reduction without reduction in contaminant mass. This is accomplished by normalizing the measured concentration of each of the BTEX compounds to the concentration of a tracer that is at least as sorptive as the BTEX compounds, but which is biologically inactive. Two trace chemicals found in fuel hydrocarbon plumes are trimethylbenzene and tetramethylbenzene (Cozzarelli *et al., 1994*). *This aspect of the data collection is very important for the calibration phase of the* BIOPLUME III model. These parameters are considered as constant parameters throughout the duration of the simulation. Dialog boxes allow to enter their appropriate values.

Dilution

Dilution results in a reduction in contaminant concentrations. It can be caused by the improper vertical extent of the screened interval of the monitoring wells, or by infiltration which causes an apparent reduction in contaminant mass by mixing with the contaminant plume, thereby causing dilution. Monitoring wells screened over large vertical distances may dilute ground water

samples by mixing water from clean aquifer zones with contaminated water during sampling. This problem is especially relevant for dissolved-phase BTEX contamination which may remain near the ground water table for some distance downgradient of the source. To avoid potential dilution, monitoring wells should be screened over relatively short vertical intervals (less than 5 feet), and nested wells should be used to define the vertical extent of contamination in the saturated zone.

Sorption (Retardation)

The retardation of organic solutes caused by sorption is an important consideration when modeling intrinsic remediation. Sorption of a contaminant to the aquifer matrix results in an apparent decrease in contaminant mass that must be accounted for. Dissolved oxygen and other electron acceptors present in the ground water travel at the advective transport velocity of the ground water. Any slowing of the solute relative to the advective transport velocity of the ground water allows replenishment of electron acceptors into upgradient areas of the plume. Sorption and retardation are explicitly taken into account in the Platform (menu "Domain/Chemical Properties").

Hydrodynamic Dispersion

Dispersion is the expansion of a plume in the apparent absence of ground water flow (due to subgrid scale movement, from subgrid scale to Brownian motion). For intrinsic bioremediation the dispersion of organic solutes in an aquifer is an important consideration because the dispersion of a contaminant into uncontaminated portions of the aquifer allows the solute plume to mix with uncontaminated ground water containing higher concentrations of electron acceptors.

B.2.4   Optional Confirmation of Biologic Activity

Extensive evidence showing that biodegradation of fuel hydrocarbons frequently occurs under natural conditions can be found in the literature. The following sections describe two techniques that may be used to show that microorganisms capable of degrading fuel hydrocarbons are present at a given site.

Field Dehydrogenase Test

The field dehydrogenase test is a qualitative method used to determine if aerobic bacteria are present in an aquifer in quantities capable of biodegrading fuel hydrocarbons. Positive results indicate that a sufficient number of microorganisms capable of aerobic metabolism and/or denitrification are present in the aquifer. However, a negative result for the dehydrogenase test gives no indication of the relative abundance of anaerobic microorganisms capable of utilizing sulfate, iron III, or carbon dioxide during biodegradation.

Microcosm Studies

Microcosm studies are necessary only when there is considerable skepticism about the biodegradation of fuel hydrocarbons at a specific site. If more evidence of intrinsic remediation of fuel hydrocarbons is required, then a microcosm study using site-specific aquifer materials and contaminants can be undertaken. Microcosm studies conducted using aquifer materials collected in a contaminated area at a site can be used to show that the microorganisms necessary for biodegradation are present and can be used as a good line of evidence to support the intrinsic remediation demonstration. Microcosm studies also provide site-specific estimates of biodegradation rate constants that can be used to verify rates of biodegradation measured in the field. It should be kept in mind, however, that the preferable method of fuel hydrocarbon biodegradation rate constant determination is by in situ field measurement. The collection of material for the microcosm study, the procedures used to set up and analyze the microcosm study, and the interpretation of the results of the microcosm study, must follow EPA standards.

B.3 Refining the Conceptual Model

The additional site investigation data must first be used to refine the conceptual model. This refinement is facilitated by estimation of the rate of ground water flow, and the rates of dispersion, sorption, dilution, and biodegradation. The results of these calculations are then used to scientifically document the occurrence and the rates of natural biodegradation and to help model intrinsic remediation. No single piece of data is sufficient to successfully support the intrinsic remediation option at a given site. Because the burden of proof is on the proponent, all available data must be integrated in such a way that the evidence in support of intrinsic remediation is sufficient and irrefutable.

Conceptual model refinement involves integrating newly gathered field data to the preliminary conceptual model that was developed based on previously existing site-specific data. This involves integrating into the Platform the newly obtained data to develop an accurate three-dimensional representation of the hydrogeologic and contaminant migration system. Conceptual model refinement consists of several steps including boring log preparation, hydrogeologic section preparation, potentiometric surface map preparation, contaminant contour map preparation, and preparation of electron acceptor and metabolic byproduct contour maps.

Geologic Boring Logs

Geologic boring logs are entered in the Platform for all subsurface materials encountered during the soil boring or cone penetrometer testing (CPT) phase of the field work. Description of the aquifer matrix includes relative density, color, major textural constituents, minor constituents, porosity, relative moisture content, plasticity of fines, cohesiveness, grain size distribution, structure or stratification, relative permeability, and any other significant observations such as visible fuel or fuel odor. It is also important to correlate the results of volatiles screening using headspace vapor analysis with depth intervals of geologic materials. The depth of lithologic contacts and/or significant textural changes should be recorded to the nearest 0.1 foot. This resolution is necessary because preferential flow and contaminant migration paths may be limited to stratigraphic units as thin as a few inches.

Cone Penetrometer Data

Cone penetrometer logs data come in the form of the ratio of sleeve friction to tip pressure. Cone penetrometer logs may also contain fluid resistivity data and estimates of aquifer hydraulic conductivity. To provide meaningful data, the cone penetrometer must be capable of providing stratigraphic resolution on the order of 3 inches. To provide accurate stratigraphic information, cone penetrometer logs must be correlated with continuous subsurface cores. Cone penetrometer logs are a cost effective means of completing the hydrogeologic section information initially based on cores.

B.3.1   Hydrogeologic Sections

Hydrogeologic sections are entered in the Platform based on boring logs or CPT data. A minimum of two hydrogeologic sections are required, one parallel to the direction of ground water flow and one perpendicular to the direction of ground water flow. Hydraulic head data including potentiometric surface and/or water table elevation data are automatically generated by the Platform. These sections are useful in locating potential preferential contaminant migration paths and in modeling the site using the simulation models of the program.

