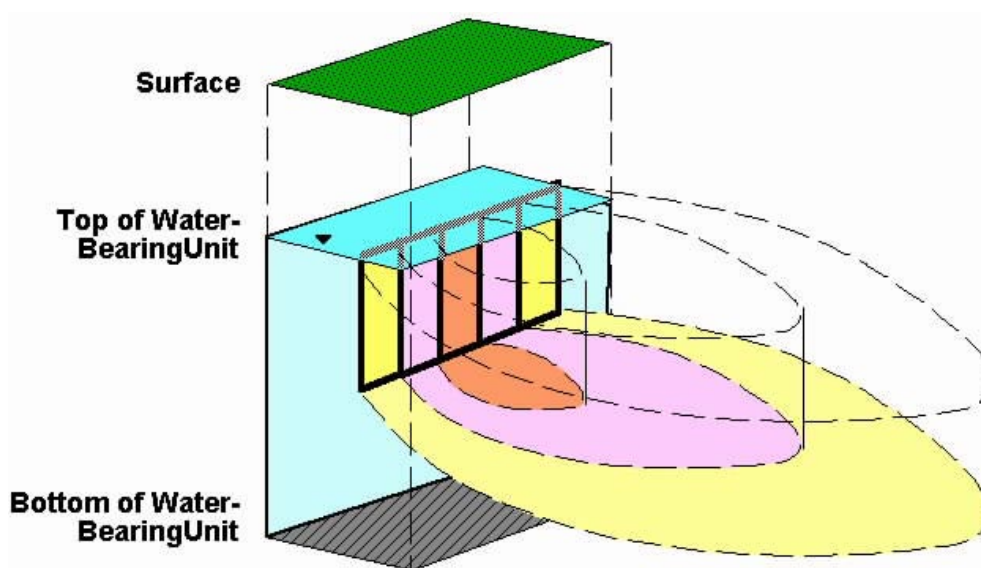




BIOSCREEN

Natural Attenuation Decision Support System

User's Manual Version 1.3



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by

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NOTICE

The information in this document was 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 BIOSCREEN mathematical model. To illustrate the appropriate application of BIOSCREEN, EPA 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 BIOSCREEN was developed by Ground Water Services, Inc. through a contract with the U.S. Air Force. Ground Water Services, Inc. also provided field data to illustrate the application of the model.

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.

An extensive investment in site characterization and mathematical modeling is often necessary to establish the contribution of natural attenuation at a particular site. BIOSCREEN is offered as a screening tool to determine whether it is appropriate to invest in a full-scale evaluation of natural attenuation at a particular site. Because BIOSCREEN incorporates a number of simplifying assumptions, it is not a substitute for the detailed mathematical models that are necessary for making final regulatory decisions at complex sites.

BIOSCREEN and its User's Manual have undergone external and internal peer review conducted by the U.S. EPA and the U.S. Air Force. However, BIOSCREEN is made available on an *as-is* basis without guarantee or warranty of any kind, express or implied. Neither the United States Government (U.S. EPA or U.S. Air Force), Ground Water Services, Inc., any of the authors nor reviewers accept any liability resulting from the use of BIOSCREEN or its documentation. Implementation of BIOSCREEN and interpretation of the predictions of the model are the sole responsibility of the user.

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.

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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Air Force Center for Environmental Excellence Technology Transfer
Division

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INTRODUCTION

BIOSCREEN is an easy-to-use screening model which simulates remediation through natural attenuation (RNA) of dissolved hydrocarbons at petroleum fuel release sites. The software, programmed in the Microsoft® Excel spreadsheet environment and based on the Domenico analytical solute transport model, has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions that have been shown to be the dominant biodegradation processes at many petroleum release sites. BIOSCREEN includes three different model types:

- 1) *Solute transport without decay,*
- 2) *Solute transport with biodegradation modeled as a first-order decay process (simple, lumped-parameter approach),*
- 3) *Solute transport with biodegradation modeled as an "instantaneous" biodegradation reaction (approach used by BIOPLUME models).*

The model is designed to simulate biodegradation by both aerobic and anaerobic reactions. It was developed for the Air Force Center for Environmental Excellence (AFCEE) Technology Transfer Division at Brooks Air Force Base by Groundwater Services, Inc., Houston, Texas.

INTENDED USES FOR BIOSCREEN

BIOSCREEN attempts to answer two fundamental questions regarding RNA:

1. How far will the dissolved contaminant plume extend if no engineered controls or further source zone reduction measures are implemented?

BIOSCREEN uses an analytical solute transport model with two options for simulating in-situ biodegradation: first-order decay and instantaneous reaction. The model will predict the maximum extent of plume migration, which may then be compared to the distance to potential points of exposure (e.g., drinking water wells, groundwater discharge areas, or property boundaries). Analytical groundwater transport models have seen wide application for this purpose (e.g., ASTM 1995), and experience has shown such models can produce reliable results when site conditions in the plume area are relatively uniform.

2. How long will the plume persist until natural attenuation processes cause it to dissipate?

BIOSCREEN uses a simple mass balance approach based on the mass of dissolvable hydrocarbons in the source zone and the rate of hydrocarbons leaving the source zone to estimate the source zone concentration vs. time. Because an exponential decay in source zone concentration is assumed, the predicted plume lifetimes can be large, usually ranging from 5 to 500 years. Note: This is an unverified relationship as there are few data showing source concentrations vs. long time periods, and the results should be considered order-of-magnitude estimates of the time required to dissipate the plume.

BIOSCREEN is intended to be used in two ways:

1. As a screening model to determine if RNA is feasible at a site.

In this case, BIOSCREEN is used early in the remedial investigation to determine if an RNA field program should be implemented to quantify the natural attenuation occurring at a site. Some data, such as electron acceptor concentrations, may not be available, so typical values are used. In addition, the model can be used to help develop long-term monitoring plans for RNA projects.

2. As the primary RNA groundwater model at smaller sites.

The Air Force Intrinsic Remediation Protocol (Wiedemeier, Wilson, *et al.*, 1995) describes how groundwater models may be used to help verify that natural attenuation is occurring and to help predict how far plumes might extend under an RNA scenario. At large, high-effort sites such as Superfund and RCRA sites, a more sophisticated model such as BIOPLUME is probably more appropriate. At less complicated, lower-effort sites such as service stations, BIOSCREEN may be sufficient to complete the RNA study. **(Note: "Intrinsic remediation" is a risk-based strategy that relies on RNA).**

BIOSCREEN has the following limitations:

1. As an analytical model, BIOSCREEN assumes simple groundwater flow conditions.

The model should not be applied where pumping systems create a complicated flow field. In addition, the model should not be applied where vertical flow gradients affect contaminant transport.

2. As a screening tool, BIOSCREEN only approximates more complicated processes that occur in the field.

The model should not be applied where extremely detailed, accurate results that closely match site conditions are required. More comprehensive numerical models should be applied in these cases.

FUNDAMENTALS OF NATURAL ATTENUATION

Biodegradation Modeling

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.*

These themes are supported by the following literature. Borden *et al.* (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. Borden *et al.* (1986) incorporated a simplifying assumption that the microbial kinetics are instantaneous into the USGS two-dimensional solute transport model (Konikow and Bredehoeft, 1978) using a simple superposition algorithm. The resulting model, BIOPLUME, was able to simulate solute transport and fate under the effects of instantaneous, oxygen-limited in-situ biodegradation.

Rifai and Bedient (1990) 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) and Rifai *et al.* (1991) 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 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.

The Air Force Natural Attenuation Initiative

Over the past several years, the high cost and poor performance of many pump-and-treat remediation systems have led many researchers to consider RNA as an alternative technology for groundwater remediation. A detailed understanding of natural attenuation processes is needed to support the development of this remediation approach. Researchers associated with the U.S. EPA's R.S. Kerr Environmental Research Laboratory (now the Subsurface Protection and Remediation Division of the National Risk Management Laboratory) have suggested that anaerobic pathways could be a significant, or even the dominant, degradation mechanism at many petroleum fuel sites (Wilson, 1994). The natural attenuation initiative, developed by the AFCEE Technology Transfer Division, was designed to investigate how natural attenuation processes affect the migration of plumes at petroleum release sites. Under the guidance of Lt. Col. Ross Miller, a three-pronged technology development effort was launched in 1993 which will ultimately consist of the following elements:

- 1) *Field data collected at over 30 sites around the country (Wiedemeier, Miller, et al., 1995) 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 RNA Study (Wiedemeier, Wilson, et al., 1995).*

- 3) *Two RNA modeling tools: the BIOPLUME III model being developed by Dr. Hanadi Rifai at Rice University (Rifai et al., 1995), and the BIOSCREEN model developed by Groundwater Services, Inc. (BIOPLUME III, a more sophisticated biodegradation model than BIOSCREEN, employs particle tracking of both hydrocarbon and alternate electron acceptors using a numerical solver. The model employs sequential degradation of the biodegradation reactions based on zero order, first order, instantaneous, or Monod kinetics).*

Relative Importance of Different Electron Acceptors

The Intrinsic Remediation Technical Protocol and modeling tools focus on evaluating both aerobic (in the presence of oxygen) and anaerobic (without oxygen) degradation processes. 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 principal factors influencing the utilization of the various electron acceptors by fuel-hydrocarbon-degrading bacteria 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.

Preferred Reactions by Energy Potential

Biologically mediated degradation reactions are reduction/oxidation (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 can serve as electron acceptors for alternative anaerobic pathways. This transfer of electrons releases energy which is utilized for microbial 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 the reaction. 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	Reaction Preference
Oxygen	Aerobic	CO ₂	<i>Most Preferred</i>
Nitrate	Anaerobic	N ₂ , CO ₂	↓
Ferric Iron (solid)	Anaerobic	Ferrous Iron (dissolved)	↓
Sulfate	Anaerobic	H ₂ S	↓
Carbon Dioxide	Anaerobic	Methane	<i>Least Preferred</i>

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 consumed, leading to a pattern where preferred electron acceptors are consumed one at a time, in sequence. Based on this principle, 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 monitoring wells that are completely depleted in one or more electron acceptors. Two processes are probably responsible for this observation:

1. *Alternative biochemical mechanisms exhibiting 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 (bacteria able to utilize electron acceptors in both aerobic and anaerobic environments), for example, can shift from aerobic metabolism to nitrate reduction when oxygen is still present but at low concentrations (i.e. 1 mg/L oxygen; Snoeyink and Jenkins, 1980). Similarly, the nearly equivalent redox potentials for sulfate and carbon dioxide (see Wiedemeier, Wilson, et al., 1995) indicate that sulfate reduction and methanogenic reactions may also occur together.*
2. *Standard monitoring wells, with 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 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 BIOSCREEN software attempts to account for the majority of these biodegradation mechanisms.

Distribution of Electron Acceptors at Sites

The utilization of electron acceptors is generally based on the energy of the reaction and the availability of the electron acceptor at the site. 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 among sites. For example, a study of several sites yielded the following summary of available electron acceptors and metabolic by-products:

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
Site ST-29, Patrick AFB, Florida*	3.8	0	2.0	0	13.6
Bldg. 735, Grissom AFB, Indiana	9.1	1.0	2.2	59.8	1.0
SW MU 66 Site, Keesler AFB, MS	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 collected by Parsons Engineering Science, Inc.; all other data collected by Groundwater Services, Inc.

At the Patrick AFB site, nitrate and sulfate are not important electron acceptors while the oxygen and the methanogenic reactions dominate (Wiedemeier, Swanson, *et al.*, 1995). At Hill AFB and Grissom 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.

Kinetics of Aerobic and Anaerobic Reactions

As described above, 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 (Wilson *et al.*, 1985). 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.

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

TABLE 1
BIODEGRADATION CAPACITY (EXPRESSED ASSIMILATIVE CAPACITY) AT AFCEE NATURAL ATTENUATION SITES
 BIOSCREEN Natural Attenuation Decision Support System

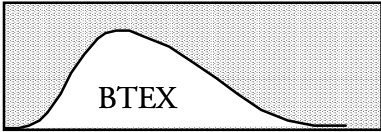
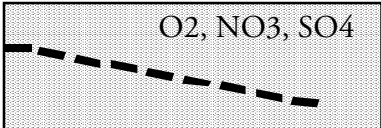
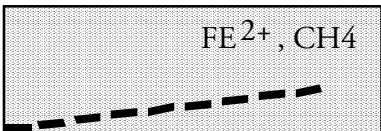
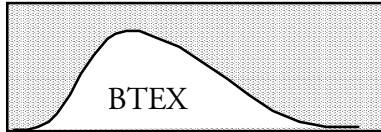
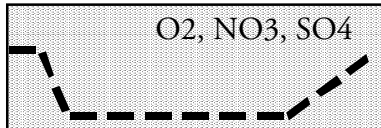
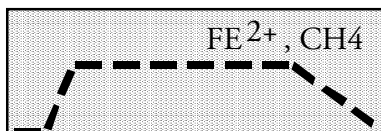
Site Number	Base	State	Site Name	Maximum Total BTEX Concentration (mg/L)	Observed Change in Concentration (mg/L)					Biodegradation Capacity/Expressed Assimilative Capacity (mg/L)					Total Biodegradation Capacity (mg/L)	Source of Data	
					O2	Nitrate	Iron	Sulfate	Methane	Aerobic		Iron	Sulfate	Methanogenesis			
										Respiration	Denitrification						Reduction
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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	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	PES	
23	Travis AFB	California		-	3.8	15.8	8.5	109.2	0.2	1.2	3.2	0.4	23.7	0.3	28.9	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	PES	
25	Seymour AFB	Johnson North Carolina		13.8	8.3	4.3	31.6	38.6	2.7	2.6	0.9	1.5	8.4	3.5	16.8	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	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	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	GSI	
				Average	14.2	5.6	17.7	49.3	39.5	8.4	1.8	3.6	2.3	8.6	10.8	27.0	
				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	12.7	69.7	599.5	109.2	48.4	4.0	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	

Note:

- Utilization factors of the electron acceptors/by-products are as follows (mg of electron acceptor or by-product/mg of BTEX): Dissolved Oxygen: 3.14, Nitrate: 4.9, Iron: 21.8, Sulfate: 4.7, Methane: 0.78.
- = Data not available.
- PES = Parsons Engineering Science (Wiedemeier, Miller, et al. 1995). GSI = Groundwater Services, Inc.

Recent results from the AFCEE Natural Attenuation Initiative indicate that the anaerobic reactions, which were originally thought to be too slow to be of significance in groundwater, can also be simulated as instantaneous reactions (Newell *et al.*, 1995). For example, Davis *et al.* (1994) also ran microcosm studies with sulfate reducers and methanogens that indicated that benzene could be degraded in a period of a few weeks (after acclimation). When compared to the time required to replenish electron acceptors in a plume, it appears appropriate to simulate anaerobic biodegradation of dissolved hydrocarbons with an instantaneous reaction, just as for aerobic biodegradation processes.

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

If microbial kinetics were limiting the rate of biodegradation:	If microbial kinetics were relatively fast (instantaneous):
<ul style="list-style-type: none"> Anaerobic electron acceptors (nitrate and sulfate) would be constantly decreasing in concentration as one moved downgradient from the source zone, and 	<ul style="list-style-type: none"> Anaerobic electron acceptors (nitrate and sulfate) would be mostly or totally consumed in the source zone, and
<ul style="list-style-type: none"> Anaerobic by-products (ferrous iron and methane) would be constantly increasing in concentration as one moved downgradient from the source zone. 	<ul style="list-style-type: none"> Anaerobic by-products (ferrous iron and methane) would be found in the highest concentrations in the source zone.
<p>Observed Conc. </p> <p>Conc. </p> <p>Conc. </p> <p style="text-align: center;">————— X —————></p>	<p>Observed Conc. </p> <p>Conc. </p> <p>Conc. </p> <p style="text-align: center;">————— X —————></p>

The second pattern is observed at RNA demonstration sites (see Figure 1), supporting the hypothesis that anaerobic reactions can be considered to be relatively instantaneous at most or almost all petroleum release sites. From a theoretical basis, the only sites where the instantaneous reaction assumption may not apply are sites with very low hydraulic residence times (very high groundwater velocities and short source zone lengths).

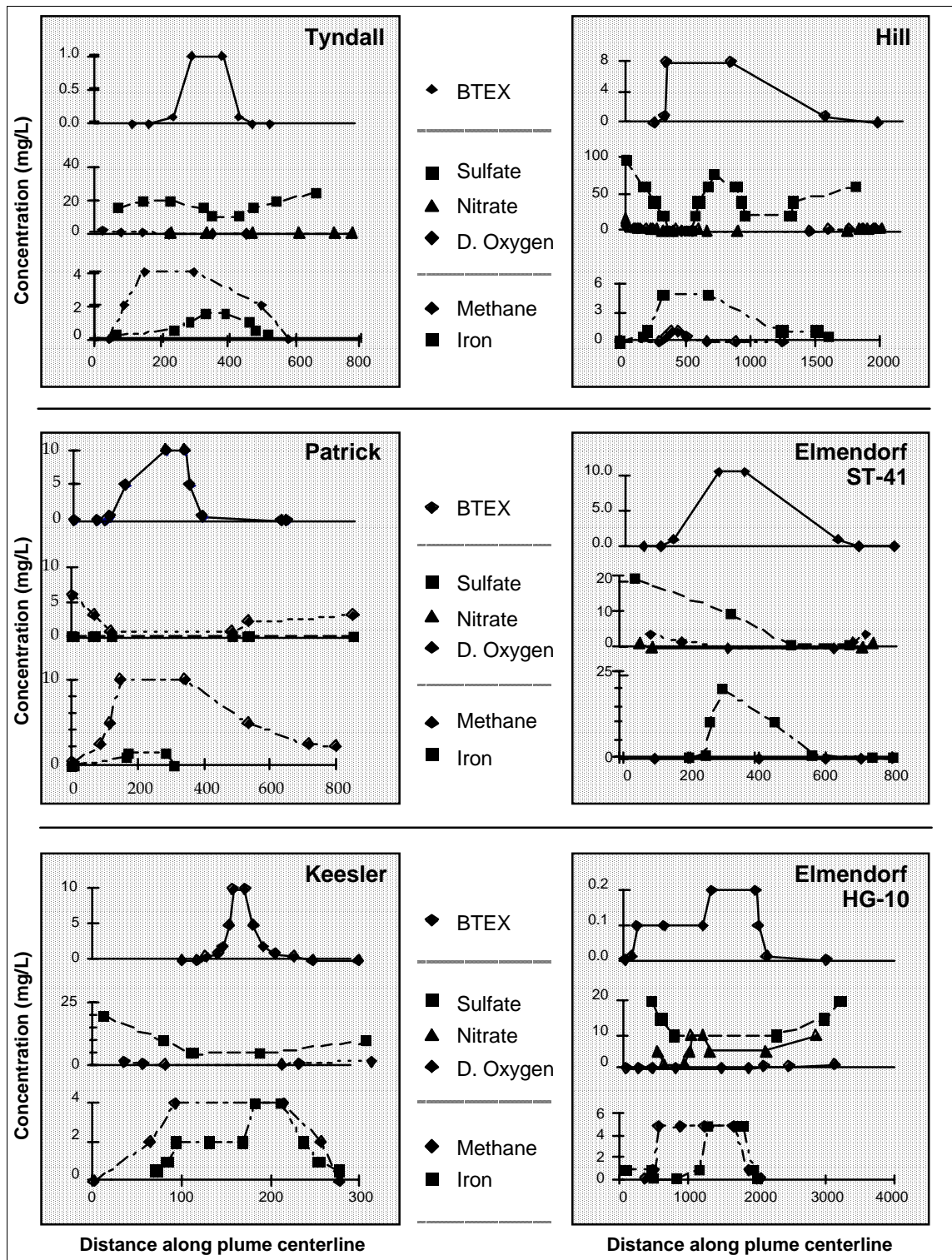


Figure 1. Distribution of BTEX, Electron Acceptors, and Metabolic By-Products vs. Distance Along Centerline of Plume.