B.3.2   Potentiometric Surface or Water Table Maps

A potentiometric surface or water table map is a two-dimensional graphic representation of equipotential lines shown in plan view. These maps are generated automatically by the Platform based on water level measurements and surveyor's data. Because ground water flows from areas of high hydraulic head to areas of low hydraulic head, such maps are used to estimate the probable direction of plume migration and to calculate hydraulic gradients. Care must be exercised to use water levels measured in wells screened in the same relative position within the same hydrogeologic unit. To document seasonal variations in ground water flow, separate potentiometric surface or water table maps should be prepared for quarterly water level measurements taken over a period of at least one year. In areas with mobile NAPL, a correction must be made for the water table deflection caused by the NAPL. Typical contours of the hydraulic heads are shown in Figure B.8 as they appear on the computer screen.
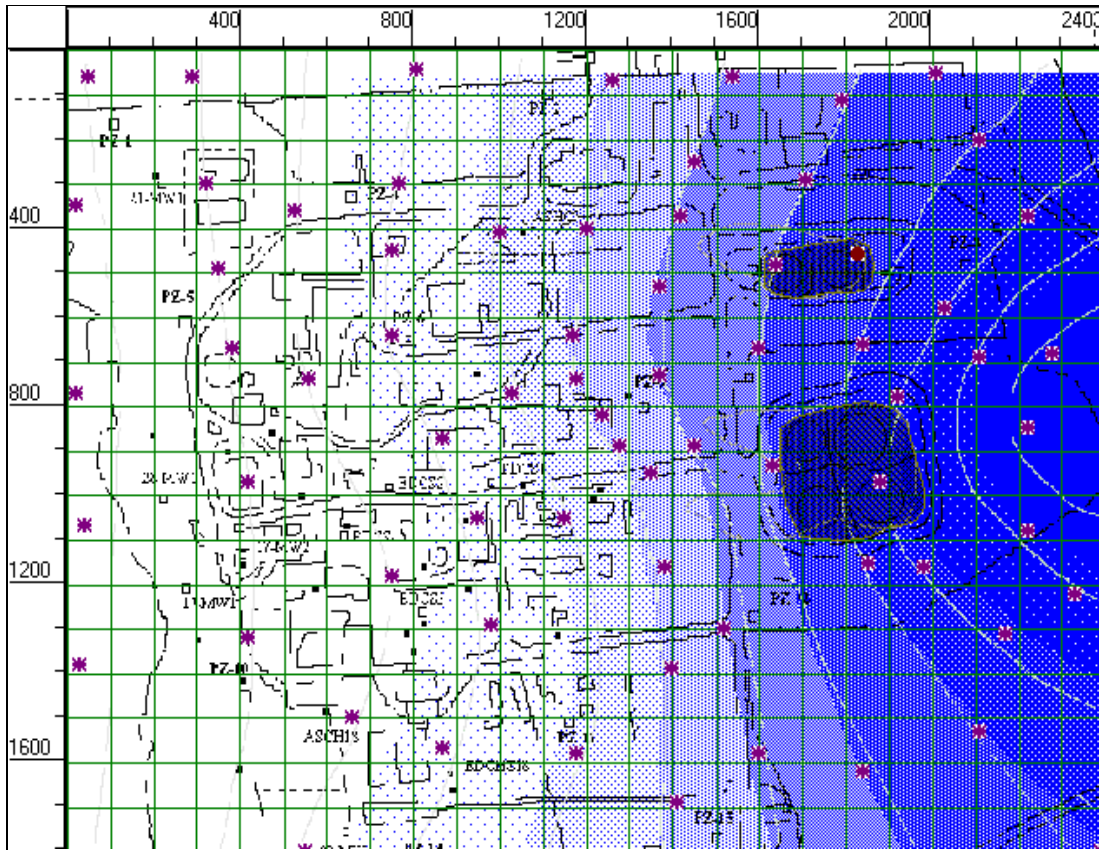
Figure B.8 Contours of Hydraulic Heads.

B.3.3   Contaminant Concentration Contour Maps

Contaminant concentration contour maps are also automatically prepared for each of the BTEX compounds present and for total BTEX. Such maps allow interpretation of data on the distribution and the relative transport and degradation rates of contaminants in the subsurface.

If mobile and residual NAPL are present at the site, a contour map showing the thickness and distribution of each phase should also be determined. These maps allow interpretation of the distribution and the relative migration rate of NAPL in the subsurface. In addition, these maps help in partitioning calculations and numerical model development. It is important to note that because of the differences between the magnitude of capillary suction in the aquifer matrix and the different surface tension properties of fuel and water, NAPL thickness observations made at monitoring points may not provide an accurate estimate of the actual volume of mobile and residual NAPL in the aquifer. To accurately determine the distribution of NAPLs, it is necessary to take continuous soil cores.

B.3.4   Electron Acceptor and Metabolic Byproduct Contour Maps

Contour maps should be prepared for electron acceptors consumed (dissolved oxygen, nitrate, and sulfate) and metabolic byproducts produced (iron II, sulfide, and methane) during

biodegradation. The electron acceptor and metabolic byproduct contour maps provide evidence of the occurrence of intrinsic remediation at a site.

Electron Acceptor Contour Maps

Contour maps are needed for the electron acceptors including dissolved oxygen, nitrate, and sulfate. During aerobic biodegradation, dissolved oxygen concentrations will decrease to levels below background. Similarly, during anaerobic degradation, the concentrations of nitrate and sulfate will be seen to decrease to levels below background. The electron acceptor contour maps allow interpretation of data on the relative migration and degradation rates of contaminants in the subsurface. The Platform allows direct input of all these parameters. Thus, electron acceptor contour maps provide visible evidence of biodegradation and a visual indication of the relationship between the contaminant plume and the various electron acceptors.

Metabolic Byproduct Contour Maps

Contour maps should be prepared for the metabolic byproducts iron II, sulfide, and methane. During anaerobic degradation, the concentrations of iron II, sulfide, and methane are seen to increase to levels above background concentrations. These maps allow interpretation of data on the microbial degradation of fuel hydrocarbons and the relative migration and degradation rates of contaminants in the subsurface. Thus, metabolic byproduct contour maps provide visible evidence of biodegradation and a visual indication of the relationship between the contaminant plume and the various metabolic byproducts.

Typical contour maps of BTEX, electron acceptors and by-products as generated by the Platform are shown below:

- Figure B.9 shows a typical BTEX contour map

- Figure B.10 shows the measured Oxygen plume

- Figure B.11 shows the measured Nitrate plume

- Figure B.12 shows the measured Sulfate plume

- Figure B.13 shows the measured Methane plume

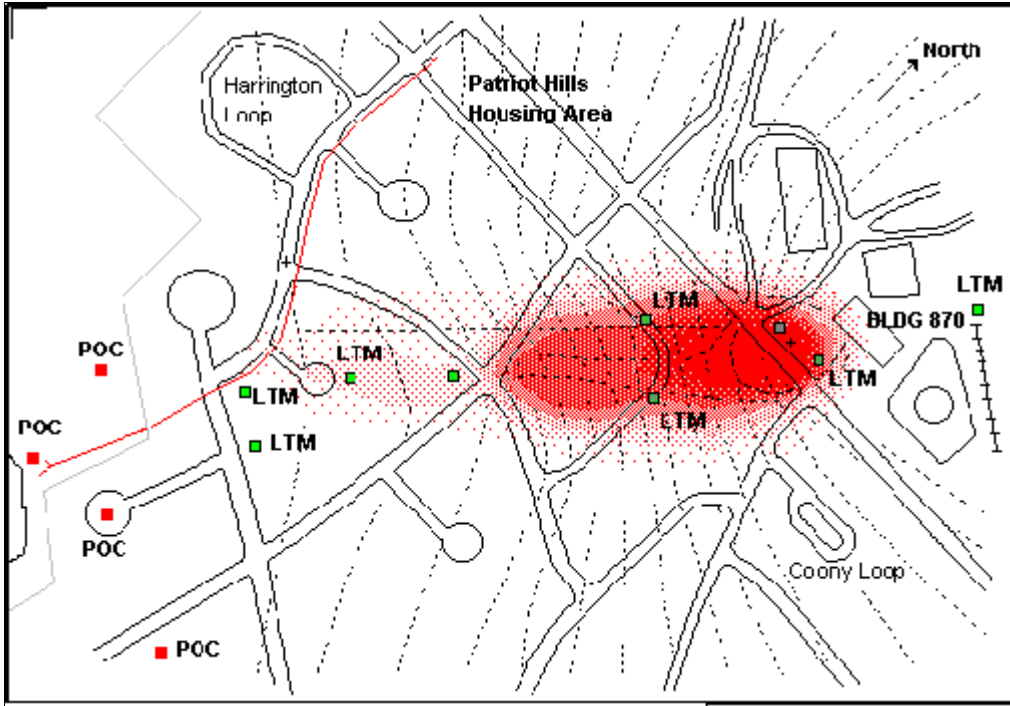- Figure B.14 shows the measured Ferrous Iron plume.
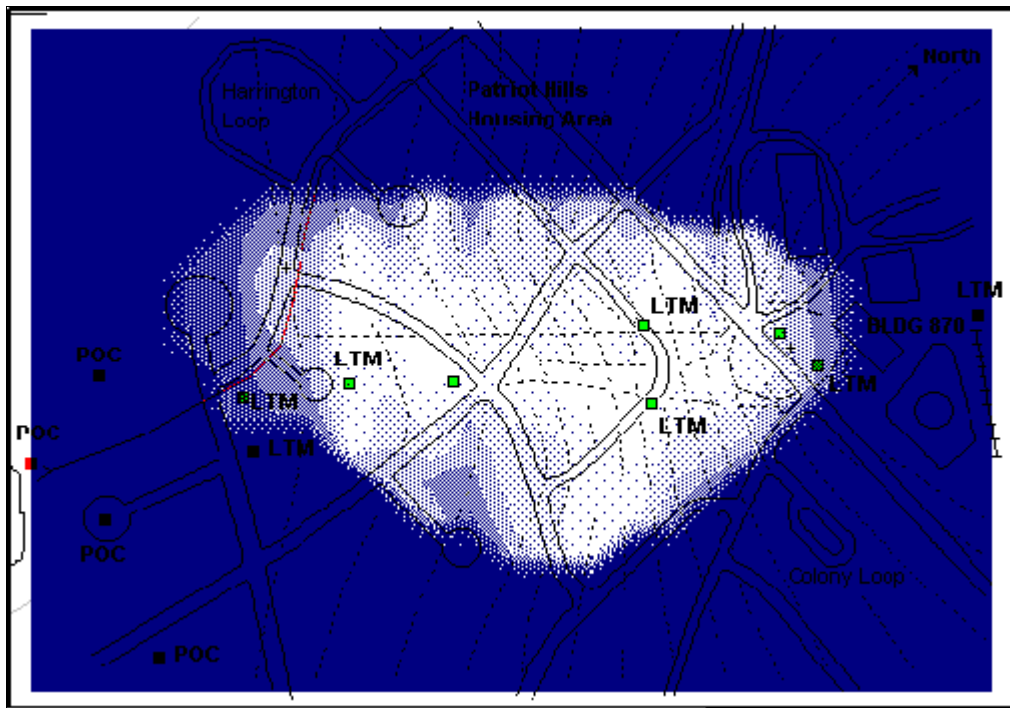
Figure B.9 Typical BTEX Contour Map.
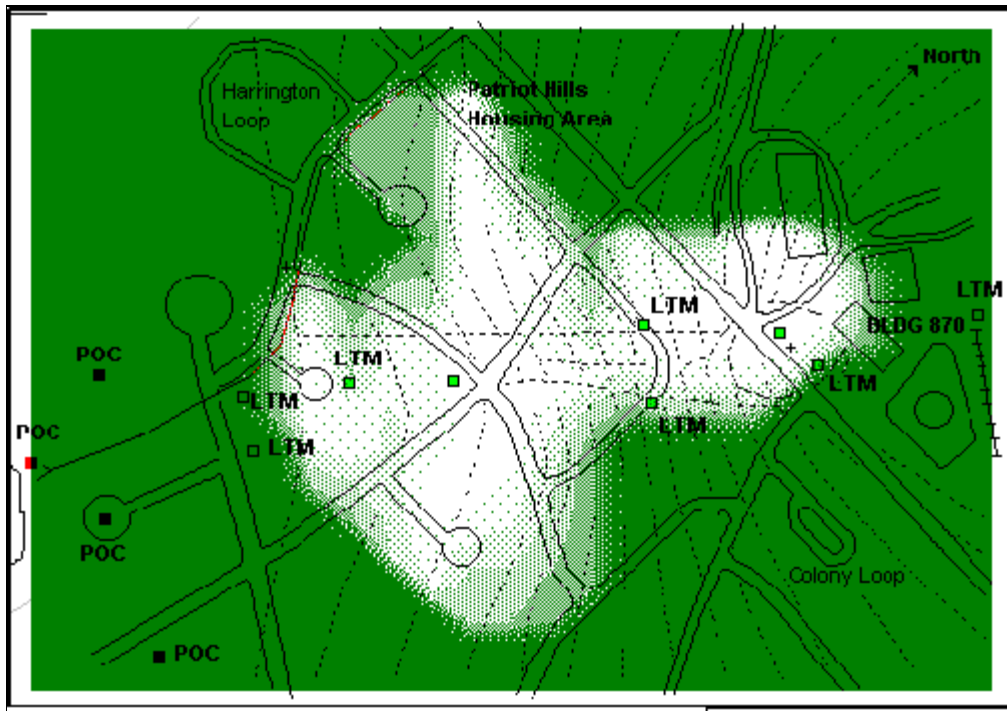

Figure B.10 Measured Oxygen Plume.

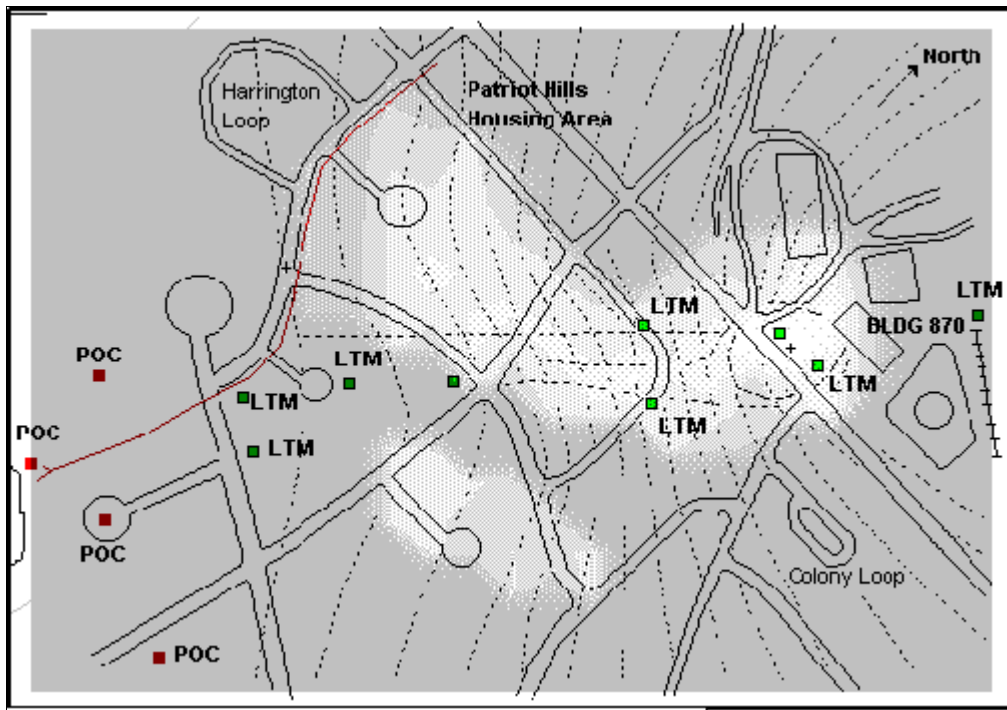Figure B.11 Measured Nitrate Plume.
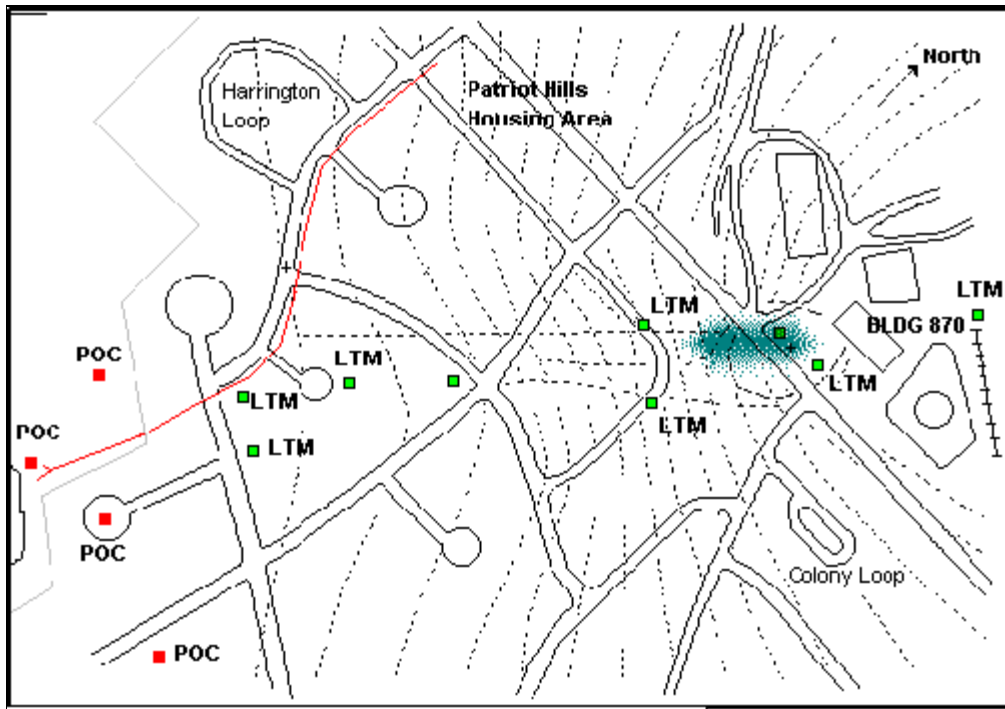

Figure B.12 Measured Sulfate Plume.

264

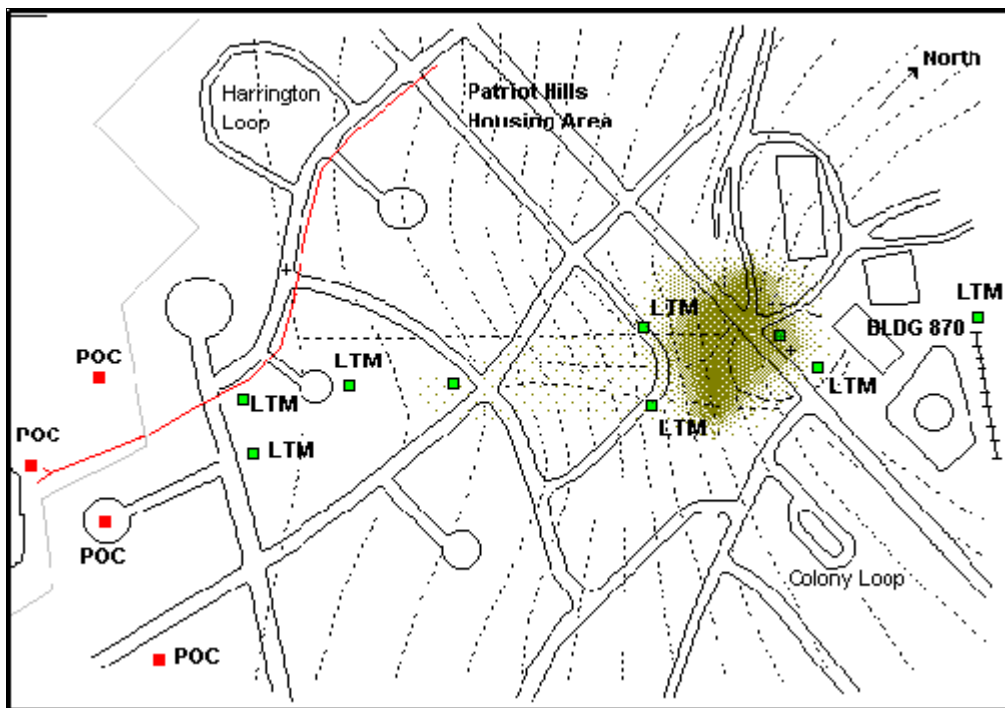Figure B.13 Measured Methane Plume.

Figure B.14 Measured Ferrous Iron Plume.

B.4 Calculations and Sorting of Raw Data

Several estimations must be made prior to the full implementation of the simulation model to predict future trends of contaminant migration. These calculations include:

- An in depth comparison of the hydrocarbons, electron acceptors and by-products plumes to estimate biodegradation rate constants,

- Sorption and retardation rates,

- fuel/water partitioning calculations,

- ground water flow velocity calculations.

Each of these calculations is discussed in the following sections.

B.4.1 Analysis of Contaminant, Electron Acceptor and Metabolic Byproduct Data

The extent and distribution (vertical and horizontal) of contaminant and electron acceptor and metabolic byproduct concentrations are of paramount importance in documenting the occurrence of biodegradation of fuel hydrocarbons and in simulation model implementation.

Electron Acceptors and BTEX Data

Dissolved oxygen concentrations below background in an area with fuel hydrocarbon contamination are indicative of aerobic hydrocarbon biodegradation. Similarly, nitrate and sulfate concentrations below background in an area with fuel hydrocarbon contamination are indicative of anaerobic hydrocarbon biodegradation. These relationships can be established on the basis of the Platform generated contour maps. Generally, dissolved oxygen and nitrate are used in areas with dissolved-phase fuel- hydrocarbon contamination at rates which are instantaneous relative to the average advective transport ground water velocity. This results in the consumption of these compounds at a rate approximately equal to the rate at which they are replenished by advective flow processes. For this reason, the use of these compounds as electron acceptors in the biodegradation of dissolved-phase fuel-hydrocarbons is a mass-transport-limited process (Borden and Bedient, 1986; Wilson *et* al., 1985). The use of dissolved oxygen and nitrate in the biodegradation of dissolved-phase fuel-hydrocarbons can be modeled using the Platform.

Microorganisms generally utilize sulfate, iron III, and carbon dioxide in areas with dissolved-phase fuel-hydrocarbon contamination at rates that are slow relative to the advective transport velocity of ground water. This results in the consumption of these compounds at a rate that could be slower than the rate at which they are replenished by advective flow processes. Therefore, the use of these compounds as electron acceptors in the biodegradation of dissolved-phase fuel-hydrocarbons may be a reaction-limited process that can be approximated by first-order kinetics.

The BIOPLUME III model uses a first-order rate constant to model such biodegradation. Determination of first-order decay rate constants is discussed in the next section.

Metabolic Byproduct and BTEX Data

Elevated concentrations of the metabolic byproducts Iron II and methane in areas with fuel hydrocarbon contamination are indicative of hydrocarbon biodegradation. Contour maps can be used to provide visible evidence of these relationships.