Sampling Date and Source of Data: Tyndall 3/95, Keesler 4/95 (Groundwater Services, Inc.), Patrick 3/94 (note: one NO₃ outlier removed, sulfate not plotted), Hill 7/93, Elmendorf Site ST41 6/94, Elmendorf Site HG 10 6/94, (Parsons Engineering Science).

Kinetic-limited sites, however, appear to be relatively rare as the instantaneous reaction pattern is observed even at sites such as Site 870 at Hill AFB, with residence times of a month or less. As shown in Figure 1, this site has an active sulfate reducing and methane production zone within 100 ft of the upgradient edge of plume. With a 1600 ft/yr seepage velocity is considered, this highly anaerobic zone has an effective residence time of 23 days. Despite this very short residence time, significant sulfate depletion and methane production were observed in this zone (see Figure 1). If the anaerobic reactions were significantly constrained by microbial kinetics, the amount of sulfate depletion and methane production would be much less pronounced. Therefore this site supports the conclusion that the instantaneous reaction assumption is applicable to almost all petroleum release sites.

Biodegradation Capacity

To apply an electron-acceptor-limited kinetic model, such as the instantaneous reaction, the amount of biodegradation able to be supported by the groundwater that moves through the source zone must be calculated. The conceptual model used in BIOSCREEN is:

1. Groundwater upgradient of the source contains electron acceptors.
2. As the upgradient groundwater moves through the source zone, non-aqueous phase liquids (NAPLs) and contaminated soil release dissolvable hydrocarbons (in the case of petroleum sites, the BTEX compounds benzene, toluene, ethylbenzene, xylene are released).
3. Biological reactions occur until the available electron acceptors in groundwater 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, CO₂ is also produced as an end-product of the reactions. For these reactions, the metabolic by-products, ferrous iron and methane, can be used as proxies for the potential amount of biodegradation that could occur from the iron-reducing and methanogenesis reactions.)
4. The total amount of available electron acceptors for biological reactions can be estimated by a) calculating the difference between upgradient concentrations and source zone concentrations for oxygen, nitrate, and sulfate; and b) measuring the production of metabolic by-products (ferrous iron and methane) in the source zone.
5. Using stoichiometry, a utilization factor can be developed showing the ratio of the oxygen, nitrate, and sulfate consumed to the mass of dissolved hydrocarbon degraded in the biodegradation reactions. Similarly, utilization factors can be developed to show the ratio of the mass of metabolic by-products that are generated to the mass of dissolved hydrocarbon degraded in the biodegradation reactions. Wiedemeier, Wilson, *et al.*, (1995) provides the following utilization factors based on the degradation of combined BTEX constituents:

Electron Acceptor/By-Product	BTEX Utilization Factor gm/gm
Oxygen	3.14
Nitrate	4.9
Ferrous Iron	21.8

Sulfate	4.7
Methane	0.78

- 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. Dividing the background concentration of an electron acceptor by its utilization factor provides an estimate (in BTEX concentration units) of the assimilative capacity of the aquifer by that mode of biodegradation.

Note that BIOSCREEN is based on the BTEX utilization provided above. If other constituents are modeled, the utilization factors in the software (scroll down from the input screen to find the utilization factors) should be changed or the available oxygen, nitrate, iron, sulfate, and methane data should be adjusted accordingly to reflect alternate utilization factors.

When the available electron acceptor/by-product concentrations (No. 4) are divided by the appropriate utilization factor (No. 5), an estimate of the "biodegradation capacity" of the groundwater flowing through the source zone and plume can be developed. The biodegradation capacity is then used directly in the BIOSCREEN model to simulate the effects of an instantaneous reaction. The suggested calculation approach to develop BIOSCREEN input data is:

Biodegradation Capacity (mg/L) =

$$\begin{aligned}
 & \{ (\text{Average Upgradient Oxygen Conc.}) - (\text{Minimum Source Zone Oxygen Conc}) \} / 3.14 \\
 + & \{ (\text{Average Upgradient Nitrate Conc.}) - (\text{Minimum Source Zone Nitrate Conc}) \} / 4.9 \\
 + & \{ (\text{Average Upgradient Sulfate Conc.}) - (\text{Minimum Source Zone Sulfate Conc}) \} / 4.7 \\
 + & \{ \text{Average Observed Ferrous Iron Conc. in Source Area} \} / 21.8 \\
 + & \{ \text{Average Observed Methane Conc. in Source Area} \} / 0.78
 \end{aligned}$$

Biodegradation capacity is similar to "expressed assimilative capacity" described in the AFCEE Technical Protocol, except that expressed assimilative capacity is based on the *maximum* observed concentration observed in the source zone for iron and methane, while the biodegradation capacity term used in BIOSCREEN is based on the *average* concentration in the source zone for iron and methane. BIOSCREEN uses the more conservative biodegradation capacity approach to provide a conservative screening tool to users. Calculated biodegradation capacities (from Groundwater Services sites) and expressed assimilative capacities (from Parsons Engineering-Science sites) at different U.S. Air Force RNA research sites have ranged from 7 to 70 mg/L (see Table 1). The median capacity for 28 AFCEE sites is 28.5 mg/L.

Note that one criticism of this lumped biodegradation capacity approach is that it assumes that all of the various aerobic and anaerobic reactions occur over the entire area of the contaminant plume, and that the theoretical "zonation" of reactions is not simulated in BIOSCREEN (e.g. typically dissolved oxygen utilization occurs at the downgradient portion and edges of the plume, nitrate utilization a little closer to the source, iron reduction in the middle of the plume, sulfate reduction near the source, and methane production in the heart of the source zone). A careful inspection of actual field data (see Figure 1) shows little or no evidence of this theoretical zonation of reactions; in

fact all of the reactions appear to occur simultaneously in the source zone. The most common pattern observed at petroleum release sites is that ferrous iron and methane seems to be restricted to the higher-concentration or source zone areas, with the other reactions (oxygen, nitrate, and sulfate depletion), occurring throughout the plume.

BIOSCREEN assumes that all of the biodegradation reactions (aerobic and anaerobic) occur almost instantaneously relative to the hydraulic residence time in the source area and plume. Because iron reduction and methane production appear to occur only in the source zone (probably due to the removal of these metabolic by-products) it is recommended to use the *average* iron and methane concentrations observed in the source zone for the calculation of biodegradation capacity instead of maximum concentrations. In addition, the iron and methane concentrations are used during a secondary calibration step (see below). Beta testing of BIOSCREEN indicated that the use of the maximum concentration of iron and methane tended to overpredict biodegradation at many sites by assuming these reactions occurred over the entire plume area. Use of an average value (or some reduced value) helps match actual field data.

7. Note that at some sites the instantaneous reaction model will appear to overpredict the amount of biodegradation that occurs, and underpredict at others. As with the case of the first-order decay model, some calibration to actual site conditions is required. With the first-order decay, the decay coefficient is adjusted arbitrarily until the predicted values match observed field conditions. With the instantaneous reaction model, there is no first-order decay coefficient to adjust, so the following procedure is recommended:
 - A) The primary calibration step (if needed) is to manipulate the model's dispersivity values. As described in the BIOSCREEN Data Entry Section below, values for dispersivity are related to aquifer scale (defined as the plume length or distance to the measurement point) and simple relationships are usually applied to estimate dispersivities. Gelhar *et al.* (1992) cautions that dispersivity values vary between 2-3 orders of magnitude for a given scale due to natural variation in hydraulic conductivity at a particular site. Therefore dispersivity values can be manipulated within a large range and still be within the range of values observed at field test sites. In BIOSCREEN, adjusting the transverse dispersivity alone will usually be enough to calibrate the model.
 - B) As a secondary calibration step, the biodegradation capacity calculation may be reevaluated. There is some judgment involved in averaging the electron acceptor concentrations observed in upgradient wells; determining the minimum oxygen, nitrate and sulfate in the source zone; and estimating the average ferrous iron and methane concentrations in the source zone. Although probably not needed in most applications, these values may be adjusted as a final level of calibration.

BIOSCREEN CONCEPTS

The BIOSCREEN Natural Attenuation software is based on the Domenico (1987) three-dimensional analytical solute transport model. The original model assumes a fully-penetrating vertical plane source oriented perpendicular to groundwater flow, to simulate the release of organics to moving groundwater. In addition, the Domenico solution accounts for the effects of advective transport, three-dimensional dispersion, adsorption, and first-order decay. In BIOSCREEN, the Domenico solution has been adapted to provide three different model types representing i) transport with no decay, ii) transport with first-order decay, and iii) transport with

"instantaneous" biodegradation reaction (see Model Types). Guidelines for selecting key input parameters for the model are outlined in BIOSCREEN Input Parameters. For help on Output, see BIOSCREEN Output.

BIOSCREEN Model Types

The software allows the user to see results from three different types of groundwater transport models, all based on the Domenico solution:

1. **Solute transport with no decay.** This model is appropriate for predicting the movement of conservative (non-degrading) solutes such as chloride. The only attenuation mechanisms are dispersion in the longitudinal, transverse, and vertical directions, and adsorption of contaminants to the soil matrix.
2. **Solute transport with first-order decay.** With this model, the solute degradation rate is proportional to the solute concentration. The higher the concentration, the higher the degradation rate. This is a conventional method for simulating biodegradation in dissolved hydrocarbon plumes. Modelers using the first-order decay model typically use the first-order decay coefficient as a calibration parameter, and adjust the decay coefficient until the model results match field data. With this approach, uncertainties in a number of parameters (e.g., dispersion, sorption, biodegradation) are lumped together in a single calibration parameter.

Literature values for the half-life of benzene, a readily biodegradable dissolved hydrocarbon, range from 10 to 730 days while the half-life for TCE, a more recalcitrant constituent, is 10.7 months to 4.5 years (Howard *et al.*, 1991). Other applications of the first-order decay approach include radioactive solutes and abiotic hydrolysis of selected organics, such as dissolved chlorinated solvents. One of the best sources of first-order decay coefficients in groundwater systems is *The Handbook of Environmental Degradation Rates* (Howard *et al.*, 1991).

The first-order decay model does not account for site-specific information such as the availability of electron acceptors. In addition, it does not assume any biodegradation of dissolved constituents in the source zone. In other words, this model assumes biodegradation starts immediately downgradient of the source, and that it does not depress the concentrations of dissolved organics in the source zone itself.

3. **Solute transport with "instantaneous" biodegradation reaction.** Modeling work conducted by GSI indicate first-order expressions may not be as accurate for describing natural attenuation processes as the instantaneous reaction assumption (Connor *et al.*, 1994). Biodegradation of organic contaminants in groundwater is more difficult to quantify using a first-order decay equation because electron acceptor limitations are not considered. A more accurate prediction of biodegradation effects may be realized by incorporating the instantaneous reaction equation into a transport model. This approach forms the basis for the BIOSCREEN instantaneous reaction model.

To incorporate the instantaneous reaction in BIOSCREEN, a superposition method was used. By this method, contaminant mass concentrations at any location and time within the flow field are corrected by subtracting 1 mg/L organic mass for each mg/L of biodegradation capacity provided by all of the available electron acceptors, in accordance with the instantaneous reaction assumption. Borden *et al.* (1986) concluded that this

simple superposition technique was an exact replacement for more sophisticated oxygen-limited expressions, as long as the oxygen and hydrocarbon had the same transport rates (e.g., retardation factor, $R = 1$). Connor *et al.* (1994) revived this approach for use in spreadsheets and compared the results to those from more sophisticated but difficult to use numerical models. They found this approach to work well, even for retardation factors greater than 1, so this superposition approach was incorporated into the BIOSCREEN model (see Appendix A.2).

Which Kinetic Model Should One Use in BIOSCREEN?

BIOSCREEN gives the user three different models to choose from to help see the effect of biodegradation. At almost all petroleum release sites, biodegradation is present and can be verified by demonstrating the consumption of aerobic and anaerobic electron acceptors. Therefore, results from the No Biodegradation model are intended only to be used for comparison purposes and to demonstrate the effects of biodegradation on plume migration.

Some key factors for comparison of the First-order Decay model and the Instantaneous Reaction model are presented below:

FACTOR	First-Order Decay Model	Instantaneous Reaction Model
Able to Utilize Data from AFCEE Intrinsic Remediation Protocol?	<ul style="list-style-type: none"> No - Does not account for electron acceptors/by-products 	<ul style="list-style-type: none"> Yes - Accounts for availability of electron acceptors and by-products
Simple to Use?	<ul style="list-style-type: none"> Yes 	<ul style="list-style-type: none"> Yes
Simplification of Numerical Model?	<ul style="list-style-type: none"> Yes - many numerical models include first-order decay 	<ul style="list-style-type: none"> Yes - Simplification of BIOPLUME III model
Familiar to Modelers?	<ul style="list-style-type: none"> More commonly used 	<ul style="list-style-type: none"> Used less frequently
Key Calibration Parameter	<ul style="list-style-type: none"> First-Order Decay Coefficients 	<ul style="list-style-type: none"> Source Term/Dispersivity
Over - or Underestimates Source Decay Rate?	<ul style="list-style-type: none"> May underpredict rate of source depletion (see Newell <i>et al.</i>, 1995) 	<ul style="list-style-type: none"> May be more accurate for estimating rate of source depletion (see Newell <i>et al.</i>, 1995)

A key goal of the AFCEE Natural Attenuation Initiative is to quantify the magnitude of RNA based on field measurements of electron acceptor consumption and metabolic by-product production. Therefore, the Instantaneous Reaction model is recommended either alone or in addition to the first-order decay model (if appropriate calibration is performed) for most sites where the Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, *et al.*, 1995) has been applied. For a more rigorous analysis of natural attenuation, the BIOPLUME III model (to be released in late 1996) may be more appropriate.

BIOSCREEN DATA ENTRY

Three important considerations regarding data input are:

- 1) To see the example data set in the input screen of the software, click on the "Paste Example Data Set" button on the lower right portion of the input screen.
- 2) Because BIOSCREEN is based on the Excel spreadsheet, you have to click outside of the cell where you just entered data or hit "return" before any of the buttons will work.

- 3) Several cells have data that can be entered directly or can be calculated by the model using data entered in the grey cells (e.g., seepage velocity can be entered directly or calculated using hydraulic conductivity, gradient, and effective porosity). If the calculation option does not appear to work, check to make sure that there is still a formula in the cell. If not, you can restore the formula by clicking on the "Restore Formulas" button on the bottom right hand side of the input screen. If there still appears to be a problem, click somewhere outside of the last cell where you entered data and then click on the "Recalculate" button on the input screen.

1. HYDROGEOLOGIC DATA

Parameter	Seepage Velocity (Vs)
Units	ft/yr
Description	Actual interstitial groundwater velocity, equaling Darcy velocity divided by effective porosity. Note that the Domenico model and BIOSCREEN are not formulated to simulate the effects of chemical diffusion. Therefore, contaminant transport through very slow hydrogeologic regimes (e.g., clays and slurry walls) should probably not be modeled using BIOSCREEN unless the effects of chemical diffusion are proven to be insignificant. Domenico and Schwartz (1990) indicate that chemical diffusion is insignificant for Peclet numbers (seepage velocity times median pore size divided by the bulk diffusion coefficient) > 100.
Typical Values	0.5 to 200 ft/yr
Source of Data	Calculated by multiplying hydraulic conductivity by hydraulic gradient and dividing by effective porosity. It is strongly recommended that actual site data be used for hydraulic conductivity and hydraulic gradient data parameters; effective porosity can be estimated.
How to Enter Data	1) Enter directly or 2) Fill in values for hydraulic conductivity, hydraulic gradient, and effective porosity as described below and have BIOSCREEN calculate seepage velocity. Note: if the calculation option does not appear to work, check to make sure that the cell still contains a formula. If not, you can reincarnate the formula by clicking on the "Restore Formulas" button on the bottom right hand side of the input screen. If there is still a problem, make sure to click somewhere outside of the last cell where you entered data and then click on the "Recalculate" button on the input screen.

Parameter	Hydraulic Conductivity (K)
Units	cm/sec
Description	Horizontal hydraulic conductivity of the saturated porous medium.
Typical Values	Clays: 1×10^{-6} cm/s Silts: 1×10^{-6} - 1×10^{-3} cm/s Silty sands: 1×10^{-5} - 1×10^{-1} cm/s

	Clean sands: $1 \times 10^{-3} - 1 \text{ cm/s}$ Gravels: $> 1 \text{ cm/s}$
Source of Data	Pump tests or slug tests at the site. It is strongly recommended that actual site data be used for most RNA studies.
How to Enter Data	Enter directly. If seepage velocity is entered directly, this parameter is not needed in BIOSCREEN.

Parameter	Hydraulic Gradient (i)
Units	ft/ft
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table.
Typical Values	0.0001 - 0.05 ft/ft
Source of Data	Calculated by constructing potentiometric surface maps using static water level data from monitoring wells and estimating the slope of the potentiometric surface.
How to Enter Data	Enter directly. If seepage velocity is entered directly, this parameter is not needed in BIOSCREEN.

Parameter	Effective Porosity (n)																								
Units	unitless																								
Description	Dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix. Note that "total porosity" is the ratio of all voids (included non-connected voids) to the bulk volume of the aquifer matrix. Difference between total and effective porosity reflect lithologic controls on pore structure. In unconsolidated sediments coarser than silt size, effective porosity can be less than total porosity by 2-5% (e.g. 0.28 vs, 0.30) (Smith and Wheatcraft, 1993).																								
Typical Values	<p>Values for Effective Porosity:</p> <table border="0"> <tr> <td>Clay</td> <td>0.01 - 0.20</td> <td>Sandstone</td> <td>0.005 - 0.10</td> </tr> <tr> <td>Silt</td> <td>0.01 - 0.30</td> <td>Unfract. Limestone</td> <td>0.001- 0.05</td> </tr> <tr> <td>Fine Sand</td> <td>0.10 - 0.30</td> <td>Fract. Granite</td> <td>0.00005 - 0.01</td> </tr> <tr> <td>Medium Sand</td> <td>0.15 - 0.30</td> <td></td> <td></td> </tr> <tr> <td>Coarse Sand</td> <td>0.20 - 0.35</td> <td></td> <td></td> </tr> <tr> <td>Gravel</td> <td>0.10 - 0.35</td> <td></td> <td></td> </tr> </table> <p><i>(From Wiedemeier, Wilson, et al., 1995; originally from Domenico and Schwartz, 1990 and Walton, 1988).</i></p> <p><i>(From Domenico and Schwartz, 1990)</i></p>	Clay	0.01 - 0.20	Sandstone	0.005 - 0.10	Silt	0.01 - 0.30	Unfract. Limestone	0.001- 0.05	Fine Sand	0.10 - 0.30	Fract. Granite	0.00005 - 0.01	Medium Sand	0.15 - 0.30			Coarse Sand	0.20 - 0.35			Gravel	0.10 - 0.35		
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Medium Sand	0.15 - 0.30																								
Coarse Sand	0.20 - 0.35																								
Gravel	0.10 - 0.35																								
Source of Data	Typically estimated. One commonly used value for silts and sands is an effective porosity of 0.25. The ASTM RBCA Standard (ASTM, 1995) includes a default value of 0.38 (to be used primarily for																								

	unconsolidated deposits).
How to Enter Data	Enter directly. Note that if seepage velocity is entered directly, this parameter is still needed to calculate the retardation factor and plume mass.

2. DISPERSIVITY	
Parameter	Longitudinal Dispersivity (alpha x) Transverse Dispersivity (alpha y) Vertical Dispersivity (alpha z)
Units	ft
Description	Dispersion refers to the process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, simple estimation techniques based on the length of the plume or distance to the measurement point ("scale") are available from a compilation of field test data. Note that researchers indicate that dispersivity values can range over 2-3 orders of magnitude for a given value of plume length or distance to measurement point (Gelhar <i>et al.</i> , 1992). In BIOSCREEN, dispersivity is used as the primary calibration parameter (see pg 12). For more information on dispersivity, see Appendix A.4, pg 47).
Typical Values	<p>Typical dispersivity relationships as a function of L_p (plume length or distance to measurement point in ft) are provided below. BIOSCREEN is programmed with some commonly used relationships representative of typical and low-end dispersivities:</p> <ul style="list-style-type: none"> <p>• Longitudinal Dispersivity</p> $\text{Alpha } x = 3.28 \cdot 0.83 \cdot \left[\log_{10} \left(\frac{L_p}{3.28} \right) \right]^{2.414} \quad (\text{Xu and Eckstein, 1995})$ <p style="text-align: center;"><i>(L_p in ft)</i></p> <p>• Transverse Dispersivity</p> <p>Alpha y = 0.10 alpha x <i>(Based on high reliability points from Gelhar et al., 1992)</i></p> <p>• Vertical Dispersivity</p> <p>Alpha z = very low (i.e. 1 x 10⁻⁹⁹ ft) <i>(Based on conservative estimate)</i></p> <hr style="border: 1px solid #cccccc;"/> <p>Other commonly used relationships include:</p> <p>Alpha x = 0.1 L_p <i>(Pickens and Grisak, 1981)</i></p> <p>Alpha y = 0.33 alpha x <i>(ASTM, 1995) (EPA, 1986)</i></p> <p>Alpha z = 0.05 alpha x <i>(ASTM, 1995)</i></p> <p>Alpha z = 0.025 alpha x to 0.1 alpha x <i>(EPA, 1986)</i></p>
Source of Data	Typically estimated using the relationships provided above (see

	Appendix A.4, pg 47).
How to Enter Data	1) Enter directly or 2) Fill in value of the estimated plume length and have BIOSCREEN calculate the dispersivities.

Parameter	Estimated Plume Length (Lp)
Units	ft
Description	Estimated length (in feet) of the existing or hypothetical groundwater plume being modeled. This is a key parameter as it is generally used to estimate the dispersivity terms (dispersivity is difficult to measure and field data are rarely collected).
Typical Values	For BTEX plumes, 50 - 500 ft. For chlorinated solvents, 50 to 1000 ft.
Source of Data	<p>To simulate an actual plume length or calibrate to actual plume data, enter the actual length of the plume. If trying to predict the maximum extent of plume migration, use one of the two methods below.</p> <p>1) Use seepage velocity, retardation factor, and simulation time to estimate plume length. While this may underestimate the plume length for a non-degrading solute, it may overestimate the plume length for either the first-order decay model or instantaneous reaction model if biodegradation is significant.</p> <p>2) Estimate a plume length, run the model, determine how long the plume is predicted to become (this will vary depending on the type of kinetic expression that is used), reenter this value, and then rerun the model. Note that considerable time and effort can be expended trying to adjust the estimated plume length term to match exactly the predicted modeling length. In practice, most modelers make the assumption that dispersivity values are not very precise, and therefore select ball-park values based on estimated plume lengths that are probably $\pm 25\%$ of the actual plume length used in the simulations. Note that BIOSCREEN is very sensitive to the dispersion estimates, particularly for the instantaneous reaction model.</p>
How to Enter Data	Enter directly. If dispersivity data are entered directly, this parameter is not needed in BIOSCREEN.

3. ADSORPTION DATA	
Parameter	Retardation Factor (R)
Units	unitless
Description	<p>The rate at which dissolved contaminants moving through an aquifer can be reduced by sorption of contaminants to the solid aquifer matrix. The degree of retardation depends on both aquifer and constituent properties. The retardation factor is the ratio of the groundwater seepage velocity to the rate that organic chemicals migrate in the groundwater. A retardation value of 2 indicates that if the groundwater seepage velocity is 100 ft/yr, then the organic chemicals migrate at approximately 50 ft/yr.</p> <p>BIOSCREEN simulations using the instantaneous reaction assumption at sites with retardation factors greater than 6 should be performed with caution and verified using a more sophisticated model such as BIOPLUME III (see Appendix A.2).</p>
Typical Values	1 to 2 (for BTEX in typical shallow aquifers)
Source of Data	<p>Usually estimated from soil and chemical data using variables described below (ρ_b = bulk density, n = porosity, K_{oc} = organic carbon-water partition coefficient, K_d = distribution coefficient, and f_{oc} = fraction organic carbon on uncontaminated soil) with the following expression:</p> $R = 1 + \frac{K_d \cdot \rho_b}{n} \quad \text{where} \quad K_d = K_{oc} \cdot f_{oc}$ <p>In some cases, the retardation factor can be estimated by comparing the length of a plume affected by adsorption (such as the benzene plume) with the length of plume that is not affected by adsorption (such as chloride). Most plumes do not have both types of contaminants, so it is more common to use the estimation technique (see data entry boxes below).</p>
How to Enter Data	1) Enter directly or 2) Fill in the estimated values for bulk density, partition coefficient, and fraction organic carbon as described below and have BIOSCREEN calculate retardation.

Parameter	Soil Bulk Density (ρ_b)
Units	kg/L or g/cm ³
Description	Bulk density, in kg/L, of the aquifer matrix (related to porosity and pure solids density).
Typical Values	Although this value can be measured in the lab, in most cases estimated values are used. A value of 1.7 kg/L is used frequently.
Source of Data	Either from an analysis of soil samples at a geotechnical lab or more commonly, application of estimated values such as 1.7 kg/L.
How to Enter Data	Enter directly. If the retardation factor is entered directly, this parameter is not needed in BIOSCREEN.

Parameter	Organic Carbon Partition Coefficient (Koc)								
Units	(mg/kg) / (mg/L) or (L/kg) or (mL/g)								
Description	Chemical-specific partition coefficient between soil organic carbon and the aqueous phase. Larger values indicate greater affinity of contaminants for the organic carbon fraction of soil. This value is chemical specific and can be found in chemical reference books. Note that many users of BIOSCREEN will simulate BTEX as a single constituent. In this case, either an average value for the BTEX compounds can be used, or it can be assumed that all of the BTEX compounds have the same mobility as benzene (the constituent with the highest potential risk to human health).								
Typical Values	<table border="0"> <tr> <td>Benzene</td> <td>38 L/kg</td> <td>Ethylbenzene</td> <td>95 L/kg</td> </tr> <tr> <td>Toluene</td> <td>135 L/kg</td> <td>Xylene</td> <td>240 L/kg</td> </tr> </table> <p>(ASTM, 1995)</p> <p>(Note that there is a wide range of reported values; for example, Mercer and Cohen (1990) report a Koc for benzene of 83 L/kg.</p>	Benzene	38 L/kg	Ethylbenzene	95 L/kg	Toluene	135 L/kg	Xylene	240 L/kg
Benzene	38 L/kg	Ethylbenzene	95 L/kg						
Toluene	135 L/kg	Xylene	240 L/kg						
Source of Data	Chemical reference literature or relationships between Koc and solubility or Koc and the octanol-water partition coefficient (Kow).								
How to Enter Data	Enter directly. If the retardation factor is entered directly, this parameter is not needed in BIOSCREEN.								

Parameter	Fraction Organic Carbon (foc)
Units	unitless
Description	Fraction of the aquifer soil matrix comprised of natural organic carbon in uncontaminated areas. More natural organic carbon means higher adsorption of organic constituents on the aquifer matrix.
Typical Values	0.0002 - 0.02
Source of Data	The fraction organic carbon value should be measured if possible by collecting a sample of aquifer material from an uncontaminated zone and performing a laboratory analysis (e.g. ASTM Method 2974-87 or equivalent). If unknown, a default value of 0.001 is often used (e.g., ASTM 1995).
How to Enter Data	Enter directly. If the retardation factor is entered directly, this parameter is not needed in BIOSCREEN.

4. BIODEGRADATION DATA	
Parameter	First-Order Decay Coefficient (λ)
Units	1/yr
Description	<p>Rate coefficient describing first-order decay process for dissolved constituents. The first-order decay coefficient equals 0.693 divided by the half-life of the contaminant in groundwater. In BIOSCREEN, the first-order decay process assumes that the rate of biodegradation depends only on the concentration of the contaminant and the rate coefficient. For example, consider 3 mg/L benzene dissolved in water in a beaker. If the half-life of the benzene in the beaker is 728 days, then the concentration of benzene 728 days from now will be 1.5 mg/L (ignoring volatilization and other losses).</p> <p>Considerable care must be exercised in the selection of a first-order decay coefficient for each constituent in order to avoid significantly over-predicting or under-predicting actual decay rates. Note that the amount of degradation that occurs is related to the time the contaminants spend in the aquifer, and that this parameter is not related to the time it takes for the source concentrations to decay by half.</p>
Typical Values	0.1 to 36 yr ⁻¹ (see half-life values)
Source of Data	<p>Optional methods for selection of appropriate decay coefficients are as follows:</p> <p>Literature Values: Various published references are available listing decay half-life values for hydrolysis and biodegradation (e.g., see Howard <i>et al.</i>, 1991). Note that many references report the half-lives; these values can be converted to the first-order decay coefficients using $k = 0.693 / t_{1/2}$ (see dissolved plume half-life).</p> <p>Calibrate to Existing Plume Data: If the plume is in a steady-state or diminishing condition, BIOSCREEN can be used to determine first-order decay coefficients that best match the observed site concentrations. One may adopt a trial-and-error procedure to derive a best-fit decay coefficient for each contaminant. For still-expanding plumes, this steady-state calibration method may over-estimate actual decay-rate coefficients and contribute to an under-estimation of predicted concentration levels.</p>
How to Enter Data	1) Enter directly or 2) Fill in the estimated half-life values as described below and have BIOSCREEN calculate the first-order decay coefficients.

Parameter	Dissolved Plume Solute Half-Life ($t_{1/2}$)
Units	years
Description	<p>Time, in years, for dissolved plume concentrations to decay by one half as contaminants migrate through the aquifer. Note that the amount of degradation that occurs is related to the time the contaminants spend in the aquifer, and that the degradation IS NOT related to the time it takes for the source concentrations to decay by half.</p> <p>Modelers using the first-order decay model typically use the first-order decay coefficient as a calibration parameter, and adjust the decay coefficient until the model results match field data. With this approach, uncertainty in a number of parameters (e.g., dispersion, sorption, biodegradation) are lumped together in a single calibration parameter.</p> <p>Considerable care must be exercised in the selection of a first-order decay coefficient for each contaminant in order to avoid significantly over-predicting or under-predicting actual decay rates.</p>
Typical Values	<p>Benzene 0.02 to 2.0 yrs Toluene 0.02 to 0.17 yr Ethylbenzene 0.016 to 0.62 yr Xylene 0.038 to 1 yr <i>(from ASTM, 1995)</i></p>
Source of Data	<p>Optional methods for selection of appropriate decay coefficients are as follows:</p> <p>Literature Values: Various published references are available listing decay half-life values for hydrolysis and biodegradation (e.g., see Howard <i>et al.</i>, 1991).</p> <p>Calibrate to Existing Plume Data: If the plume is in a steady-state or diminishing condition, BIOSCREEN can be used to determine first-order decay coefficients that best match the observed site concentrations. A trial-and-error procedure may be adopted to derive a best-fit decay coefficient for each contaminant. For expanding plumes, this steady-state calibration method may over-estimate actual decay-rate coefficients and contribute to an under-estimation of predicted concentration levels.</p>
How to Enter Data	Enter directly. If the first-order decay coefficient is entered directly, this parameter is not needed in BIOSCREEN.

Parameter	Delta Oxygen (O ₂)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The model assumes that 3.14 mg of oxygen are required to consume 1 mg of BTEX (Wiedemeier, Wilson, <i>et al.</i> , 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 5.8 mg/L Maximum = 12.7 mg/L Minimum = 0.4 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, <i>et al.</i> , 1995) should be applied. Enter the average background concentration of oxygen minus the lowest observed concentration of oxygen in the source area. BIOSCREEN automatically applies the utilization factor used to compute a biodegradation capacity.
How to Enter Data	Enter directly.

Parameter	Delta Nitrate (NO ₃)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The model assumes that 4.9 mg of nitrate are required to consume 1 mg of BTEX (Wiedemeier, Wilson, <i>et al.</i> , 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 6.3 mg/L Maximum = 69.7 mg/L Minimum = 0 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, <i>et al.</i> , 1995) should be applied. Enter the average background concentration of nitrate minus the lowest observed concentration of nitrate in the source area. BIOSCREEN automatically applies the utilization factor to

	compute a biodegradation capacity.
How to Enter Data	Enter directly.
Parameter	Observed Ferrous Iron (Fe^{2+})
Units	mg/L
Description	<p>This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. Ferrous iron is a metabolic by-product of the anaerobic reaction where solid ferric iron is used as an electron acceptor. The model assumes that 21.8 mg of ferrous iron represents the consumption of 1 mg of BTEX (Wiedemeier, Wilson, <i>et al.</i>, 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.</p> <p>Because ferrous iron reacts with the sulfide produced from the reduction of sulfate, some or most of the ferrous iron may not be observed during groundwater sampling. Some researchers suspect that the observed ferrous iron concentration is much less (10% or less) than the actual amount of ferrous iron that has been generated due to the sorption of ferrous iron onto the aquifer matrix (Lovely, 1995). If this is the case, then the value used for this parameter should be much higher than the observed maximum concentration of ferrous iron in the aquifer.</p>
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 16.6 mg/L Maximum = 599.5 mg/L Minimum = 0 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, <i>et al.</i> , 1995) should be applied. Enter the average observed concentration, in mg/L, of ferrous (dissolved) iron found in the source area (approximately the area where ferrous iron has been observed in monitoring wells). BIOSCREEN automatically applies the utilization factor to compute a biodegradation capacity.
How to Enter Data	Enter directly.

Parameter	Delta Sulfate (SO ₄)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The model assumes that 4.7 mg of sulfate are required to consume 1 mg of BTEX (Wiedemeier, Wilson, <i>et al.</i> , 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 24.6 mg/L Maximum = 109.2 mg/L Minimum = 0 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, <i>et al.</i> , 1995) should be applied. Enter the average background concentration of sulfate minus the lowest observed concentration of sulfate in the source area. BIOSCREEN then computes a biodegradation capacity.
How to Enter Data	Enter directly.

Parameter	Observed Methane (CH ₄)
Units	mg/L
Description	This parameter, used in the instantaneous reaction model, is one component of the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. Methane is a metabolic by-product of methanogenic activity. The model assumes that 0.78 mg of methane represents the consumption of 1 mg of BTEX (Wiedemeier, Wilson, <i>et al.</i> , 1995). Note that this parameter is used for the instantaneous reaction model, which is appropriate only for readily biodegradable compounds such as BTEX that degrade according to the assumed BIOSCREEN utilization factors, and is not appropriate for more recalcitrant compounds such as the chlorinated solvents.
Typical Values	Data from 28 AFCEE sites (see Table 1): Median = 7.2 mg/L Maximum = 48.4 mg/L Minimum = 0.0 mg/L
Source of Data	For planning studies, typical values taken from Table 1 can be used. For actual RNA studies, the Air Force Intrinsic Remediation Technical Protocol (Wiedemeier, Wilson, <i>et al.</i> , 1995) should be applied. Enter the average observed concentration of methane found in the source area (approximately the area where methane is observed in monitoring wells). BIOSCREEN automatically computes a biodegradation capacity.

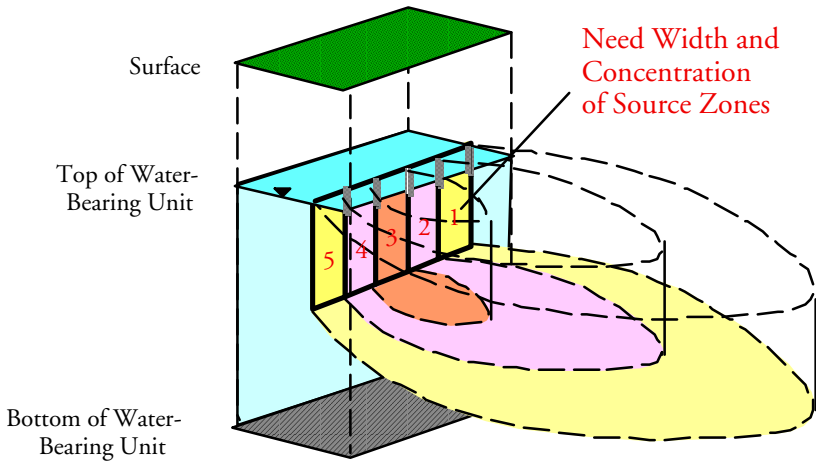
How to Enter Data	Enter directly.
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5. GENERAL DATA

Parameter	Model Area Length and Width (L and W)
Units	ft
Description	Physical dimensions (in feet) of the rectangular area to be modeled. To determine contaminant concentrations at a particular point along the centerline of the plume (a common approach for most risk assessments), enter this distance in the "Modeled Area Length" box and see the results by clicking on the "Run Centerline" button. If one is interested in more accurate mass calculations, make sure most of the plume is within the zone delineated by the Modeled Area Length and Width. Find the mass balance results using the "Run Array" button.
Typical Values	10 to 1000 ft
Source of Data	Values should be slightly larger than the final plume dimensions or should extend to the downgradient point of concern (e.g., point of exposure). If only the centerline output is used, the plume width parameter has no effect on the results.
How to Enter Data	Enter directly.