Indicative of the existence of these biodegradtion processes are the contour maps described in the previous section. To further examine their delicate interaction, the Platform offers the possibility to compare various distributions of the hydrocarbons versus the electron acceptors and by-products. Figure B.15 for example, clearly shows the Oxygen depletion in the area of the corresponding hydrocarbon plume. Similar patterns are observed for nitrates and Sulfates, (Figure B.16 and B.17). Figures B.18 and B.19 by comparison show the creation of byproducts, namely ferrous iron and methane, in plumes similar in shape to the hydrocarbon plume.
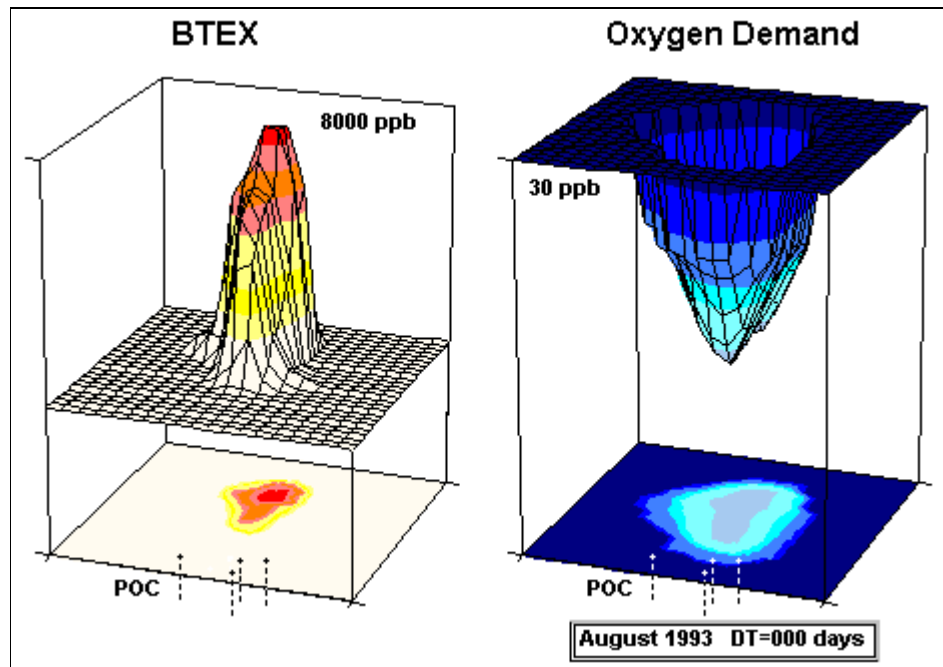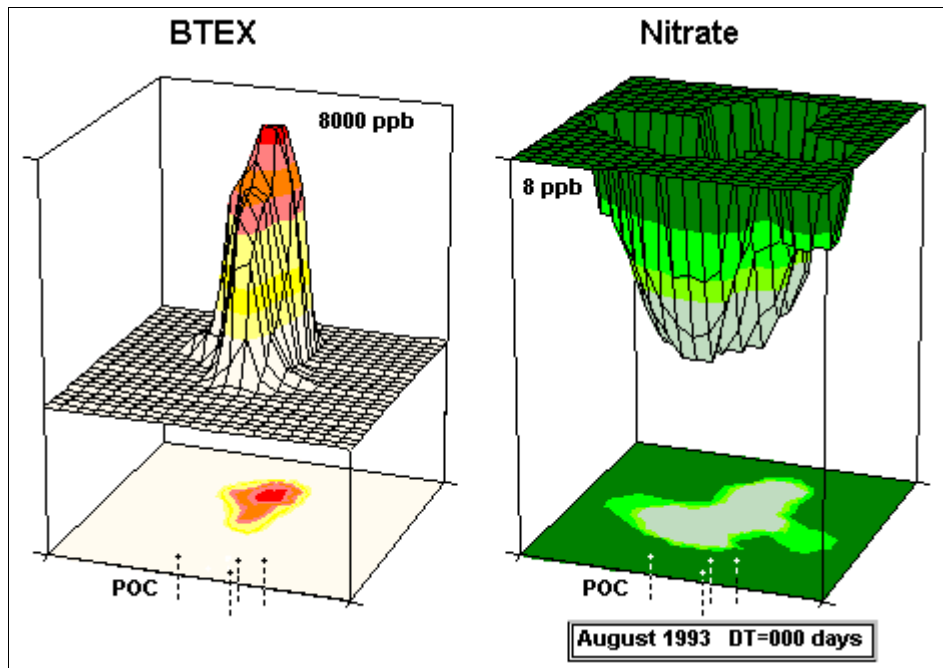

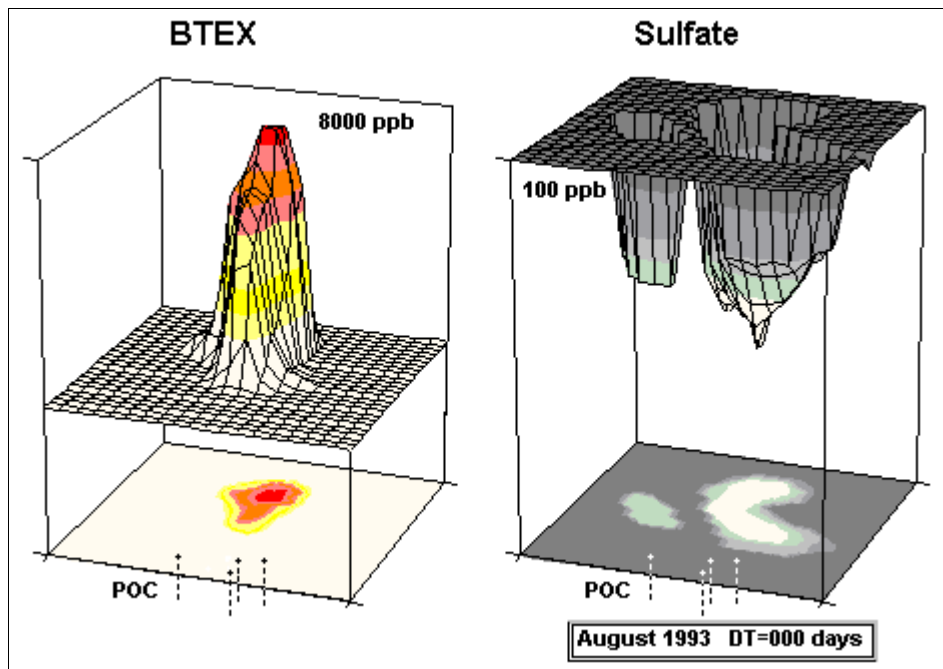Figure B.15 Oxygen Depletion.

Figure B.16 Nitrate Depletion.

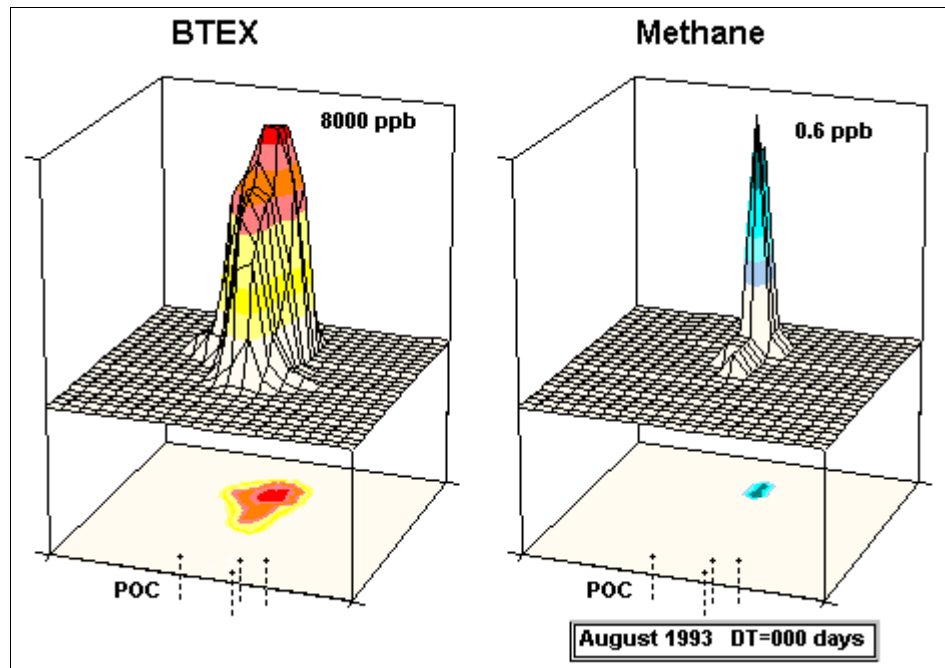Figure B.17 Sulfate Depletion.

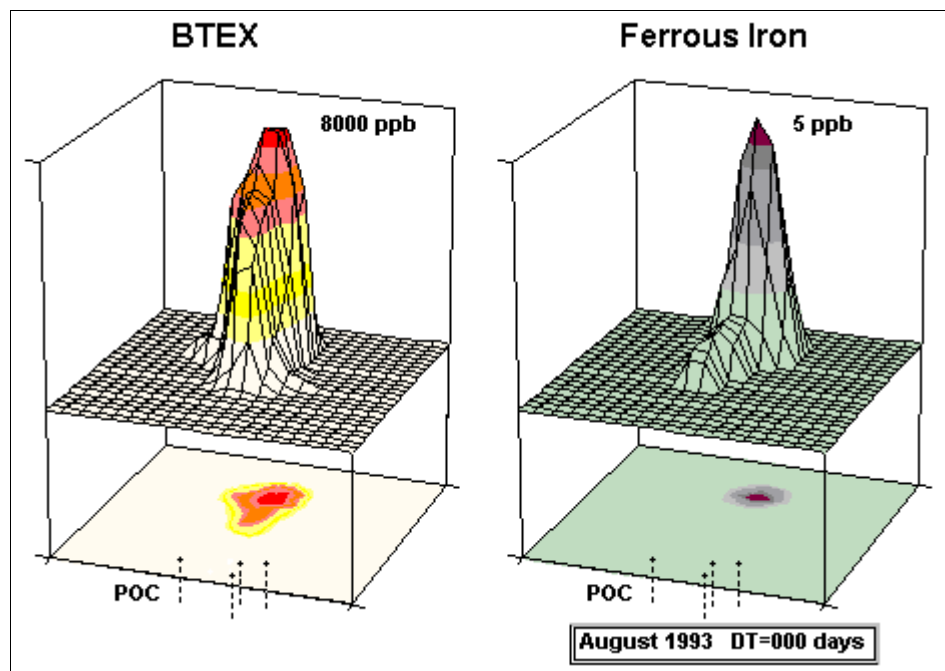Figure B.18 Methane Creation.