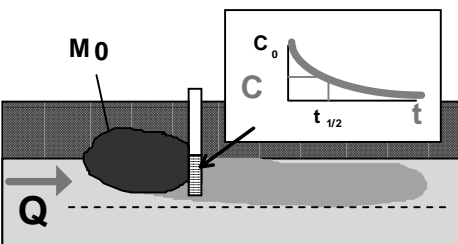
Parameter	Simulation Time (t)
Units	years
Description	Time (in years) for which concentrations are to be calculated. For steady-state simulations, enter a large value (i.e., 1000 years would be sufficient for most sites).
Typical Values	1 to 1000 years
Source of Data	To match an existing plume, estimate the time between the original release and the date the field data were collected. To predict the maximum extent of plume migration, increase the simulation time until the plume no longer increases in length.
How to Enter Data	Enter directly.

6. SOURCE DATA	
Parameter	Source Thickness In Saturated Zone (z)
Units	ft
Description	<p>The Domenico (1987) model assumes a vertical plane source of constant concentration. For many fuel spill sites the thickness of this source zone is only 5 - 20 ft, as petroleum fuels are LNAPLs (light non-aqueous phase liquids) that float on the water table. Therefore, the residual source zones that are slowly dissolving, creating the dissolved BTEX plume, are typically restricted to the upper part of the aquifer.</p> <p style="text-align: center;">Surface</p> <p style="text-align: center;">Top of Water-Bearing Unit</p> <p style="text-align: center;">Source Thickness</p> <p style="text-align: center;">Bottom of Water-Bearing Unit</p>
Typical Values	5-50 ft
Source of Data	<p>This value is usually determined by evaluating groundwater data from wells near the source zone screened at different depths. If this type of information is not available, then one could estimate the amount of water table fluctuation that has occurred since the time of the release and use this value as the source zone thickness (equating to the smear zone). Otherwise, a simple assumption of 10 feet would probably be appropriate for many petroleum release sites. Note that if DNAPLs are present at the site (e.g., a chlorinated solvent site), a larger source zone thickness would probably be required.</p>
How to Enter Data	Enter directly.

Parameter	Source Zone Width
Units	ft
Description	The Domenico (1987) model assumes a vertical plane source of constant concentration. BIOSCREEN expands the simple one source-zone approach by allowing up to five source zones with different concentrations to account for spatial variations in the source area.
Typical Values	10 - 200 ft
Source of Data	<p>To define a varying source concentration across the site:</p> <ol style="list-style-type: none"> 1) Draw a line perpendicular to the groundwater flow direction in the source zone. The source zone is typically defined as being the area with contaminated soils having high concentrations of sorbed organics, free-phase NAPLs, or residual NAPLs. If the source zone covers a large area, it is best to choose the most downgradient or widest point in the source area to draw the perpendicular-to-flow line. 2) Divide the line into 1, 3, or 5 zones. A total of 5 zones is shown on the input screen. 3) Determine the width and corresponding average concentration of Zones 1, 2, and 3. Typically Zone 3 will contain the highest concentration. Note that the model assumes the source zone is symmetrical and will automatically define source zones 4 and 5 to be identical to Zones 2 and 1. Therefore, it is not necessary to specify all 5 zones. For simpler problems, you can either use three zones to define varying source concentrations across the site (enter information in Zones 2 and 3, and the model will define Zone 4) or just use a single zone (enter data for Zone 3 only). 4) Enter the width and source concentration into the appropriate zones on the spreadsheet. For example, if a total source width of 100 ft. is divided into five zones, enter 20 ft for each zone width. Enter the average concentration observed across each zone. 
How to Enter Data	Enter directly.

Parameter	Source Zone Concentration
Units	mg/L
Description	<p>BIOSCREEN requires source zone concentrations that correspond to the source zone width data (see previous page). Suggested rules of thumb regarding how to handle multiple constituents are:</p> <p>1) If the maximum plume length is desired, model lumped constituents (such as BTEX). If a risk assessment is being performed, data on individual constituents are needed.</p> <p>2) If lumped constituents are being modeled (BTEX all together), use either average values for the chemical-specific data (Koc and lambda) or the worst-case values (e.g., use the lowest of the Koc and lambda from the group of constituents being modeled) to overestimate concentrations. Most modeling will be performed assuming that the ratio of BTEX at the edge of the plume is the same as at the source. For more detailed modeling studies, Wilson (1996) has proposed the following rules of thumb to help account for different rates of reaction among the BTEX compounds:</p> <ul style="list-style-type: none"> • If the site is dominated by aerobic degradation (most of the biodegradation capacity is from oxygen, a relatively rare occurrence) assume that the benzene will degrade first and that the dissolved material at the edge of the plume is primarily TEX. • If the site is dominated by nitrate utilization (most of the biodegradation capacity is from nitrate, a relatively rare occurrence) assume that benzene will degrade last and that the dissolved material at the edge of the plume is primarily benzene. • If the site is dominated by sulfate reduction (most of the biodegradation capacity is due to sulfate utilization, a more common occurrence) assume that the benzene will degrade at the same rate as the TEX constituents and that the dissolved material at the edge of the plume is a mixture of BTEX. • If the site is dominated by methane production (most of the biodegradation capacity is due to methanogenesis, a more common occurrence) assume that benzene will degrade last and that the dissolved material at the edge of the plume is primarily benzene. <p>3) If individual constituents are being modeled with the instantaneous reaction assumption, note that the total biodegradation capacity must be reduced to account for electron acceptor utilization by other constituents present in the plume. For example, in order to model benzene as an individual constituent using the instantaneous reaction model in a BTEX plume containing equal source concentrations of benzene, toluene, ethylbenzene and xylene, the amount of oxygen, nitrate, sulfate, iron, and methane should be reduced by 75% to account for utilization by toluene, ethylbenzene, and xylene.</p>
Typical Values	0.010 to 120 mg/L
Source of Data	Source area monitoring well data (see figure on previous page).

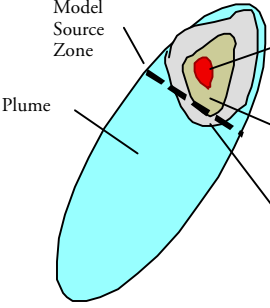
How to Enter Data	Enter directly.
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Parameter	Source Half-Life (Value Calculated by Model)
Units	years
Description	<p>The Domenico (1987) model assumes the source is infinite, i.e. the source concentrations are constant. In BIOSCREEN, however, an approximation for a declining source concentration has been added. Note that this is an experimental relationship, and it should be applied with caution. The declining source term is based on the following assumptions:</p> <ul style="list-style-type: none"> • There is a finite mass of organics in the source zone present as a free-phase or residual NAPL. The NAPL in the source zone dissolves slowly as fresh groundwater passes through. • The change in source zone concentration can be approximated as a first-order decay process. For example, if the source zone concentration "half-life" is 10 years and the initial source zone concentration is 1 mg/L, then the source zone concentration will be 0.5 mg/L after 10 years, and 0.25 mg/L after 20 years. <p>Note that the assumption that dissolution is a first-order process is only an approximation, and that source attenuation is best described by first-order decay when concentrations are relatively low (< 1 mg/L). For more information on dissolution, see Newell <i>et al.</i>, (1994). The source half-life IS NOT related to lambda, the biodegradation half-life for dissolved constituents. Lambda is used to calculate the amount of biodegradation of dissolved organics <i>after</i> they leave the source zone and travel through the plume area. The source half-life is related to the rate of dissolution occurring in the source zone, and describes the change in source concentrations over time.</p> <ul style="list-style-type: none"> • The BIOSCREEN software automatically calculates the source zone concentration half-life if the user enters a best estimate for the mass of dissolvable organics zone (soluble organic constituents sorbed on the soil, residual NAPLs, and free product) in the source. The half-life of the dissolution process can be approximated if one knows the mass of dissolvable organics in the source zone (in mg or kg), the flow rate through the source zone, and the average concentration of dissolved organics that leave the source zone. The equation is based on integrating the concentration vs. time relationship (first-order decay) and using the relationship that the mass in the source zone over time is proportional to the source concentration over time. This yields the following expression for the half-life of the concentration of dissolved organics in the source zone (see Appendix A.3): $t_{\text{half source}} = (0.693 * M_0) / (Q * C_0) \quad \text{where:}$ <div style="display: flex; align-items: flex-start;"> <div style="flex: 1;">  </div> <div style="flex: 1; padding-left: 20px;"> <p>$t_{\text{half source}}$ = Half-life of source concentration (yrs)</p> <p>Q = Groundwater flow through source zone (L/yr)</p> <p>C_0 = Effective source zone conc. (observed concentration + biodegradation capacity for inst. react. assumption) at $t = 0$ (mg/L)</p> </div> </div>

		M_0 = Mass of dissolvable organics in source zone at $t = 0$ (mg)
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Parameter	Source Half-Life (Value Calculated by Model)(Cont'd)
<p>Description (cont'd)</p> <p>Key Questions:</p>	<p>Why are there two source half-lives reported? Note that BIOSCREEN automatically selects the correct source half-life value depending on which kinetic model is being used (see Which Model Should One Use? under BIOSCREEN Concepts).</p> <p>Two source half-lives are reported by the model in the source half-life cell: the smaller number will be the source half-life from dissolution if Instantaneous Reaction kinetics are used, and the larger value will be for No Degradation or First-order Decay kinetics. The first-order decay model assumes biodegradation starts immediately downgradient of the source, and that the rate of dissolution is reflected by the concentration of dissolved organics actually measured in monitoring wells. In other words, the first-order decay model assumes C_0 is equal to the observed source concentration.</p> <p>The instantaneous reaction model assumes biodegradation is occurring directly in the source zone, and that the effective source zone concentration C_0 is equal to the measured concentration in the source zone plus any "missing" concentration due to biodegradation. For example, if the source zone concentration in monitoring wells is 5 mg/L, and the biodegradation capacity is 10 mg/L, the effective source concentration C_0 (concentration before biodegradation) is 15 mg/L. In other words, C_0 is equal to the measured source concentration plus the biodegradation capacity provided by the electron acceptor concentration. This means use of the instantaneous reaction assumption will result in higher dissolution rates and shorter source lifetimes (see Newell <i>et al.</i>, 1995).</p> <p>Does BIOSCREEN account for travel time away from the declining source? With the declining source option in BIOSCREEN, the concentration for any location and any time is calculated using a source concentration determined by the first-order decay calculations shown above. The time used to determine the source concentration is adjusted to account for the travel time between the source and measurement point.</p> <p>For example, consider the case where a declining source term is used with a source half-life of 10 years and a solute velocity of 100 ft/yr. To calculate the concentration at a point 2000 ft away at time = 30 years, BIOSCREEN follows these steps</p> <ol style="list-style-type: none"> 1) Calculates travel time from point to source: $2000/100 = 20$ years 2) Subtracts travel time from simulation time: $30 \text{ yrs} - 20 \text{ yrs} = 10 \text{ yrs}$ 3) Calculates source decay coeff.: $k_{\text{source}} = 0.693/(\text{source half-life})$ 4) Calculates source conc. at $t = 10$ yr: $C_{10} = C_0 \exp(-k_{\text{source}} \times 10 \text{ yrs})$
Typical Values	1 to 10,000 years
Source of Data	Calculated by model from soluble mass in NAPL and soil (see below), source concentrations, and groundwater velocity.
How to Enter	Calculated directly by model. Change by changing soluble mass.

Data	
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Parameter	Soluble Mass in NAPL, Soil																																
Units	kg																																
Description	<p>The best estimate of dissolvable organics in the source zone is obtained by adding the mass of dissolvable organics on soils, free-phase NAPLs, and residual NAPLs. This quantity is used to estimate the rate that the source zone concentration declines. Note that this is an experimental and unverified model that should be applied with care (the model probably underpredicts removal rate).</p> <p>For gasoline or JP-4 spills, BTEX is usually assumed to comprise the bulk of dissolvable organics in the source zone. To simulate a declining source, use the method described below. For constant-source simulations, either enter a very large number for soluble mass in the source zone (e.g., 1,000,000 kg) or type "Infinite".</p>																																
Typical Values	0.1 to 100,000 kg																																
Source of Data	<p>This information will most likely come from either:</p> <ol style="list-style-type: none"> 1) Estimates of the mass of spilled fuel (remember to convert the total mass of spilled fuel to the dissolvable mass; for example BTEX represents only 5-15% of the total mass of gasoline). 2) Integration of maps showing contaminated soil zones (data in mg/kg) and/or NAPL zones (usually product thickness). The user should estimate the volume of contaminated soil, convert to kg of contaminated soil, and multiply by the average soil concentration. To make the estimate more accurate, the user might have to divide the soil into different zones of soil concentrations, into unsaturated vs. saturated soil, and/or into different depths. (One standard approach is to divide into a vertically averaged unsaturated zone map and a vertically averaged saturated zone map.) If the user is making estimates from NAPL data, remember the thickness of product in a aquifer is only 10-50% of the actual product thickness in the well (Bedient <i>et al.</i>, 1994). <p>Note that the data is to be entered in kg, and the model will convert the results to estimate the source half-life. An example is provided below assuming a bulk density of 1.7 kg/L (e.g., 100 ft² x 20 ft x 28.3 L/ft³ x 1.7 kg/L x 600 mg/Kg x 10⁻⁶ kg/mg = 58 kg):</p> <div style="display: flex; align-items: center;">  <table style="margin-left: 20px;"> <thead> <tr> <th></th> <th></th> <th></th> <th>SOLUBLE MASS</th> </tr> </thead> <tbody> <tr> <td>Soil Area 1:</td> <td>100 sq. ft</td> <td>Depth 20 ft</td> <td></td> </tr> <tr> <td></td> <td colspan="2">Average Soil Concentration = 600 mg/Kg BTEX</td> <td>58 Kg</td> </tr> <tr> <td>Soil Zone 2:</td> <td>220 sq. ft</td> <td>Depth 20 ft</td> <td></td> </tr> <tr> <td></td> <td colspan="2">Average Soil Concentration = 50 mg/Kg BTEX</td> <td>11 Kg</td> </tr> <tr> <td>Soil Zone 3:</td> <td>400 sq. ft</td> <td>Depth 20 ft</td> <td></td> </tr> <tr> <td></td> <td colspan="2">Average Soil Concentration = 10 mg/Kg BTEX</td> <td>4 Kg</td> </tr> <tr> <td colspan="3" style="text-align: right;">TOTAL SOLUBLE MASS</td> <td>73 Kg</td> </tr> </tbody> </table> </div>				SOLUBLE MASS	Soil Area 1:	100 sq. ft	Depth 20 ft			Average Soil Concentration = 600 mg/Kg BTEX		58 Kg	Soil Zone 2:	220 sq. ft	Depth 20 ft			Average Soil Concentration = 50 mg/Kg BTEX		11 Kg	Soil Zone 3:	400 sq. ft	Depth 20 ft			Average Soil Concentration = 10 mg/Kg BTEX		4 Kg	TOTAL SOLUBLE MASS			73 Kg
			SOLUBLE MASS																														
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	Average Soil Concentration = 10 mg/Kg BTEX		4 Kg																														
TOTAL SOLUBLE MASS			73 Kg																														
How to Enter	Enter directly.																																

Data	
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7. FIELD DATA FOR COMPARISON

Parameter	Field Data for Comparison
Units	mg/L
Description	These parameters are concentrations of dissolved organics in wells near the centerline of the plume. These data are used to help calibrate the model and are displayed with model results in the "Run Centerline" option.
Typical Values	0.001 to 50 mg/L
Source of Data	Monitoring wells located near the centerline of the plume.
How to Enter Data	Enter as many or as few of these points as needed. The data are used only to help calibrate the model when comparing the results from the centerline option. Note that the distance from source values cannot be changed; use the closest value possible.

ANALYZING BIOSCREEN OUTPUT

The output shows concentrations along the centerline (for all three kinetic models at the same time) or as an array (one kinetic model at a time). Note that the results are all for the time entered in the "Simulation Time" box.

Centerline Output

Centerline output is displayed when the "Run Centerline" button is pressed on the input screen. The centerline output screen shows the average concentration at the top of the saturated zone (Z=0) along the centerline of the plume (Y=0). Clicking on "Animate" divides the simulation into 10 separate time periods and shows the movement of the plume based on the three BIOSCREEN models (red: no degradation, blue: first-order decay, green: instantaneous reaction). Note that all concentrations are displayed in units of mg/L.

Array Output

The array output is displayed when the "Run Array" button is pressed on the Input screen. The user is asked to select one of the three model types (no degradation, first-order decay, or instantaneous reaction). A 3-D graphic shows results on a 10-point-long by 5-point-wide grid. To alter the modeled area, adjust the Model Area Length and Width parameters on the input screen.

To see the plume array that exceeds a certain target level (such as an MCL or risk-based cleanup level), enter the target level in the box and push "Plot Data > Target". Only sections of the plume exceeding the target level will be displayed. To see all the data again, push "Plot All Data". Note that BIOSCREEN automatically resets this button to "Plot All Data" when the "Run Array" button is pressed on the input screen. An approximate mass balance is presented on the array output screen as described below.