Figure B.19 Ferrous Iron Creation.

B.4.2   Sorption and Retardation Calculations

Contaminant sorption and retardation calculations should be made based on the total organic carbon (TOC) content of the aquifer matrix and the organic carbon partition coefficient (Y) of each contaminant. The average TOC concentration from the most transmissive zone in the aquifer should be used for retardation calculations. At a minimum, these calculations should be completed for each of the BTEX compounds and any tracers.   Sorption and retardation calculations are described in the next section.

B.4.3   Fuel/Water Partitioning Calculations

If NAPL remains at the site, fuel/water partitioning calculations should be made to account for the partitioning from these phases into the dissolved phase in ground water. Several models for fuel/water partitioning have been proposed in recent years, including those by Hunt *et al. (1988), Johnson and Pankow (1992), Cline et al. (1991) and Bruce et al (1991).* The models presented by *Cline et al. (1991) and Bruce et al. (1991)* represent equilibrium partitioning, i.e. they are the most conservative models. Equilibrium partitioning is conservative because it predicts the maximum dissolved-phase concentration when LNAPL in contact with water is allowed to reach equilibrium.   The results of these equilibrium partitioning calculations can be used in a simulation model to simulate a continuous source of contamination.

B.4.4   Ground Water Flow Velocity Calculations

The average linear ground water flow velocity of the most transmissive aquifer zone containing contamination should be calculated to check the accuracy of the ground water flow simulation model and to allow calculation of first-order biodegradation rate constants.

B.4.5   Anaerobic Biodegradation Rate Constant Calculations

One of the advantages of BIOPLUME III is that it does account for anaerobic degradation to the same degree of accuracy as for aerobic degradation, i.e. one can also use a first-order anaerobic decay constant.

In order to calculate anaerobic rate constants for each chemical, the apparent degradation rate must be dissociated from the effects of dilution and volatilization.

This is accomplished by normalizing the concentration of each contaminant to the concentration of a tracer that is at least as sorptive, but which is biologically inactive. Two chemicals that have good potential as tracers that are found in fuel hydrocarbon plumes are trimethylbenzene and tetramethylbenzene. Both have been shown to be recalcitrant under anaerobic conditions. It is important to note however, that all refined fuel components will degrade in a ground water system undergoing intrinsic remediation. Trimethylbenzene and tetraethylbenzene, while being recalcitrant under anaerobic conditions, will degrade under aerobic conditions.

When sulfate is being used as an electron acceptor and sulfate concentrations are greater than 10 milligrams per liter (mg/L), the first-order rate constant is appropriate. To adequately describe biodegradation rates using a first-order rate constant during methanogenesis, the total alkalinity for the system should be greater than about 50 mg/L. An example anaerobic biodegradation rate constant calculation is given in the next section. The Platform allows direct input of anaerobic electron acceptor data so that both aerobic and anaerobic degradation can be simulated.

B.5   Simulate Intrinsic Remediation Using the Platform

Modeling of the intrinsic bioremediation processes is necessary because we need to predict the migration and attenuation of the contaminant plume over time. Unlike other technologies, Intrinsic Remediation requires the ability to predict the future behavior of a contaminant plume. Indeed the whole IR technology is based on the claim that the applicant has deep knowledge of the behavior of the contaminant plume over time, and can guarantee with a high degree of reliability that the plume will experience loss of contaminant mass and that in any event it will not reach receiving points along established exposure pathways, and that concentrations will not exceed regulatory standards at compliance points.

Simulation can be used to do site-specific predictions of the fate and migration of solutes under governing physical, chemical, and biological processes, provided the model has been calibrated and verified to site data. Therefore, the simulation model cannot prove or disprove that intrinsic remediation is occurring at a given site alone. But in conjunction with site-specific data analysis simulation models can be very powerful indeed. A calibrated and verified model can prove the case that it reproduces historical data and can be used in a predictive mode.

Scenario analysis vs. Prediction

A calibrated and verified model will be used in one of two capacities: 1/ to predict (exactly) what will happen in the immediate or longer term future (like the weather forecast in the nightly news); and, 2/ to predict extreme conditions (scenario analysis). The distinction is subtle but important: any difference between scenario predictions and the subsequent plume behavior should not be used to discredit the model. Instead, these differences should be first explained (e.g. wet year, or presence of new contaminant source) and then used to strengthen the validity of the scenario predictions. The exact future prediction depends on imponderables such as the hydrological cycle (wet/ dry year), exact behavior of the contamination source, which may be of lesser importance in ascertaining that contamination will be contained. The scenario analysis will have fulfilled its role if under the simulation conditions the plume does not exceed the safety envelope around the site as monitored by the long term monitoring wells and the compliance wells.

B.5.1 Requirements for a Contaminant Biodegradation Simulation

A ground water simulation model for intrinsic remediation is developed to formulate and substantiate ground water restoration decisions. It is used for the following reasons:

1. To give insight into the physical bioremediation processes influencing the study area,

2. To provide predictions of system behavior under changing circumstances, and

3. To test hypotheses on system behavior by organizing the collection of additional data to improve site characterization and increase the confidence level in the management decisions.

B.5.2 Context of the Conceptual Model

A conceptual model is a word description of the components of a prototype contaminated aquifer system, the "loads" or "forcing" to the system, and the processes operative on the system. This description is made on the basis of preexisting data, regional aquifer atlases, or previous site studies. Pictures complement word descriptions (proverbially "worth a thousand words"). A graphical representation of the contaminated aquifer is part of the conceptual model. Figure B.20 illustrates a typical conceptual representation of a contaminated aquifer system.

Present in this conceptual model are a source of contamination, a fuel tank leaking at the surface (a typical problem that can be handled with intrinsic remediation); the vadose or unsaturated zone through which the 'free product' seeps; the mass of free product that "floats" atop the water table, i.e. that portion of the aquifer is saturated with fuel; a vapor zone, i.e. unsaturated zone filled with fuel vapors; and a zone of contact between free product and water table, where fuel is dissolved into the saturated aquifer. The dissolved contaminant creates a plume which is advected and dispersed by the flow of the aquifer. In most instances, the immediate concern is about the quality of the aquifer and therefore how to control the level of concentration of the dissolved contaminant. The rest of the phases, leaking source, free product, characterize the release mechanism.

Of course, any long term remediation will have to start with the removal of the source and the free product. But even that cannot be achieved one hundred percent, and therefore is controlled by the desirable or achievable concentration levels of dissolved contaminants in the aquifer which represents the major 'end point'. A modern approach to risk assessment then works backwards from the accepted concentration level in the aquifer to target residual levels in the soil.

This document deals primarily with the dissolved plume, its origin, its evolution, its simulation and its remediation by biodegradation. And of course, a fuel leakage does not produce one contaminant plume but many, as many as the constituents of the fuel. Not all are toxic, and therefore the discussion focuses on the stable toxic constituents. For fuel hydrocarbons these are the BTEX sequence (Benzene, Toluene, Ethylene, Xylene). All above discussion deals with light

hydrocarbons (LNAPLs -light non-aqueous phase liquids). Dense organic liquids, DNAPLs, form free product masses which tend to sink in the aquifer, that is they have a higher mobility. They are mostly solvents which are significantly more difficult to degrade biologically.

This completes the component description of the conceptual model. But a conceptual model is not complete without providing additional information about boundary conditions, or how the vicinity of the aquifer near the site of interest relates to the surrounding aquifers at the regional scale; the presence and interaction with other surface features such as rivers and ponds or drains; and the "forcing" mechanisms or loads to the system, wells, recharge, evapotranspiration and other losses.

The conceptual model development is arguably the most important phase for a modeling exercise, where experience counts the most. The automated/integrated Platform breaks rank with this tradition in two important ways:

1. Because data entry and model setup are performed by the program very efficiently, the user can concentrate on the physical, chemical, and biological aspects of the problem and gain experience very quickly.

2. The user does not need to switch from simple (analytic) to more complicated models: all entered data are immediately accessible for use in testing new model setups, adjusted numerical grids, boundary conditions etc.

These are extraordinary advantages that the Platform offers when dealing with a subject as complicated as the modern multi-disciplinary theory of biodegradation.
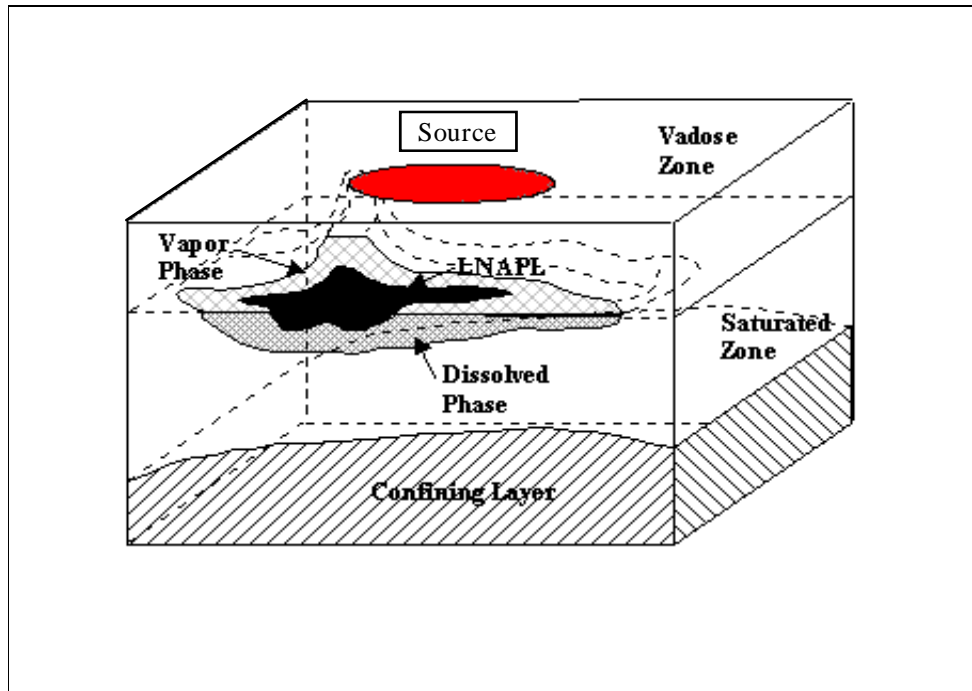
Figure B.20 A conceptual Intrinsic Remediation Model

B.5.3   Steps Specific to Biodegradation Modeling

Most of the elements that go into preparing for a biodegradation modeling exercise are already mentioned in the conceptual model phase described above.

The first thing that needs to be done is the determination of the modeling domain, that is the geographic extent of the simulation area. Typically this domain will start from the area of interest (for example a waste site or a well field) and extend to where secure boundary conditions may exist (that is conditions that are unaltered by 'forcing' that may be imposed within the simulation domain), or beyond the radius of influence of anticipated forcing mechanisms. With variable spacing grids available one should err on the side of safety and retain a larger rather than a narrower domain. The element to consider in defining the simulation domain is a bitmap of the site showing as many features as available, including topographic contour lines, surface features, lakes, rivers, drains, observed hydraulic heads and plume delineation. This bitmap is imported in the program and "registered" to the scales of the simulation domain defined earlier. It provides the canvas on which to build the ground water intrinsic remediation model using the Platform tools.

Grid definition is automated in the Platform and offers absolutely no inconvenience to the modeler on two counts:

1. It is drawn by specifying the increments or the number of elements in the x (top) and y (left) axes spanning the domain. The drawn grid can then be graphically edited by moving horizontal or vertical grid lines at will; or inserting new lines (rows or columns) as the need arises.

274

2. The aquifer properties (conductivities, porosity, dispersion) are interpolated to the grid centers from observed data points by Kriging. A complete assortment of advanced kriging options are available for the modeler to control the geostatistical interpolation error. In fact this is one of the strong points of the Platform because once the raw data are entered the modeler does not <u>ever</u> have to revisit them although he/ she may test a wide variety of different grid configurations.

Next is the depiction of the soil medium aquifer stratification or layering. In fact a distinction is drawn between soil strata and aquifer layers: strata are physical units in the soil medium which have different conductances and other properties and can be aquitards or even confining units.

The last piece of data necessary to perform a simulation pertains to the initial and boundary conditions. Contaminant and oxygen or other terminal electron acceptor concentrations must be known or assumed (constant for example) at some point in time. A simulation model always starts from some known initial conditions and marches the solution in time. Often these conditions are measured in the field from observation wells or piezocones at one or more points in time, and are interpreted into concentration contours. These data also are interpolated to the model grid via kriging as explained above. In fact, more than one set of data are needed so as to calibrate the model against one set and validate it against additional sets of observed heads.

With all the necessary data entered, the remaining tasks for the modeler are to "create" his/ her conceptual model interactively on screen with the program tools by selecting and specifying features to include, for example rivers, ponds, drains, wells and their pumping schedule, as well as man-made features such as liners, slurry walls, even geologic faults, and of course the contaminant sources. With the interactive/ graphical selection of appropriate boundary conditions, the modeler is then ready to fire up their first simulation. Nothing to be timid about: if there is an error in the data or model setup, it will become immediately apparent in the distorted simulated results. Or the Platform will guide you about any discrepancies that may not allow you to activate the ground water biodegradation model. Corrections can then be made on the spot so that one can proceed very quickly to a series of trial-and-errors.

The Platform in fact gives a good name to the old trial-and-error procedure; only it does it while increasing efficiency and productivity!

In the following sections we look in more detail into the types of data that are needed for a ground water biodegradation simulation; and into the crucial task of model calibration and validation. Of course, the specific steps for biodegradation modeling presume a calibrated/ verified flow model.

B.5.4   Calibration of the Bioremediation Model

A ground water bioremediation model is an integrated suite of interacting simulators for the flow through the porous medium, interaction with surface waters, evapotranspiration losses, drains, other forcing mechanisms such as wells and recharge, and boundary conditions; and the advection and dispersion of constituent plumes and their interaction. A calibrated model is one where there is a *balance* between grid resolution and data accuracy, layering and the vertical

structure of the hydraulic head and concentration distributions, the number of processes and their importance or influence on the simulated results. Here is how to proceed to develop a balanced model.

The calibration picture is at once complicated but also tractable because there is a hierarchy to follow. First, we must begin with a calibrated flow model, that is the flow model can be calibrated independently of the migration or biodegradation processes. Of course unresolved discrepancies at the migration or biodegradation level can point to necessary adjustments in aquifer layer thickness' or conductivities which are the primary flow model calibration parameters. This is why the calibration process is an iterative one. But do not equate iterations with confusion: iterations bring order to a complex process.

The calibrated flow model will then be used to calibrate the intrinsic remediation migration model for a conservative constituent. This will allow to calibrate the advective and dispersive properties of the aquifer. For example, starting from one set of observed concentrations as initial conditions the 1-species simulation will be used to reproduce the concentrations as observed at a later time.

With a calibrated advection/ dispersion model one then will attempt to model degradation processes, chemical reactions or biodegradation. For the case of biodegradation, a second plume will be simulated of dissolved oxygen for aerobic conditions, or a "compound" plume for the case where additional degradation conditions exist, for example denitrifying conditions. The calibration consists of comparing the simulated degraded hydrocarbon plume (dissolved BTEX) and the corresponding depletion of dissolved oxygen, nitrates, other electron acceptors and by-products against the observed (measured) concentrations. The calibration parameters are the stoichiometric ratio of hydrocarbon consumption to oxygen or nitrate; alternatively, the interaction between electron acceptor and hydrocarbon plumes may be modeled instantaneously or using Monod kinetics theory. Additional tuning parameters such as the reaeration coefficient can also be used to resolve any residual discrepancies.