Calculating the Mass Balance

Plume Mass if No Biodegradation(kg)
<p>The model calculates the total amount of dissolved contaminant that has left the source zone. If the source is an infinite source, then the calculation is based on the discharge of groundwater through the source zone (Darcy velocity for groundwater times the total source width times the source depth) times the average concentration of the source zone (a weighted average of concentration and source length for each of the different source zones) times the simulation time.</p> <p>If the source is a declining source, an exponential source decay term is used to estimate the mass of organics that have left the source zone (see Source Data: Varying Concentrations Over Time). Note that the source decay term is for dissolution of soluble organics from the source zone and is not related to the first-order decay term for the dissolved constituents.</p> <p>Note that the total mass in the plume is the same for the No Degradation and First-order Decay models but is different for the Instantaneous Reaction model. The source zone dissolution rate is calculated to be much higher if the instantaneous reaction model is selected. The instantaneous reaction assumes that active biodegradation reactions occur in the source zone, and that the observed concentrations of organics in source zone monitoring wells reflect conditions after biodegradation. In this case, the actual concentration of organics coming off the source zone is equal to the measured concentration plus the biodegradation capacity of the upgradient groundwater. The resulting higher effective dissolution rate equates to a greater amount of mass leaving the source area, leading to different mass values for the Instantaneous Reaction model.</p>

Actual Plume Mass(kg)
<p>BIOSCREEN calculates the mass of organics in the 5x10 plume array for the three models:</p> <p>1) No Degradation 2) 1st Order Decay 3) Instantaneous Reaction</p> <p>The mass is calculated by assuming that each point represents a cell equal to the incremental width and length (except for the first column which is assumed to be half as long as the other columns because the source is assumed to be in the middle of the cell). The volume of affected groundwater in each cell is calculated by multiplying the area of each cell by the source depth and by porosity (the mass balance calculation assumes 2-D transport). The mass of organics in each cell is then determined by multiplying the volume of groundwater by the concentration and then by the retardation factor (to account for sorbed constituents).</p>
<p>How BIOSCREEN Estimates Actual Plume Mass for Biodegradation Models</p> <p>If the mass of organics in the 5x10 plume array is within 50% to 150% of the mass of organics that have left the source (see box above), then two values are calculated:</p> <p>% Biodegraded, 1st order decay = (Plume Mass, 1st order decay) * 100 / (Plume mass, no biodeg)</p> <p>% Biodegraded, inst. react. = (Plume Mass, inst. react) * 100 / (Plume mass, no biodeg)</p> <p>These percentages are multiplied against the Plume Mass if No Biodegradation Value (first box) to estimate the actual plume mass for the two biodegradation models. If the No Degradation model has been selected, there is no biodegradation, and the Actual Plume Mass (second box) will equal the Plume Mass if No Biodegradation (first box).</p>

If BIOSCREEN Says " Can't Calc"

If the mass of organics in the plume does not fall within 50% to 150% of the mass of organics that have left the source (first box), then the model concludes that the modeled area (see Input Screen, Section 5: General Data) is not sized correctly to capture enough mass in the 5X10 array and writes "Can't Calc" in the box. The user is encouraged to adjust the modeled length and width to capture most of the No Degradation plume in the 5x10 array. In addition, sometimes source conditions with variable concentrations and widths (see input screens) can make it difficult to accurately capture the plume mass. If the user has problems obtaining a mass balance even after changing the modeled area, change the source term to a single source zone (instead of 3 or 5 zones) to improve the accuracy of the mass balance.

If problems still exist, ensure that the vertical dispersivity term (Section 2 on the Input Screen) is set to 0 (the default value). The mass balance calculations are less accurate for three-dimensional simulations.

Plume Mass Removed by Biodegradation (kg)

An estimate of the mass of contaminants that are biodegraded is provided in BIOSCREEN. The model subtracts the Actual Plume Mass (second box) from the Plume Mass if No Biodegradation (first box). For the No Degradation model, the first box equals the second box, and **Plume Mass Removed by Biodeg** is zero. For the other two cases, the 2 boxes will differ, and the amount of biodegradation will be calculated. The value beneath the third box shows the % of organics that have left the source and have been biodegraded.

Change in Electron Acceptor/Byproduct Masses (kg)

BIOSCREEN uses the Plume Mass Removed by Biodegradation to back-calculate the amount of measurable electron acceptors consumed and the amount of measurable metabolic by-products that have been produced.

For example, the amount of oxygen consumed is calculated by:

$$\text{Oxygen Consumed (kg)} = (\text{Plume Mass Removed by Biodeg}) * \frac{(\text{Delta O}_2/\text{Util. Fact.})}{(\text{Biodeg. Capacity})}$$

(see Biodegradation Capacity section to see how this term is calculated)

Note that the total sum of consumed electron acceptors does not equal the Plume Mass Removed by Biodegradation. This is because the stoichiometry of the biodegradation reactions do not represent a 1:1 relationship between the mass of hydrocarbon and electron acceptor consumed (see Utilization Factor section).

Original Mass in Source (kg)

Equal to the Soluble Mass in NAPL and Soil entered by the user on the Input Screen. If the user has selected an "Infinite" mass to simulate a non-declining source, this box will show "Infinite."

Mass in Source Now (kg)

The amount of mass remaining in the source zone at the end of the simulation period is calculated and displayed in this box. This calculation is performed as follows:

$$(\text{Mass in the Source Now}) = (\text{Original Mass in Source}) - (\text{Actual Plume Mass} + \text{Plume Mass Removed by Biodeg})$$

Current Volume of Groundwater in Plume (ac-ft)

If the mass of organics in the plume falls within 50% to 150% of the mass of organics that have left the source (first box), then the model concludes the modeled area (see Input Screen, Section 5: General Data) is appropriately sized to estimate the volume of the plume. In this case BIOSCREEN counts the number of cells in the 5 x 10 array with concentration values greater than 0, and multiplies this by the volume of groundwater in each cell (length * width * source thickness * porosity).

If the user wishes to estimate the volume of the plume above a certain target level, enter the target level in the appropriate box and press the appropriate model to display the result (No Degradation, 1st Order Decay, or Instantaneous Reaction).

Note that the model does not account for the effects of any vertical dispersion.

Flowrate of Water Through Source Zone (ac-ft/yr)

Using the Darcy velocity, the source thickness, and the source width, BIOSCREEN calculates the rate that clean groundwater moves through the source zone where it will pick up dissolved hydrocarbons. Note that the groundwater Darcy velocity is equal to the groundwater seepage velocity multiplied by porosity.

BIOSCREEN TROUBLESHOOTING TIPS

Minimum System Requirements

The BIOSCREEN model requires a computer system capable of running Microsoft® Excel 5.0 for Windows. Because of the volume of calculations required to process the numerical data generated by the model, GSI recommends running the model on a system equipped with a 486 DX or higher processor running at 66 MHz or faster. A minimum of 8 Megabytes of system memory (RAM) is strongly recommended.

The model's input and output screens are optimized for display at a monitor resolution of 640x480 (Standard VGA). If you are using a higher resolution, for example 800x600 or 1024x768, see Changing the Model's Display.

For best results, Start Excel and Load the BSCREEN.XLS file from the **File / Open** menu.

Spreadsheet-Related Problems

The buttons won't work: BIOSCREEN is built in the Excel spreadsheet environment, and to enter data one must click anywhere outside the cell where you just entered data. If you can see the numbers you just entered in the data entry part of Excel above the spreadsheet, the data has not yet been entered. Click on another cell to enter the data.

is displayed in a number box: The cell format is not compatible with the value, (e.g. the number is too big to fit into the window). To fix this, select the cell, pull down the format menu, select "Cells" and click on the "Number" tab. Change the format of the cell until the value is visible. If the values still cannot be read, select the format menu, select "Cells" and click on the "Font" tab. Reduce the font size until the value can be read.

#DIV/0! is displayed in a number box: The most common cause of this problem is that some input data are missing. In some cases, entering a zero in a box will cause this problem. Double check to make certain that all of the input cells required for your run have data. Note that for vertical dispersivity, BIOSCREEN will convert a "0" into the data entry cell into a very low number (1×10^{-99}) to avoid #DIV/0! errors.

There once were formulas in some of the boxes on the input screen, but they were accidentally overwritten: Click on the "Restore Formulas for Vs, Dispersivities, R, and lambda" button on the bottom right-hand side of the input screen. Note that this button will also restore the formulas that make the Source Width and Source Concentrations for source zones 4 and 5 equal to source zones 2 and 1, respectively.

The graphs seem to move around and change size: This is a feature of Excel. When graph scales are altered to accommodate different plotted data, the physical size of the graphs will change slightly, sometimes resulting in a graph that spreads out over the fixed axis legends. You can manually resize the graph to make it look nice again by double-clicking on the graph and resizing it (refer to the Excel User's Manual).

Common Error Messages

Unable to Load Help File: The most common error message encountered with BIOSCREEN is the message "Unable to Open Help File" after clicking on a Help button. Depending on the version of Windows you are using, you may get an Excel Dialog Box, a Windows Dialog Box, or you may see Windows Help load and display the error. This problem is related to the ease with which the Windows Help Engine can find the data file, BIOSCRN.HLP. Here are some suggestions (in decreasing order of preference) for helping WinHelp find it:

- If you are fortunate enough to be asked to find the requested datafile, do so. It's called BIOSCRN.HLP, and it was installed in the same directory/folder as the BIOSCRN.XLS file.
- Use the File/Open menus from within Excel instead of double-clicking on the filename or Program Manager icon to open the BIOSCRN.XLS file. This sets the "current directory" to the directory containing the Excel file you just opened.
- Change the WinHelp call in the VB Module to "hard code" the directory information. That way, the file name and its full path will be explicitly passed to WinHelp. Hints for doing this are in the VBA module. Select the Macro Module tab and search for the text "Helpfile".
- As a last resort, you can add the BIOSCREEN directory to your path (located in your AUTOEXEC.BAT file), and this problem will be cured. You will have to reboot your machine, however, to make this work

The BIOSCREEN system was designed to be used on a PC with Windows configured to a standard VGA resolution of 640x480 pixels. If you are using a larger monitor and your video resolution is set to 800x600 pixels or greater, you will need to change the zoom factor in the Visual Basic code.

In the first three lines in the Macro Module of the BIOSCREEN spreadsheet, change the number after the equals sign in the following line:

```
Const ZoomValue = 65
```

If your display resolution is standard VGA (640x480), use 65 for the zoom value. If your resolution is 800x600, use a zoom value of 82. If your resolution is not 640x480 or 800x600, if your video performance is seriously degraded, or if you experience display problems, you may need to change your video resolution (see the on-line help for Windows Setup or consult your Windows installation manuals) and experiment with other values for ZoomValue.

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APPENDIX A.1 DOMENICO ANALYTICAL MODEL

The Domenico (1987) analytical model, used by BIOSCREEN, is designed for the multidimensional transport of a decaying contaminant species. The model equation, boundary conditions, assumptions, and limitations are discussed below.

Domenico Model with Instantaneous Reaction Superposition Algorithm	
	$\frac{C(x,y,o,t)}{(C_o + BC)} = \frac{1}{8} \exp\left[\frac{x}{\alpha_x} \left(1 - (1 + 4\lambda\alpha_x/v)^{1/2}\right)\right]$ $\operatorname{erfc}\left[\frac{\left(x - vt(1 + 4\lambda\alpha_x/v)^{1/2}\right)}{2(\alpha_x vt)^{1/2}}\right]$ $\left\{ \operatorname{erf}\left[\frac{(y + Y/2)}{2(\alpha_y x)^{1/2}}\right] - \operatorname{erf}\left[\frac{(y - Y/2)}{2(\alpha_y x)^{1/2}}\right] \right\}$ $\left\{ \operatorname{erf}\left[\frac{(Z)}{2(\alpha_z x)^{1/2}}\right] - \operatorname{erf}\left[\frac{(-Z)}{2(\alpha_z x)^{1/2}}\right] \right\} - BC$ <p>where: $v = \frac{K \cdot i}{\theta_e R}$ $BC = \sum \frac{C(ea)_n}{UF_n}$</p>
Definitions	
<p>BC Biodegradation capacity (mg/L)</p> <p>$C(x,y,z,t)$ Concentration at distance x downstream of source and distance y off centerline of plume at time t (mg/L)</p> <p>C_s Concentration in Source Zone (mg/L)</p> <p>C_o Concentration in Source Zone at t=0 (mg/L)</p> <p>x Distance downgradient of source (ft)</p> <p>y Distance from plume centerline of source (ft)</p> <p>z Distance from surface to measurement point (assumed to be 0; concentration is always assumed to be at top of water table).</p> <p>$C(ea)_n$ Concentration of electron acceptor n in groundwater (mg/L)</p>	<p>UF_n Utilization factor for electron acceptor n (i.e., mass ratio of electron acceptor to hydrocarbon consumed in biodegradation reaction)</p> <p>α_x Longitudinal groundwater dispersivity (ft)</p> <p>α_y Transverse groundwater dispersivity (ft)</p> <p>α_z Vertical groundwater dispersivity (ft)</p> <p>θ_e Effective Soil Porosity</p> <p>λ First-Order Degradation Rate (day^{-1})</p> <p>v Groundwater Seepage Velocity (ft/yr)</p> <p>K Hydraulic Conductivity (ft/yr)</p> <p>R Constituent retardation factor</p> <p>i Hydraulic Gradient (cm/cm)</p> <p>Y Source Width (ft)</p> <p>Z Source Depth (ft)</p>

The initial conditions are:

- 1) $c(x, y, z, 0) = 0$ (Initial concentration = 0 for x, y, z, > 0)
- 2) $c(0, Y, Z, 0) = C_0$ (Source concentration for each vertical plane source = C_0 at time 0)

The key assumptions in the model are:

- 1) The aquifer and flow field are homogenous and isotropic.
- 2) The groundwater velocity is fast enough that molecular diffusion in the dispersion terms can be ignored (may not be appropriate for simulation of transport through clays).
- 3) Adsorption is a reversible process represented by a linear isotherm.

The key limitations to the model are:

- 1) The model should not be applied where pumping systems create a complicated flow field.
- 2) The model should not be applied where vertical flow gradients affect contaminant transport.
- 3) The model should not be applied where hydrogeologic conditions change dramatically over the simulation domain.

The most important modifications to the original Domenico model are:

- 1) The addition of "layer cake" source terms where three Domenico models are superimposed one on top of another to yield the 5-source term used in BIOSCREEN (see Connor et al., 1994; and the Source Width description in the BIOSCREEN Data Entry Section).
- 2) Addition of the instantaneous reaction term using the superposition algorithm (see Appendix A.2, below). For the instantaneous reaction assumption, the source concentration is assumed to be an "effective source concentration" (Coe) equal to the observed concentration in the source zone plus the biodegradation capacity (see "Source Concentration" on the BIOSCREEN Data Entry section).

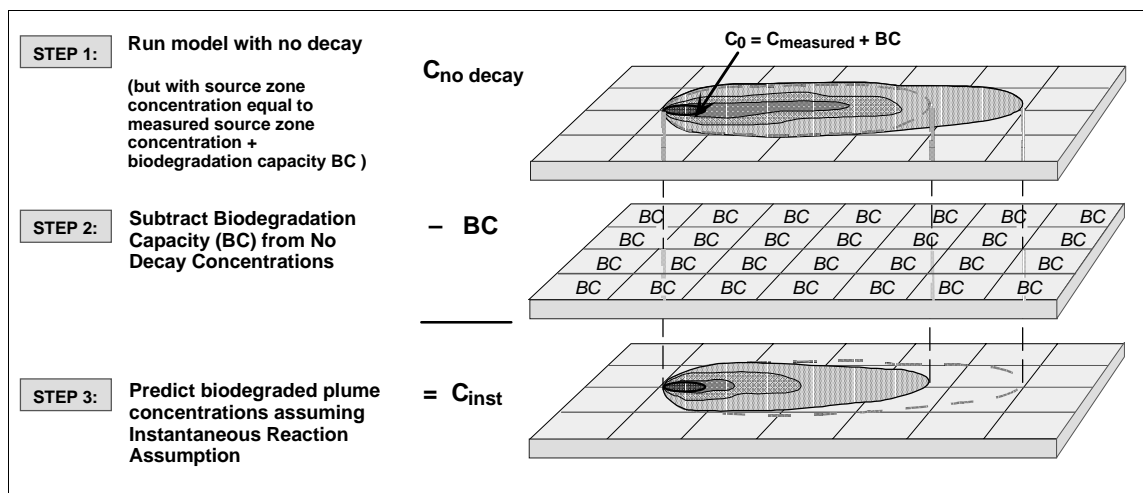
APPENDIX A.2 INSTANTANEOUS REACTION - SUPERPOSITION ALGORITHM

Early biodegradation research focused on the role of dissolved oxygen in controlling the rate of biodegradation in the subsurface (Borden *et al.*, 1986; Lee *et al.*, 1987). Because microbial biodegradation kinetics are relatively fast in comparison to the rate of oxygen transport in the groundwater flow system, Borden demonstrated that the biodegradation process can be simulated as an instantaneous reaction between the organic contaminant and oxygen. This simplifying assumption was incorporated into the BIOPLUME I numerical model which calculated organic mass loss by superposition of background oxygen concentrations onto the organic contaminant plume. In BIOPLUME II, a dual-particle mover procedure was incorporated to more accurately simulate the separate transport of oxygen and organic contaminants within the subsurface (Rifai *et al.*, 1987; Rifai, *et al.*, 1988).

In most analytical modeling applications, contaminant biodegradation is estimated using a first-order decay equation with the biodecay half-life values determined from research literature or site data. However, by ignoring oxygen limitation effects such first-order expressions can significantly overestimate the rate and degree of biodegradation, particularly within low-flow regimes where the rate of oxygen exchange in a groundwater plume is very slow (Rifai, 1994). As a more accurate method of analysis, Newell recommended incorporation of the concept of oxygen superposition into an analytical model (Connor *et al.*, 1994) in a manner similar to that employed in the original BIOPLUME model (Borden *et al.*, 1986). By this method, contaminant mass concentrations at any location and time within the flow field are corrected by subtracting 1 mg/L organic mass for each 3 mg/L of background oxygen, in accordance with the instantaneous reaction assumption. Borden *et al.* (1986) concluded this simple superposition technique was an exact replacement for more sophisticated oxygen-limited models, as long as the oxygen and the hydrocarbon had the same transport rates (e.g., retardation factor, $R = 1$).

In their original work, Borden *et al.* (1986) noted that for highly sorptive contaminants the oxygen-superposition method might erroneously characterize biodegradation due to the differing transport rates of dissolved oxygen and the organic contaminant within the aquifer matrix. However, as demonstrated by Connor *et al.* (1994), the oxygen superposition method and BIOPLUME II (dual particle transport) are in reasonable agreement for contaminant retardation factors as high as 6. Therefore, the superposition method can be employed as a reasonable approximation in BIOSCREEN regardless of contaminant sorption characteristics.

BIOSCREEN employs the same superposition approach for all of the aerobic and anaerobic biodegradation reactions (based on evaluation of O_2 , NO_3 , SO_4 , Fe^{2+} , and CH_4). Based on work reported by Newell *et al.* (1995), the anaerobic reactions (nitrate, ferric iron, and sulfate reduction and methanogenesis) are amenable to simulation using the instantaneous reaction assumption. The general approach is presented below:



Based on the biodegradation capacity of electron acceptors present in the groundwater system, this algorithm will correct the non-decayed groundwater plume concentrations predicted by the Domenico model (Appendix A.1) for the effects of organic constituent biodegradation.

To summarize:

- 1) The original BIOPLUME model (Borden *et al.* 1986) used a superposition method to simulate the fast or “instantaneous” reaction of dissolved hydrocarbons with dissolved oxygen in groundwater.
- 2) Borden *et al.* (1986) reported that this version of BIOPLUME was mathematically exact for the case where the retardation factor of the contaminant was 1.0.
- 3) Rifai and Bedient (1990) developed the BIOPLUME II model with a dual-particle tracking routine that expanded the original BIOPLUME model to handle contaminants with retardation factors other than 1.0, in addition to other improvements.
- 4) Connor *et al.* (1994) compared the superposition method with the more sophisticated BIOPLUME II model and determined that the two approaches yielded very similar results for readily biodegradable contaminants with retardation factors between 1.0 and 6.0.
- 5) BIOSCREEN was developed using the superposition approach to simulate the “instantaneous” reaction of aerobic and anaerobic reactions in groundwater. The biodegradation term in BIOSCREEN is mathematically identical to the approach used in the original BIOPLUME model. This mathematical approach (superposition) matches the more sophisticated BIOPLUME II model very closely for readily biodegradable contaminant retardation factors of up to 6.0. BIOSCREEN simulations using the instantaneous reaction assumption at sites with retardation factors greater than 6.0 should be performed with caution and verified using a more sophisticated model such as BIOPLUME III.

APPENDIX A.3 DERIVATION OF SOURCE HALF-LIFE

Purpose: Determine the source half-life relationship used in BIOSCREEN (see Source Half-Life discussion in BIOSCREEN Data Entry Section, pg 30).

Given: 1) There is a finite amount of soluble organic compounds in source zone (the area with contaminated soils and either free-phase or residual NAPL).
 2) These organics dissolve slowly as fresh groundwater passes through source zone. Assume the change in mass due to dissolution can be approximated as a first order process:

$$M(t) = M_0 e^{-k_s t} \quad (1)$$

Procedure: 1) Calculate initial mass of dissolvable organics in source zone, M_0
 2) Determine initial source concentration from monitoring well data, C_0
 3) Apply conservation of mass to a control surface containing source zone.
 4) Set the expressions for mass at time $t \geq 0$ based on dissolution and conservation of mass equal to each other and solve for an expression describing the concentration at time $t \geq 0$.
 5) Apply initial conditions for concentration at time $t=0$ and solve for the first order decay constant, k_s .

Assumptions: 1) Groundwater flowrate is constant, $Q(t)=Q_0$
 2) Groundwater flowing through the source zone is free of organic compounds. This implies that no mass is added to the system, only dissolution occurs.

Calculations: 1) Calculate initial mass of dissolved/soluble organic compound, M_0 by using procedure described under "Soluble Mass in NAPL, Soil" page in BIOSCREEN Data Input section.
 2) Determine initial concentration, C_0 of organic compound in groundwater leaving the source zone. This may be a spatial average, maximum value, or other value representative of the groundwater concentration leaving the source area. (Note that for the instantaneous reaction assumption, C_0 equals the concentration observed in monitoring wells plus the biodegradation capacity to account for rapid biodegradation reactions in the source zone. See "Soluble Mass in NAPL, Soil" page in BIOSCREEN Data Input section).

$$C(t=0) = C_0 \quad (2)$$

3) Apply conservation of mass to a control surface that contains the source zone. The mass present in the source zone at time $t \geq 0$ is the initial mass minus the change in mass.

$$M(t) = M_0 + \int_{c.s.} \int_t Q(t) C(t) dt dA \tag{3}$$

DERIVATION OF SOURCE HALF-LIFE, Cont'd

Applying the assumptions equation (3) simplifies to

$$M(t) = M_0 - \int_t Q_0 C(t) dt \tag{4}$$

- 4) Set the two expressions for mass of organic compound in the source zone at time $t \geq 0$ (equations (1) and (4)) equal to each other and solve for an expression describing the concentration leaving the source zone.

$$M_0 e^{-k_s t} = M_0 - \int_t Q_0 C(t) dt \tag{5}$$

$$\frac{d}{dt} \left[\int_t Q_0 C(t) dt = M_0 - M_0 e^{-k_s t} \right] \tag{6}$$

$$Q_0 C(t) = k_s M_0 e^{-k_s t} \tag{7}$$

$$C(t) = \frac{k_s M_0}{Q_0} e^{-k_s t} \tag{8}$$

- 5) Apply the initial condition for concentration leaving the source zone at time $t=0$, eqn (2) to the expression for $C(t)$, eqn (8) and solve for the first order decay coefficient, k_s

$$C_0 = \frac{k_s M_0}{Q_0} \tag{9}$$

$$\therefore k_s = \frac{Q_0 C_0}{M_0} \tag{11}$$

Summary: The decay coefficient for the source zone in BIOSCREEN is:

$$k_s = \frac{Q_0 C_0}{M_0}$$

The expression for mass at any time $t \geq 0$ is:

$$M(t) = M_0 e^{-k_s t}$$

Noting that the change in source concentration is directly related to the change in source mass, the expression for source zone concentration any time $t \geq 0$ is:

$$C(t) = C_0 e^{-k_s t}$$

Acknowledgments: Original derivation developed by C. Newell. Detailed derivation developed by Xiaoming Liu, Anthony Holder, and Thomas Reeves.

APPENDIX A.4 DISPERSIVITY ESTIMATES

Dispersion refers to the process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion. Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. However, dispersivity data from over 50 sites has been compiled by Gelhar *et al.* (1992) (see figures A.1 and A.2, next page).

The empirical data indicates that longitudinal dispersivity, in units of length, is related to scale (distance between source and measurement point; the plume length; L_p in BIOSCREEN). Gelhar *et al.* (1992) indicate 1) there is a considerable range of dispersivity values at any given scale (on the order of 2 - 3 orders of magnitude), 2) suggest using values at the low end of the range of possible dispersivity values, and 3) caution against using a single relationship between scale and dispersivity to estimate dispersivity. However, most modeling studies do start with such simple relationships, and BIOSCREEN is programmed with some commonly used relationships representative of typical and low-end dispersivities:

• **Longitudinal Dispersivity**

$$\text{Alpha } x = 3.28 \cdot 0.83 \cdot \left[\log_{10} \left(\frac{L_p}{3.28} \right) \right]^{2.414} \quad (\text{Xu and Eckstein, 1995})$$

$(L_p \text{ in ft})$

• **Transverse Dispersivity**

$$\text{Alpha } y = 0.10 \text{ alpha } x \quad (\text{Based on high reliability points from Gelhar et al., 1992})$$

• **Vertical Dispersivity**

$$\text{Alpha } z = \text{very low (i.e. } 1 \times 10^{-99} \text{ ft)} \quad (\text{Based on conservative estimate})$$

Other commonly used relationships include:

- Alpha x = 0.1 L_p *(Pickens and Grisak, 1981)*
- Alpha y = 0.33 alpha x *(ASTM, 1995) (EPA, 1986)*
- Alpha z = 0.05 alpha x *(ASTM, 1995)*
- Alpha z = 0.025 alpha x to 0.1 alpha x *(EPA, 1986)*

The BIOSCREEN input screen includes Excel formulas to estimate dispersivities from scale. BIOSCREEN uses the Xu and Eckstein (1995) algorithm for estimating longitudinal dispersivities because 1) it provides lower range estimates of dispersivity, especially for large values of L_p , and 2) it was developed after weighting the reliability of the various field data compiled by Gelhar *et al.* (1992) (see Figure A.1). BIOSCREEN also employs low-end estimates for transverse and vertical dispersivity estimates (0.10 alpha x and 0, respectively) because: 1) these relationships better fit observed field data reported by Gelhar *et al.* to have high reliability (see Figure A.2), 2) Gelhar *et al.* recommend use of values in the lower range of the observed data, and 3) better

results were realized when calibrating BIOSCREEN to actual field sites using lower dispersivities. The user can override these formulas by directly entering dispersivity values in the input screen cell.

Note that the Domenico model and BIOSCREEN are not formulated to simulate the effects of chemical diffusion. Therefore, contaminant transport through very slow hydrogeologic regimes (e.g., clays and slurry walls) should probably not be modeled using BIOSCREEN unless the effects of chemical diffusion are proven to be insignificant. Domenico and Schwartz (1990) indicate that chemical diffusion is small for Peclet numbers (seepage velocity times median pore size divided by the bulk diffusion coefficient) greater than 100.

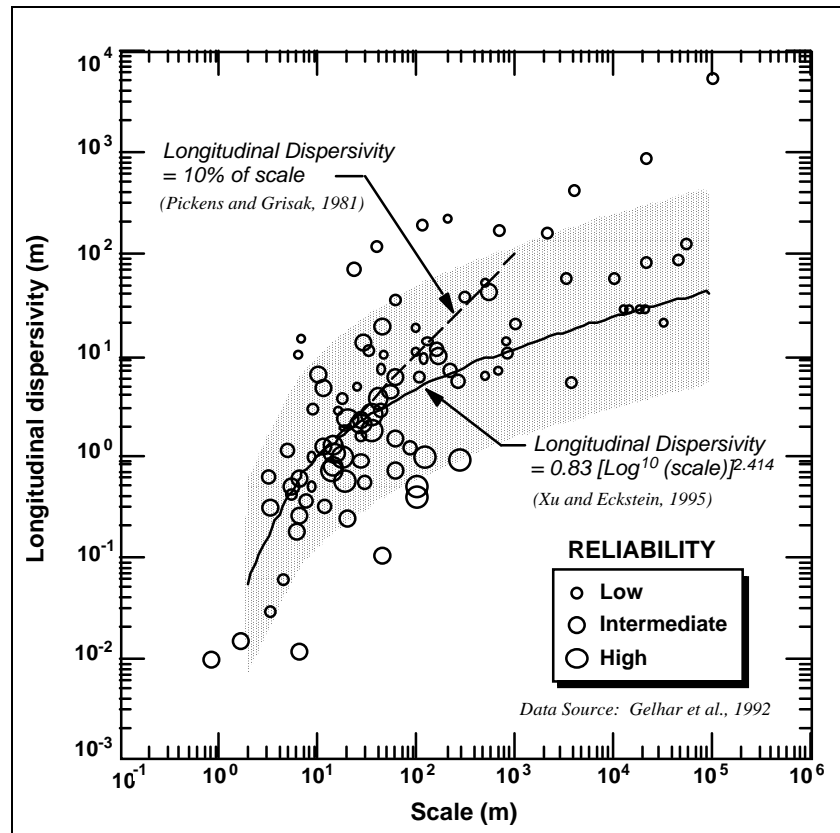


Figure A.1. Longitudinal dispersivity vs. scale data reported by Gelhar *et al.* (1992). Data includes Gelhar's reanalysis of several dispersivity studies. Size of circle represents general reliability of dispersivity estimates. Location of 10% of scale linear relationship plotted as dashed line (Pickens and Grisak, 1981). Xu and Eckstein's regression (used in BIOSCREEN) shown as solid line. Shaded area defines ± 1 order of magnitude from the Xu and Eckstein regression line and represents general range of acceptable values for dispersivity estimates. Note that BIOSCREEN defines scale as L_p , the plume length or distance to measurement point in ft, and employs the Xu and Eckstein algorithm with a conversion factor.

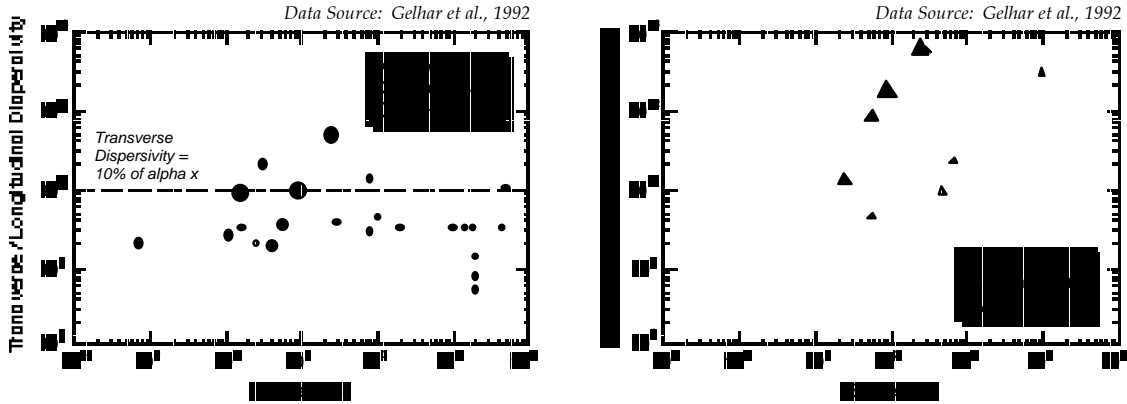


Figure A.2 Ratio of transverse dispersivity and vertical dispersivity to longitudinal dispersivity data vs. scale reported by Gelhar *et al.* (1992). Data includes Gelhar's reanalysis of several dispersivity studies. Size of symbol represents general reliability of dispersivity estimates. Location of transverse dispersivity relationship used in BIOSCREEN is plotted as dashed line.

APPENDIX A.5 ACKNOWLEDGMENTS

BIOSCREEN was developed for the Air Force Center for Environmental Excellence, Brooks AFB, San Antonio, Texas by Groundwater Services, Inc.

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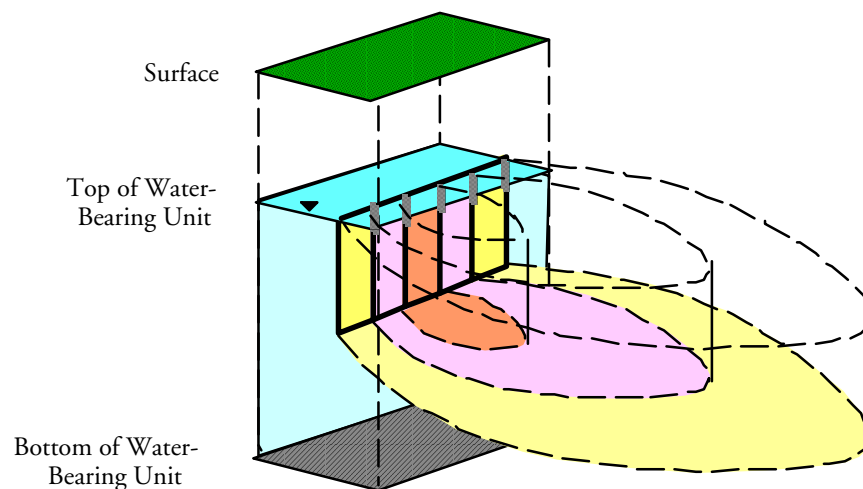
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BIOSCREEN

Natural Attenuation
Decision Support System

Version 1.4
July 1997

VERSION 1.4 REVISIONS



by

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INTRODUCTION

BIOSCREEN is an easy-to-use screening model which simulates remediation through natural attenuation (RNA) of dissolved hydrocarbons at petroleum fuel release sites. The software, programmed in the Microsoft® Excel spreadsheet environment and based on the Domenico analytical solute transport model, has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions, which have been shown to be the dominant biodegradation processes at many petroleum release sites. BIOSCREEN includes three different model types:

- 1) *Solute transport without decay,*
- 2) *Solute transport with biodegradation modeled as a first-order decay process (simple, lumped-parameter approach),*
- 3) *Solute transport with biodegradation modeled as an "instantaneous" biodegradation reaction (approach used by BIOPLUME models).*

The model is designed to simulate biodegradation by both aerobic and anaerobic reactions. It was developed for the Air Force Center for Environmental Excellence (AFCEE) Technology Transfer Division at Brooks Air Force Base by Groundwater Services, Inc., Houston, Texas.

Version 1.3 of BIOSCREEN was released in October 1996. Version 1.4 of BIOSCREEN includes a new mass flux calculation feature, a modification to the vertical dispersion term in the Domenico model, a revised description of the Domenico analytical model equation, and a minor change to the input display. This document describes these updates and provides new biodegradation modeling information for BIOSCREEN users. Continue to refer to the existing BIOSCREEN version 1.3 User's Manual as the primary source of information about BIOSCREEN.

NEW MASS FLUX CALCULATION FEATURE IN VERSION 1.4

Version 1.4 of BIOSCREEN includes a new feature to assist users in estimating the mass flux of contaminants entering surface water bodies via groundwater plume discharge. This feature, included on the "Run Array" Output, provides an estimate of the mass flux of contaminants in units of mg/day computed at specific distances away from the source (see Figure 1).

Example Application

Set up BIOSCREEN to simulate the Keesler AFB SWMU 66 plume (Example 1 in the Version 1.3 User's Manual, page 52). Assume that the plume at Keesler AFB discharges into a hypothetical stream located 210 ft away from the source zone as shown in Figure 1 (note that no such stream actually exists at this location). Using BIOSCREEN 1.4 with the Instantaneous Reaction model, calculate the mass flux of contaminants discharging into the stream (see Example 1 in Appendix A).

As shown in the attached Figure 4 (see Example 1 in Appendix A), the computed mass flux of BTEX constituents within the groundwater plume at 224 ft away from the source is 1500 mg/day. Therefore, in order to achieve a target concentration in the stream of < 0.001 mg/L total BTEX, a minimum naturally-occurring flowrate of 1.5×10^6 L/day (0.61 cubic feet per second) is required.

Obtaining Streamflow Data

Two types of stream flowrates can be used for estimating exposure concentrations, depending on the nature of the contaminant. For contaminants with *acute* effects on human or aquatic receptors (such as ammonia), a minimum flowrate such as the 2-year 7-day average low flow value may be appropriate. For contaminants with *chronic* effects on human or aquatic receptors (such as the BTEX compounds), a harmonic mean or other form of average flow could be used.

The harmonic mean is defined as:

$$Q_{hm} = \frac{n}{\sum_{i=1}^n \frac{1}{Q_i}}$$

where

Q_i = daily average discharge data
n = number of days with data

Calculation of 10-year 7-day average low flow values is discussed in several hydrology texts, including the *Handbook of Hydrology*, David R. Maidment, ed. McGraw-Hill, 1993. Daily average discharge data are often available through state or local agencies which regulate wastewater treatment discharges. Streamflow data are also available through the U.S. Geological Survey (USGS) for many larger streams (see the USGS World-Wide Web page: <http://water.usgs.gov/swr/>).

For smaller, ungaged streams, or for locations not near a gaging station, data from an alternative location having similar watershed characteristics (i.e., landuse, land cover, topography, channel type, drainage area, etc.) may be used. For two locations that differ in size of the drainage area, but are otherwise similar, streamflow data from the gaged location may be adjusted by the ratio of drainage areas to provide an estimate of the flow at the ungaged location.

Description of Calculation

The contaminant mass flux is determined using a simple calculation technique. The concentration in each cell of the array is multiplied by: 1) the Darcy velocity, 2) the width associated with each cell in the array, and 3) the thickness of the source zone. The plume mass flux for a particular cross section is then determined by summing the five values in the array for that cross section. The calculation technique is disabled when vertical dispersion is used, as the vertical concentration profile is no longer uniform. In addition, the mass flux calculation should only be used for gaining streams (streams where groundwater discharges into surface water) and should not be used for losing streams (streams that recharge groundwater).

The calculation approach is approximate, and other averaging techniques (use of geometric means, etc.) might provide different results. Because the model defines the plume cross section with only 5 points, the computed plume mass flux may appear to be slightly higher for a downgradient point than an upgradient point in some instances. As illustrated in the example, the mass flux estimates are sensitive to the model width, and for best results users should adjust the model width so that the contaminant plume covers most of the calculated array (compare mass flux results from a simulation using a 200 ft model width, Figure 4, to mass flux results from a simulation using a 50 ft model width, Figure 6). Users should assume that the mass flux estimates are probably accurate to $\pm 50\%$.