These are the essential steps to follow for a systematic biodegradation simulation model calibration. In the foregoing discussion little mention is made about source mechanisms. This and other features are discussed next.

Identifying Loadings, Sources for the Simulation Model

First determine what drives the contaminant migration system: how does recharge from precipitation, influx from neighboring regions of the aquifer or surface water impoundments affect the migration process; and where are the withdrawals, pumping wells, drains, seepage into rivers or lakes. Then determine how the cyclicity of the aquifer regime, either annual or drought-wet year cycle can affect the long term behavior of contaminant plumes. Then consider the contamination source mechanism. There are several possibilities depending on the data available: it can be simulated as a recharge zone with a given flux and concentration; or it can be simulated as a zone of constant concentration at the maximum dissolution rate below the free product mass; or it can be emulated by a series of injection wells. Before proceeding with a simulation however, there is a series of boundary and initial conditions to define.

Identifying Boundary and Initial Conditions of the Simulation Model

Boundary conditions are usually the concentrations prevailing at the boundary of the modeled domain. When they are known from observations and when they are not affected by processes taking place in the simulation domain (e.g. cone of depression from pumping wells) they may as well be considered as constant. Under these conditions the model can be calibrated for conservative constituents as discussed above. If other processes are important, for example recharge from precipitation or interaction with surface waters, then the fixed boundary condition can be relaxed and the model can be calibrated explicitly for the source mechanism. Thus, the individual processes can be isolated and calibrated separately in a hierarchical manner. The Platform offers automation and integration which allow the user to perform all these formidable looking calibration tasks very efficiently, accurately and effortlessly.

Identifying Soil Layering and Grid Resolution for the Simulation Model

Finally, a word must be said about grid resolution. It should be looked at as a calibration parameter in the sense that the user should start out simple with a clearly distinctive coarse grid. After initial calibration and if the accuracy of the contaminant plume field data warrant it then the user can consider increasing the grid resolution for final calibration. Once the data have been entered in the program data structure, switching grid resolution is easy and painless. This is how with the Platform, the complicated steps for a professional model calibration do become tangible.

B.6   Conduct an Exposure Assessment

After the rates of natural attenuation have been documented and predictions of the future extent and concentration of the contaminant plume have been made using the BIOPLUME III fate and migration model, the proponent of intrinsic remediation should prepare a permit application for implementation of this remedial option. Supporting the intrinsic remediation option generally will involve implementation of an exposure assessment. The results of numerical fate and migration modeling are central to the exposure assessment. Conservative model input parameters should give conservative estimates of contaminant plume migration. From this information, the potential impacts to human health and the environment from contamination present at the site can be estimated. The exposure assessment in support of the remediation option is described in a separate Risk Assessment AFCEE document.

B.7   Prepare Long-Term Monitoring Plan

The long-term monitoring plan consists of locating ground water monitoring wells and developing a ground water sampling and analysis strategy. This plan is used to monitor plume migration over time and to verify that intrinsic remediation is occurring at rates sufficient to protect potential downgradient receptors. The long-term monitoring plan should be developed based on the results of the BIOPLUME III model simulations.

Point-of-compliance (POC) monitoring wells are wells that are installed at locations downgradient of the contaminant plume and upgradient of potential receptors. POC monitoring

wells are generally installed along a property boundary or at a location approximately 5 years downgradient of the current plume at the seepage velocity of the ground water or 1 to 2 years upgradient of the nearest downgradient receptor, whichever is more protective. The final number and location of POC monitoring wells will depend on regulatory considerations. Long-term monitoring wells are wells that are placed upgradient of, within, and immediately downgradient of the contaminant plume. These wells are used to monitor the effectiveness of intrinsic remediation in reducing the total mass of contaminant within the plume. Requirements are, one well upgradient of the contaminant plume, one well within the anaerobic treatment zone, one well in the aerobic treatment zone and one well immediately downgradient of the contaminant plume. The final number and location of longterm monitoring wells will depend on regulatory considerations.

Figure B.21 shows a hypothetical long-term monitoring scenario. The results of a numerical model such as BIOPLUME III can be used to help locate both the long-term and POC monitoring wells. In order to provide a valid monitoring instrument, all monitoring wells must be screened in the same hydrogeologic unit as the contaminant plume. This generally requires detailed stratigraphic correlation. To facilitate accurate stratigraphic correlation, detailed visual descriptions of all subsurface materials encountered during borehole drilling should be prepared prior to monitoring well installation. The final placement of all monitoring wells should be determined in collaboration with the appropriate regulators.

The ground water sampling and analysis plan should be prepared in conjunction with POC and long-term monitoring well placement. Analyses should be limited to determining BTEX, dissolved oxygen, nitrate, and sulfate concentrations. Water level and NAPL thickness measurements must be made during each sampling event. Sampling frequency is dependent on the final placement of the POC monitoring wells. For example, if the POC monitoring wells are located 2 years upgradient of the nearest downgradient receptor, then an annual sampling frequency should be sufficient. If the POC monitoring wells are located 1 year upgradient of the potential receptor, then a semiannual sampling frequency should be sufficient. The final sampling frequency should be determined in collaboration with regulators.
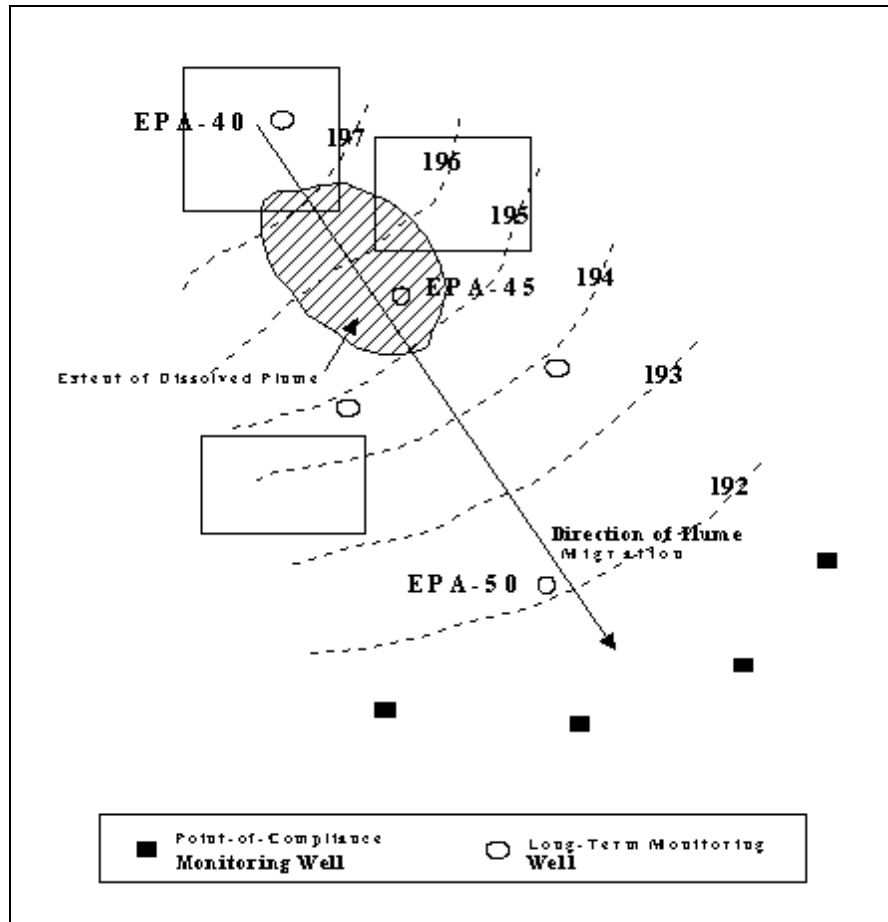
Figure B.21 Typical Long-Term Monitoring Strategy

B.8   Additional Reading

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