NEW KILOGRAM TO GALLONS CONVERSION FEATURE IN VERSION 1.4

Version 1.4 of BIOSCREEN also includes a new feature to show users how much volume the mass of contaminants displayed in the Array Output screen represents. For example, if BIOSCREEN estimates that the Actual Plume Mass is 7.8 Kg (see Figure 4), the model will convert this into an effective contaminant volume of 2.4 gallons of organic, using a density value of 0.87 g/mL (representative of the density of a BTEX mixture). The following mass values will be converted to volumes: i) Plume Mass if No Biodegradation, ii) Actual Plume Mass, iii) Plume Mass Removed by Biodegradation, iv) Original Mass in Source (Time = 0 Years), and v) Mass in Source Now (Time = X Years).

To display the data converted into gallons, the user should click the "See Gallons" button in the "Plume and Source Masses" region of the Array Output screen. A dialog box appears with several common fuel constituents (average BTEX, benzene, toluene, ethylbenzene, and para-xylene) and their densities in g/mL. If an alternative value for constituent densities is available, this number can be entered into the "Density" box. When the "OK" button is pressed, the dialog box disappears and the plume and source mass calculations in Kg are replaced with volume information in gallons. To convert back to mass values, click on the "See Kg" button.

RELATED REFERENCES FOR BIOSCREEN MODELING

Ollila (1996) provides a good comparison of the Domenico model with the instantaneous reaction superposition method against BIOPLUME II. Rifai et al. (1997) summarize the theory and use of AFCEE's BIOPLUME III model. Nevin et al. (1997) describe software for deriving first-order decay coefficients for steady-state plumes from actual site data.

Nevin, J. P., J.A. Connor, C.J. Newell, J.B. Gustafson, K.A. Lyons, 1997. "FATE 5: A Natural Attenuation Calibration Tool for Groundwater Fate and Transport Modeling," Petroleum Hydrocarbons and Organic Chemicals in Groundwater, NWWA, Houston, Texas, Nov. 1997.

Ollila, P.W., 1996. Evaluating Natural Attenuation With Spreadsheet Analytical Fate and Transport Models. Ground Water Monitoring and Remediation, Vol. XVI, No. 24, pp. 69-75.

Rifai, H.S., C.J. Newell, J.R. Gonzales, S. Dendrou, L. Kennedy, and J. Wilson, 1997. BIOPLUME III Natural Attenuation Decision Support System Version 1.0 User's Manual. Air Force Center for Environmental Excellence, Brooks AFB, Texas (in press).

IMPACT OF NON-BTEX CONSTITUENTS ON BIOSCREEN 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-phase plumes that are dominated by the BTEX compounds.

The following calculations support this conceptual model of BTEX-dominated plumes from JP-4 and gasoline. For additional supporting data and calculations, see Section 3.3.2 of Weidemeier et al., 1995.

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, Rifai, and Newell 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, two weathered gasolines, and 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) ÷ (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
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$$\% \text{ BTEX} = (112 \text{ mg/L}) + (126 \text{ mg/L}) = \underline{89 \%}$$

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

$$\% \text{ BTEX} = (44 \text{ mg/L}) + (65 \text{ mg/L}) = \underline{68 \%}$$

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

$$\% \text{ BTEX} = (87 \text{ mg/L}) \div (91 \text{ mg/L}) = \underline{95 \%}$$

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, Rifai, and Newell, 1994 for a more complete discussion).

Note that the total effective solubility of weathered gasoline #1 (126 mg/L) is greater than the total effective solubility of the fresh gasoline (93 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 mg/L vs. 93 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 appears to be generally representative of the complete JP-4 mixture.

% benzenes, alkylbenzenes in identified compounds:	14% (<i>note: equals 4.5% of 31.5%</i>)
% benzenes, alkylbenzenes in complete JP-4 mixture:	18% (<i>from Stelljes and Watkin, 1993</i>)
% 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 regard 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 using the instantaneous reaction approach 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.

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Contamination Dissolved in Groundwater (Revision 0)", Air Force Center for Environmental Excellence, Brooks AFB, Texas, Nov., 1995.

CHANGES FROM BIOSCREEN 1.3

Display of Source Half-Life Values

The input screen for Version 1.4 has been modified to emphasize that BIOSCREEN generates two different source half-lives when a value for "Soluble Mass in Source NAPL, Soil" is entered. As discussed on page 31 of the Version 1.3 User's Manual, two half-lives are reported, one for the Instantaneous Reaction model and one for the No Degradation or First Order Decay models. Version 1.3 of BIOSCREEN presented both half-lives in one black box (black input boxes designate intermediate values calculated by the model). As part of the Version 1.4 modifications, the single box for source half-lives has been replaced with two boxes, one showing the source half-life calculated using the instantaneous reaction model and one showing the source half-life calculated using the No Degradation or First Order Decay models. The change was made to emphasize that two different values are calculated by BIOSCREEN depending on which biodegradation model is employed (see page 31 of the Version 1.3 User's Manual).

Vertical Dispersion Term

As explained in the Version 1.3 User's Manual, BIOSCREEN has been configured so that the default vertical dispersivity is set to zero (see Appendix A.4 in the Version 1.3 User's Manual). In BIOSCREEN 1.3, however, if the user opts to use a non-zero vertical dispersivity estimate, the software may overestimate the effects of vertical dispersion in some cases, as described below.

BIOSCREEN 1.3 was coded so that vertical dispersion is assumed to occur in both directions as the contaminants travel away from the source zone (i.e., downwards and upwards). For source zones located in the middle of a thick aquifer, or in cases where recharge produces a clean zone on top of the plume, this would be an appropriate approach. For source zones located at the top of an aquifer (the case at most petroleum release sites), upward vertical dispersion above the water table does not occur (unless recharge is significant), and therefore the model could overestimate the effects of dispersion. While the vertical dispersion term in the Domenico analytical model expression in the Version 1.3 User's Manual was correct, showing vertical dispersion in only *one* direction (see Appendix A.1), the Version 1.3 model actually simulates vertical dispersion in *both* directions.

In BIOSCREEN 1.4, the default approach of no vertical dispersion is still recommended. The software code has been changed, however, so that there is vertical dispersion is modeled in the downward direction only. (If a user would like to use BIOSCREEN 1.4 with dispersion in both directions, multiply the vertical dispersivity estimate by a factor of 4 and enter the result as the vertical dispersivity. This will have the effect of simulating vertical dispersion occurring in two directions).

Most users will not notice any effect with this change, as BIOSCREEN's default vertical dispersivity is set near zero corresponding to no vertical dispersion. BIOSCREEN 1.3 only overestimates the effects of vertical dispersion if: 1) the default dispersivity value of zero is

replaced with a non-zero vertical value and 2) the source zone is located at the top of an aquifer that does not have significant recharge.

Appendix A.1 Domenico Analytical Model Equation

The Domenico analytical model expression provided in Appendix A.1 of the BIOSCREEN Version 1.3 User's Manual incorrectly showed how the superposition term was employed, was unclear about the separation of the first order decay model and the instantaneous reaction model, and did not include the source decay term. Revised equation descriptions are provided below and replace the single equation shown on page 41 of the Version 1.3 User's Manual. Note that the equations encoded in the software were not in error and have not been modified (except as described above with regard to vertical dispersion).

Domenico Model with First Order Decay Algorithm	
	$C(x, y, o, t) = C_o \exp[-k_s(t - x / v)]$ $\frac{1}{8} \exp\left[\frac{x}{\alpha_x} \left(1 - (1 + 4 \lambda \alpha_x / v)^{1/2}\right)\right]$ $\operatorname{erfc}\left[\frac{(x - vt(1 + 4 \lambda \alpha_x / v)^{1/2})}{2(\alpha_x vt)^{1/2}}\right]$ $\left\{ \operatorname{erf}\left[\frac{(y + Y / 2)}{2(\alpha_y x)^{1/2}}\right] - \operatorname{erf}\left[\frac{(y - Y / 2)}{2(\alpha_y x)^{1/2}}\right] \right\}$ $\left\{ \operatorname{erf}\left[\frac{(Z)}{2(\alpha_z x)^{1/2}}\right] - \operatorname{erf}\left[\frac{(-Z)}{2(\alpha_z x)^{1/2}}\right] \right\}$ <p>where: $v = \frac{K \cdot i}{\theta_e R}$</p>
Domenico Model with Instantaneous Reaction Superposition Algorithm	
	$C(x, y, o, t) = (C_o \exp[-k_s(t - x / v)] + BC)$ $\frac{1}{8} \operatorname{erfc}\left[\frac{(x - vt)}{2(\alpha_x vt)^{1/2}}\right]$ $\left\{ \operatorname{erf}\left[\frac{(y + Y / 2)}{2(\alpha_y x)^{1/2}}\right] - \operatorname{erf}\left[\frac{(y - Y / 2)}{2(\alpha_y x)^{1/2}}\right] \right\}$ $\left\{ \operatorname{erf}\left[\frac{(Z)}{2(\alpha_z x)^{1/2}}\right] - \operatorname{erf}\left[\frac{(-Z)}{2(\alpha_z x)^{1/2}}\right] \right\} - BC$ <p>where: $v = \frac{K \cdot i}{\theta_e R}$ $BC = \Sigma \frac{C(ea)_n}{UF_n}$</p>
Definitions	

BC	Biodegradation capacity (mg/L)	UF _n	Utilization factor for electron acceptor <i>n</i> (i.e., mass ratio of electron acceptor/by-product to hydrocarbon consumed in biodegradation reaction)
C(x,y,z,t)	Concentration at distance x downstream of source and distance y off centerline of plume at time t (mg/L)	α _x	Longitudinal groundwater dispersivity (ft)
C _s	Concentration in Source Zone (mg/L)	α _y	Transverse groundwater dispersivity (ft)
C _o	Concentration in Source Zone at t=0 (mg/L)	α _z	Vertical groundwater dispersivity (ft)
x	Distance downgradient of source (ft)	λ	First-order decay coefficient for dissolved contaminants (yr ⁻¹)
y	Distance from centerline of source (ft)	θ _e	Effective soil porosity
z	Vertical Distance from groundwater surface to measurement point (assumed to be 0; concentration is always assumed to be at top of water table).	v	Contaminant velocity in groundwater (ft/yr)
C(ea) _n	Concentration of electron acceptor (or by-product equivalent) <i>n</i> in groundwater (mg/L)	K	Hydraulic conductivity (ft/yr)
		R	Constituent retardation factor
		i	Hydraulic gradient (ft/ft)
		Y	Source width (ft)
		Z	Source depth (ft)
		t	Time (yr)
		k _s	First-order decay term for source concentration (yr ⁻¹)

ACKNOWLEDGMENTS

BIOSCREEN was developed for the Air Force Center for Environmental Excellence, Brooks AFB, San Antonio, Texas by Groundwater Services, Inc.

AFCEE Technology Transfer Division Chief:	Mr. Marty Faile
AFCEE Project Officer:	Mr. Jim Gonzales
BIOSCREEN Developers:	Charles J. Newell, Ph.D., P.E. and R. Kevin McLeod Groundwater Services, Inc. phone: 713 522-6300 2211 Norfolk Suite 1000 fax: 713 522-8010 Houston, Texas 77005 cjnewell@gsi-net.com rkmcleod@gsi-net.com
BIOSCREEN Manual:	Charles J. Newell, Ph.D., P.E. Groundwater Services, Inc.
Contributors to BIOSCREEN Version 1.4:	R. Todd Fisher

The Air Force Center for Environmental Excellence is distributing BIOSCREEN 1.4 via:

EPA Center for Subsurface Modeling Support (CSMoS) NRMRL/SPRD P.O. Box 1198 Ada, Oklahoma 74821-1198	<ul style="list-style-type: none"> • Phone: (405) 436-8594 • Fax: (405) 436-8718 • Bulletin Board: (405) 436-8506 (14,400 baud-8 bits -1 stop bit -no parity). • Internet: http://www.epa.gov/ada/kerrlab.html (Electronic manuals will be in .pdf format; must download Adobe Acrobat Reader to
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Note that first-time users should download:

- 1) The BIOSCREEN 1.4 software,
- 2) The BIOSCREEN 1.3 User's Manual, and
- 3) The BIOSCREEN 1.4 Revisions document.

APPENDIX 1. BIOSCREEN Version 1.4 EXAMPLE

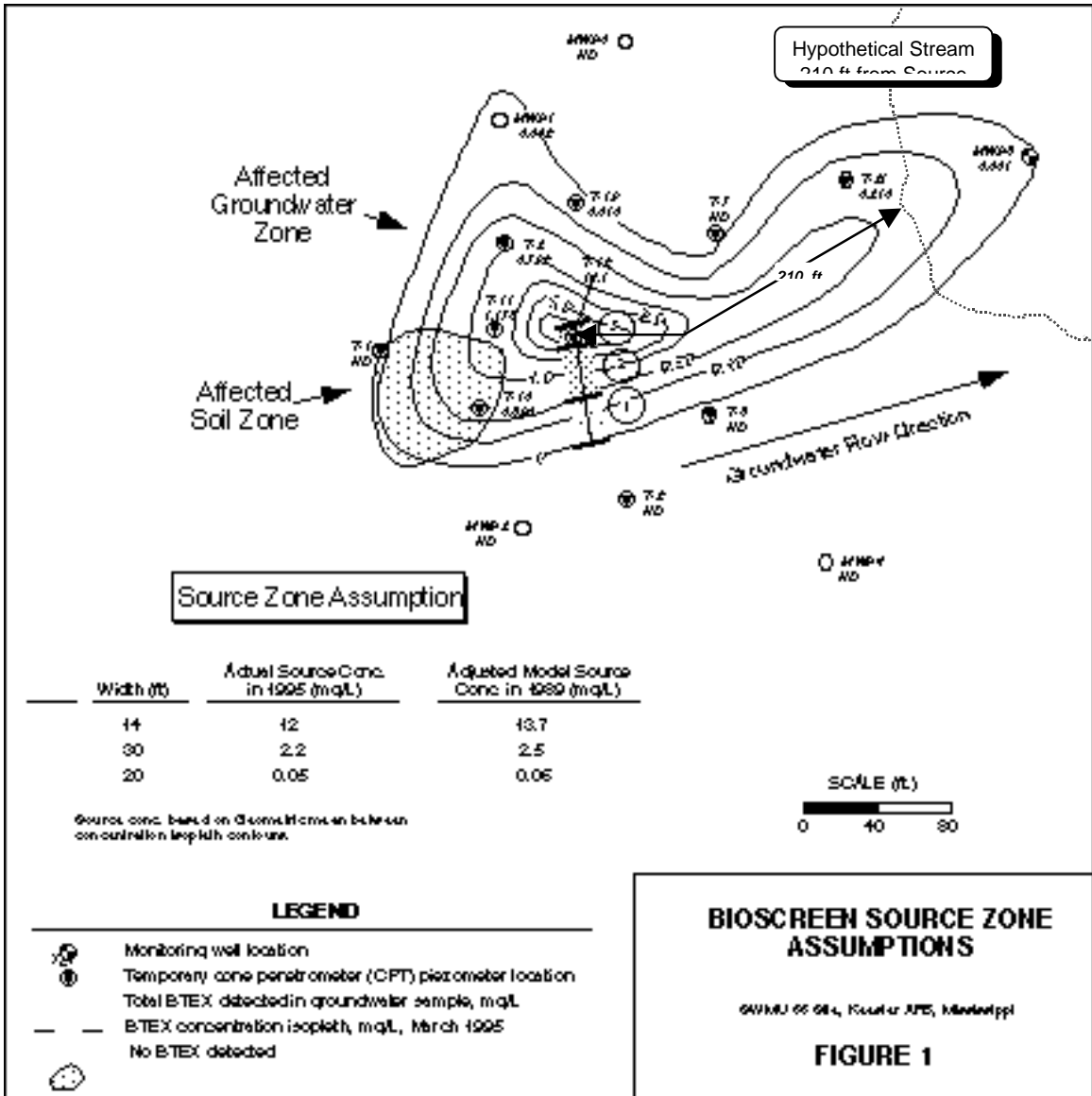
Example 1: SWMU 66, Keesler AFB, Mississippi

- Input Data
- Fig. 1 Source Map
- BIOSCREEN Modeling Summary
- Fig. 2 BIOSCREEN Input Data
- Fig. 3 BIOSCREEN Centerline Output
- Fig. 4 BIOSCREEN Array Output
- Fig. 5 BIOSCREEN Input Data, 50 ft Model Width
- Fig. 4 BIOSCREEN Array Output, 50 ft Model Width

BIOSCREEN EXAMPLE 1

Keesler Air Force Base, SWMU 66, Mississippi

DATA TYPE	Parameter	Value	Source of Data																												
Hydrogeology	<ul style="list-style-type: none"> Hydraulic Conductivity: Hydraulic Gradient: Porosity: 	1.1 x 10 ⁻² (cm/sec) 0.003 (ft/ft) 0.3	<ul style="list-style-type: none"> Slug-tests results Static water level measurements Estimated 																												
Dispersion	Original: <ul style="list-style-type: none"> Longitudinal Dispersivity: Transverse Dispersivity: Vertical Dispersivity: After Calibration: <ul style="list-style-type: none"> Longitudinal Dispersivity: Transverse Dispersivity: Vertical Dispersivity: 	13.3 (ft) 1.3 (ft) 0 (ft) 32.5 (ft) 3.25 (ft) 0 (ft)	<ul style="list-style-type: none"> Based on estimated plume length of 280 ft and Xu/Eckstein relationship Based on calibration to plume length (Note this is well within the observed range for long. dispersivity; see Fig. A.1 in Appendix A.3. Remember to convert from feet to meters before using the chart). 																												
Adsorption	<ul style="list-style-type: none"> Retardation Factor: Soil Bulk Density ρ_b: foc: Koc: 	1.0 1.7 (kg/L) 0.0057% B: 38 T: 135 E: 95 X: 240	<ul style="list-style-type: none"> Calculated from $R = 1 + K_{oc} \times f_{oc} \times \rho_b/n$ Estimated Lab analysis Literature - use Koc = 38 																												
Biodegradation	Electron Acceptor: Background Conc. (mg/L): Minimum Conc. (mg/L): Change in Conc. (mg/L): Electron Acceptor: Max. Conc. (mg/L): Avg. Conc. (mg/L):	<table border="0"> <tr> <td></td> <td><u>O2</u></td> <td><u>NO3</u></td> <td><u>SO4</u></td> </tr> <tr> <td></td> <td>2.05</td> <td>0.7</td> <td>26.2</td> </tr> <tr> <td></td> <td>- 0.4</td> <td>- 0</td> <td>- 3.8</td> </tr> <tr> <td></td> <td>1.65</td> <td>0.7</td> <td>22.4</td> </tr> <tr> <td></td> <td><u>Fe</u></td> <td><u>CH4</u></td> <td></td> </tr> <tr> <td></td> <td>36.1</td> <td>7.4</td> <td></td> </tr> <tr> <td></td> <td>16.6</td> <td>6.6</td> <td></td> </tr> </table> <p>Note: Boxed values are BIOSCREEN input values.</p>		<u>O2</u>	<u>NO3</u>	<u>SO4</u>		2.05	0.7	26.2		- 0.4	- 0	- 3.8		1.65	0.7	22.4		<u>Fe</u>	<u>CH4</u>			36.1	7.4			16.6	6.6		<ul style="list-style-type: none"> Based on March 1995 groundwater sampling program conducted by Groundwater Services, Inc.
	<u>O2</u>	<u>NO3</u>	<u>SO4</u>																												
	2.05	0.7	26.2																												
	- 0.4	- 0	- 3.8																												
	1.65	0.7	22.4																												
	<u>Fe</u>	<u>CH4</u>																													
	36.1	7.4																													
	16.6	6.6																													
General	<ul style="list-style-type: none"> Modeled Area Length: Modeled Area Width: Simulation Time: 	320 (ft) 200 (ft), 50 (ft) 6 (yrs)	<ul style="list-style-type: none"> Based on area of affected groundwater plume Steady-state flow 																												
Source Data	<ul style="list-style-type: none"> Source Thickness: Source Concentration: 	10 (ft) (See Figure 1)	<ul style="list-style-type: none"> Based on geologic logs and lumped BTEX monitoring data 																												
Actual Data	Distance From Source (ft): BTEX Conc. (mg/L):	<table border="0"> <tr> <td><u>30</u></td> <td><u>60</u></td> <td><u>180</u></td> <td><u>280</u></td> </tr> <tr> <td>5.0</td> <td>1.0</td> <td>0.5</td> <td>0.001</td> </tr> </table>	<u>30</u>	<u>60</u>	<u>180</u>	<u>280</u>	5.0	1.0	0.5	0.001	<ul style="list-style-type: none"> Based on observed concentrations at site 																				
<u>30</u>	<u>60</u>	<u>180</u>	<u>280</u>																												
5.0	1.0	0.5	0.001																												
OUTPUT	Centerline Concentration:	See Figure 3																													
	Array Concentration:	See Figure 4, 6																													



BIOSCREEN Modeling Summary, Keesler Air Force Base, SWMU 66, Mississippi:

- BIOSCREEN was used to try to reproduce the movement of the plume from 1989 (the best guess for when the release occurred) to 1995.
- The soluble mass in soil and NAPL was estimated by integrating BTEX soil concentrations contours mapped as part of the site soil delineation program. An estimated 2000 Kg of BTEX was estimated to be present at the site based on GC/MS analysis of soil samples collected from both the vadose and saturated zone. This value represented a source half-life of 60 years with the instantaneous reaction model (the first value shown in the source half-life box in Figure 2), a relatively long half-life, so the 2000 Kg measured in 1995 was assumed to be representative of 1989 conditions.
- The instantaneous reaction model was used as the primary model to try to reproduce the plume length (~ 280 ft).
- Because a decaying source was used, the source concentration on the input screen (representing concentrations 6 yrs ago) were adjusted so the source concentration on the centerline output screen (representing concentrations now) were equal to 12 mg/L. Because the source decay term is different for the first order decay and instantaneous reaction models, this simulation focused on matching the instantaneous reaction model. The final result was a source concentration of 13.68 mg/L in the center of the source zone (note on the centerline output the source concentration is 12.021 mg/L).
- The initial run of the instantaneous reaction model indicated that the plume was too long. This indicates that there is more mixing of hydrocarbon and electron acceptors at the site than is predicted by the model. Therefore the longitudinal dispersivity was adjusted upwards (more mixing) until BIOSCREEN matched the observed plume length. The final longitudinal dispersivity was 32.5 ft.
- As a check the first-order decay model was used with the BIOSCREEN default value of 2 yrs. This run greatly overestimated the plume length, so the amount of biodegradation was increased by decreasing the solute half-life. A good match of the plume was reached with a solute half-life of 0.15 years. This is within observed ranges reported in the literature (see solute half-life section, page 22).
- As shown in Figure 3, BIOSCREEN matches the observed plume fairly well. The instantaneous model is more accurate near the source while the first order decay model is more accurate near the middle of the plume. Both models reproduce the actual plume length relatively well.

- As shown in Figure 4, the current plume is estimated to contain 7.8 kg of BTEX. BIOSCREEN indicates that the plume under a no-degradation scenario would contain 126.3 kg BTEX. In other words BIOSCREEN indicates that 94% of the BTEX mass that has left the source since 1989 has biodegraded.
- Most of the source mass postulated to be in place in 1989 is still there in 1996 (2000 kg vs. 1837 kg, or 92% left).
- The current plume contains 1.0 ac-ft of contaminated water, with 1.019 acre-ft/yr of water being contaminated as it flows through the source. Because the plume is almost at steady state, 1.019 ac-ft of water become contaminated per year with the same amount being remediated every year due to in-situ biodegradation and other attenuation processes. This indicates that a long-term monitoring approach would probably be more appropriate for this site than active remediation, as the plume is no longer growing in size.
- A hypothetical stream is assumed to be located approximately 210 ft downgradient of the source (note no such stream exists at the actual site). Using an estimated model width of 200 ft (see Figure 2), a mass flux of 1500 mg/day is calculated (see Figure 4) at a distance of 224 ft away from the source (the closest point calculated by BIOSCREEN).

Users should be aware that the mass flux calculation is sensitive to the model width assigned in Section 6 of the input screen (see Figure 2). A model width of 200 ft was used in the original example so that most of the “no degradation” plume was in the array, allowing calculation of the plume and source masses (see pg. 34-35 of the BIOSCREEN Ver. 1.3 Manual for a more detailed explanation).

For the mass flux calculation, however, a more accurate result will be obtained by selecting a width where most of the plume of interest (in this case the instantaneous reaction plume) appears across the array. As shown in Figures 5 and 6, a model width of 50 ft was selected so that the instantaneous reaction plume covered most of the BIOSCREEN array. With this width, a mass flux value of 860 mg/day was calculated. This is a more accurate estimate of the mass flux than the 1500 mg/day calculated above.

BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence Version 1.4

1. HYDROGEOLOGY

Seepage Velocity* V_s (ft/yr)
 or (cm/sec)

Hydraulic Conductivity K (cm/sec)

Hydraulic Gradient i (ft/ft)

Porosity n (-)

2. DISPERSION

Longitudinal Dispersivity* α_{long} (ft)

Transverse Dispersivity* α_{trans} (ft)

Vertical Dispersivity* α_v (ft)
 or (ft)

Estimated Plume Length L_p (ft)

3. ADSORPTION

Retardation Factor* R (-)
 or (year)

Soil Bulk Density ρ (kg/l)

Partition Coefficient K_{oc} (L/kg)

Fraction Organic Carbon f_{oc} (-)

4. BIODEGRADATION

1st Order Decay Coeff* λ (per yr)
 or (year)

or Instantaneous Reaction Model

Delta Oxygen* DO (mg/L)

Delta Nitrate* NO_3 (mg/L)

Observed Ferrous Iron* Fe^{2+} (mg/L)

Delta Sulfate* SO_4 (mg/L)

Observed Methane* CH_4 (mg/L)

5. GENERAL

Modeled Area Length* (ft) L

Modeled Area Width* (ft) W

Simulation Time* (yr)

6. SOURCE DATA

Source Thickness in Sat Zone* (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
28	0.057
30	2.508
14	13.68
30	2.508
28	0.057

Source Halflife (see Help):
 (yr)
 Inst. React. 1st Order

Soluble Mass (Kg)

In Source NAPL, Soil

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	12.0	5.0	1.0			.5		.001			
Dist. from Source (ft)	0	32	64	96	128	160	192	224	256	288	320

8. CHOOSE TYPE OF OUTPUT TO SEE:

RUN CENTERLINE

View Output

RUN ARRAY

View Output

Help

Data Input Instructions:

→ 1. Enter value directly...or
 → 2. Calculate by filling in grey cells below. (To restore formulas, hit button below).

Variable* → Data used directly in model.

→ Value calculated by model. (Don't enter any data).

Figure 2. BIOSCREEN Input Screen. Keesler Air Force Base, Mississippi. (Note: longitudinal dispersivity has been changed from the original computed value of 13.3 ft. to 32.5 ft. during calibration.)

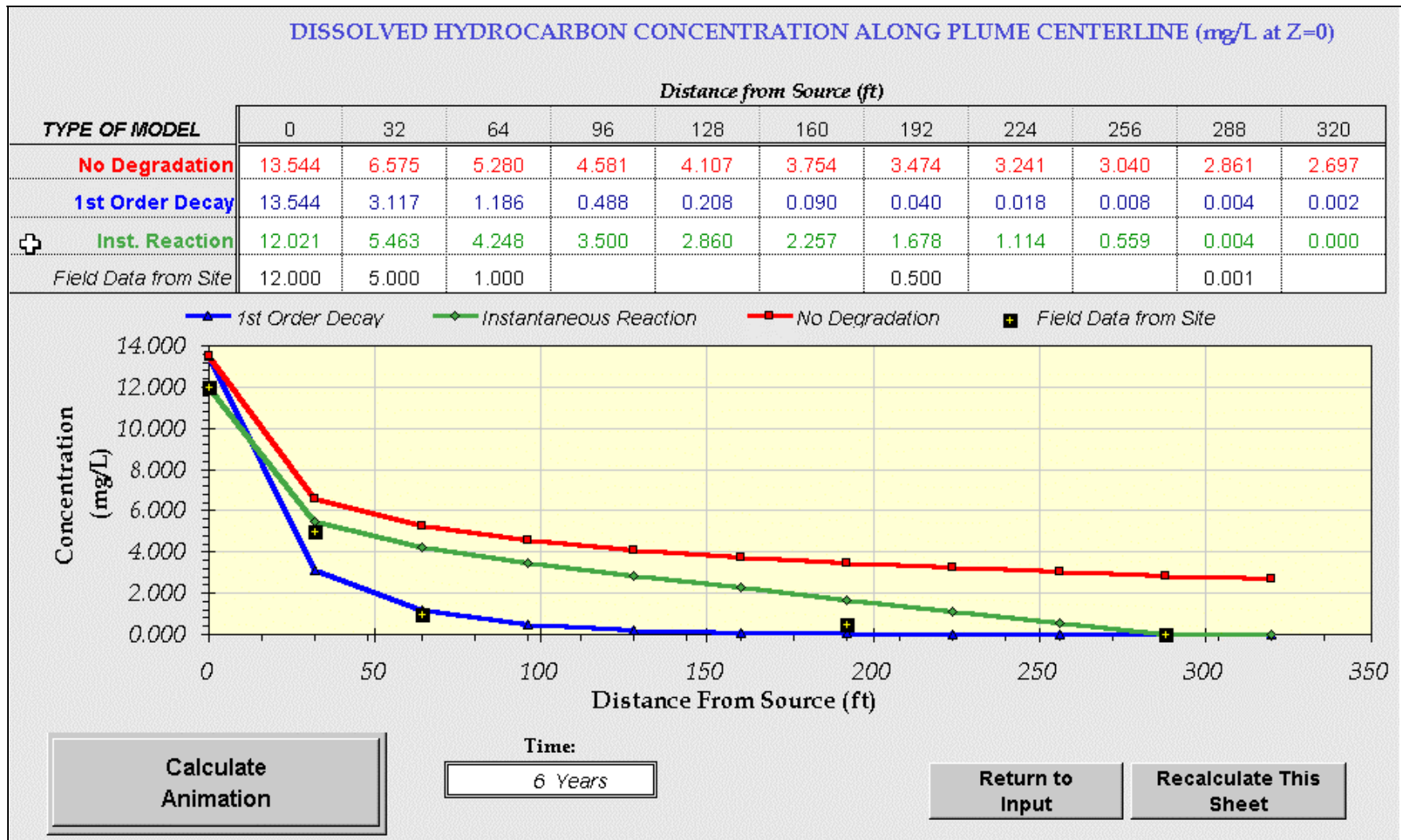


Figure 3. Centerline Output. Keesler Air Force Base, Mississippi.

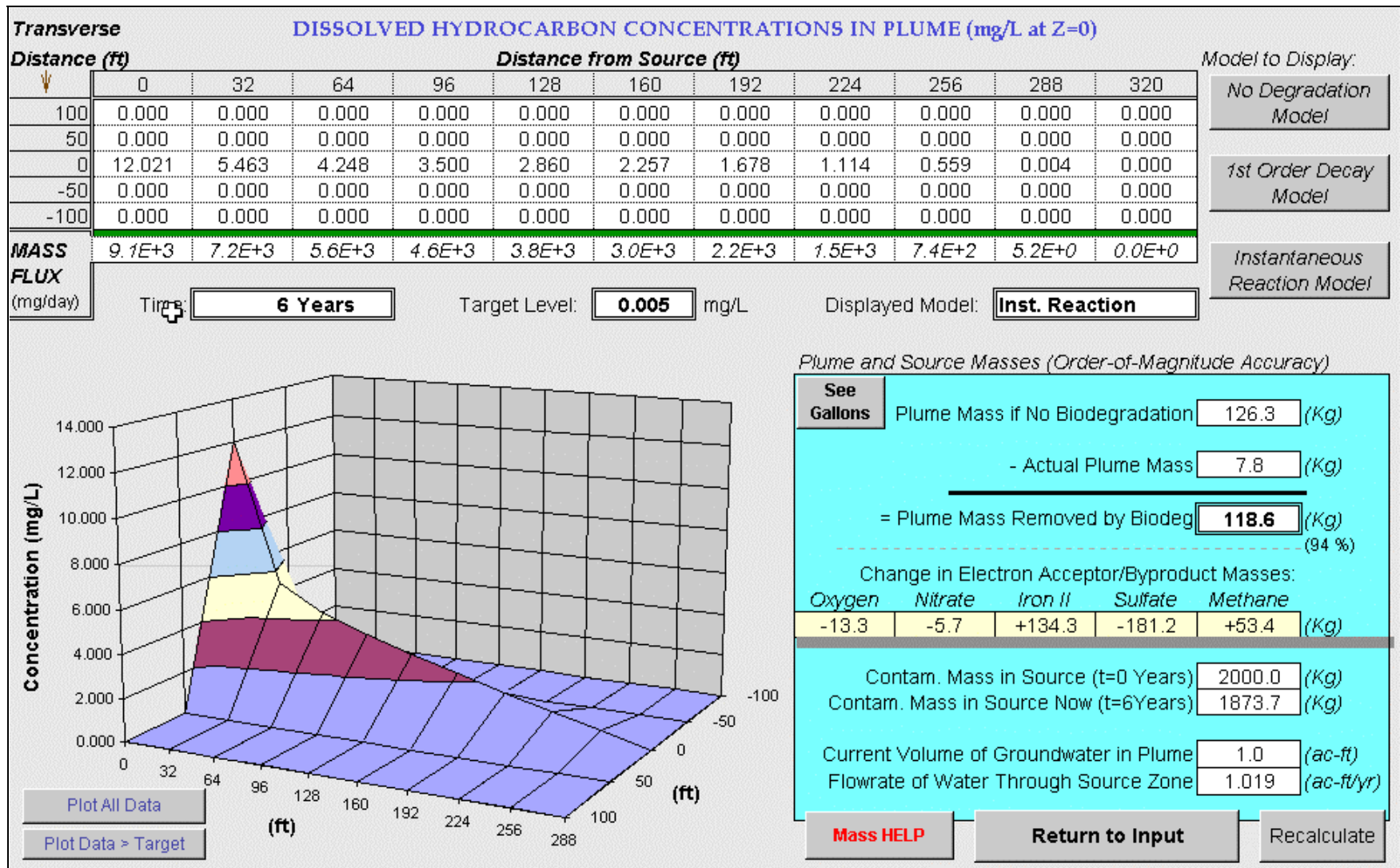


Figure 4. Array Concentration Output. Keesler Air Force Base, Mississippi.

BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence Version 1.4

Keesler AFB
SWMU 66
Run Name

Data Input Instructions:

115 → 1. Enter value directly... or
↑ or 0.02 → 2. Calculate by filling in grey cells below. (To restore formulas, hit button below).

Variable* → Data used directly in model.
20 → Value calculated by model. (Don't enter any data).

1. HYDROGEOLOGY

Seepage Velocity* Vs (ft/yr)
or

Hydraulic Conductivity K (cm/sec)

Hydraulic Gradient i (ft/ft)

Porosity n (-)

2. DISPERSION

Longitudinal Dispersivity* α_x (ft)

Transverse Dispersivity* α_y (ft)

Vertical Dispersivity* α_z (ft)
or

Estimated Plume Length Lp (ft)

3. ADSORPTION

Retardation Factor* R (-)
or

Soil Bulk Density rho (kg/l)

Partition Coefficient Koc (L/kg)

Fraction Organic Carbon foc (-)

4. BIODEGRADATION

1st Order Decay Coeff* lambda (per yr)
or

Solute Half-Life t-half (year)
or Instantaneous Reaction Model

Delta Oxygen* DO (mg/L)

Delta Nitrate* NO3 (mg/L)

Observed Ferrous Iron* Fe2+ (mg/L)

Delta Sulfate* SO4 (mg/L)

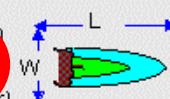
Observed Methane* CH4 (mg/L)

5. GENERAL

Modeled Area Length (ft)

Modeled Area Width (ft)

Simulation Time* (yr)



6. SOURCE DATA

Source Thickness in Sat Zone* (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
28	0.057
30	2.508
14	13.68
30	2.508
28	0.057

Source Half-life (see Help):
 (yr)
 Inst. React. 1st Order
 Soluble Mass (Kg)
 In Source NAPL, Soil

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	12.0	5.0	1.0				5		.001		
Dist. from Source (ft)	0	32	64	96	128	160	192	224	256	288	320

8. CHOOSE TYPE OF OUTPUT TO SEE:

RUN CENTERLINE

View Output

RUN ARRAY

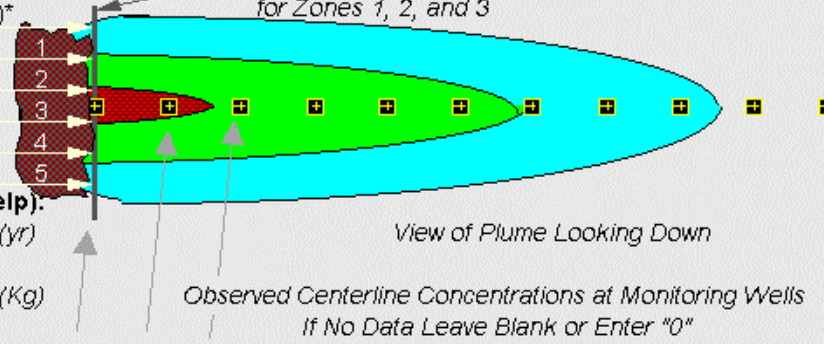
View Output

Help

Recalculate This Sheet

Paste Example Dataset

Restore Formulas for Vs, Dispersivities, R, lambda, other



View of Plume Looking Down

Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

Figure 5. BIOSCREEN Input Screen. Keesler Air Force Base, Mississippi, with 50 ft. modeled area width.

A-9

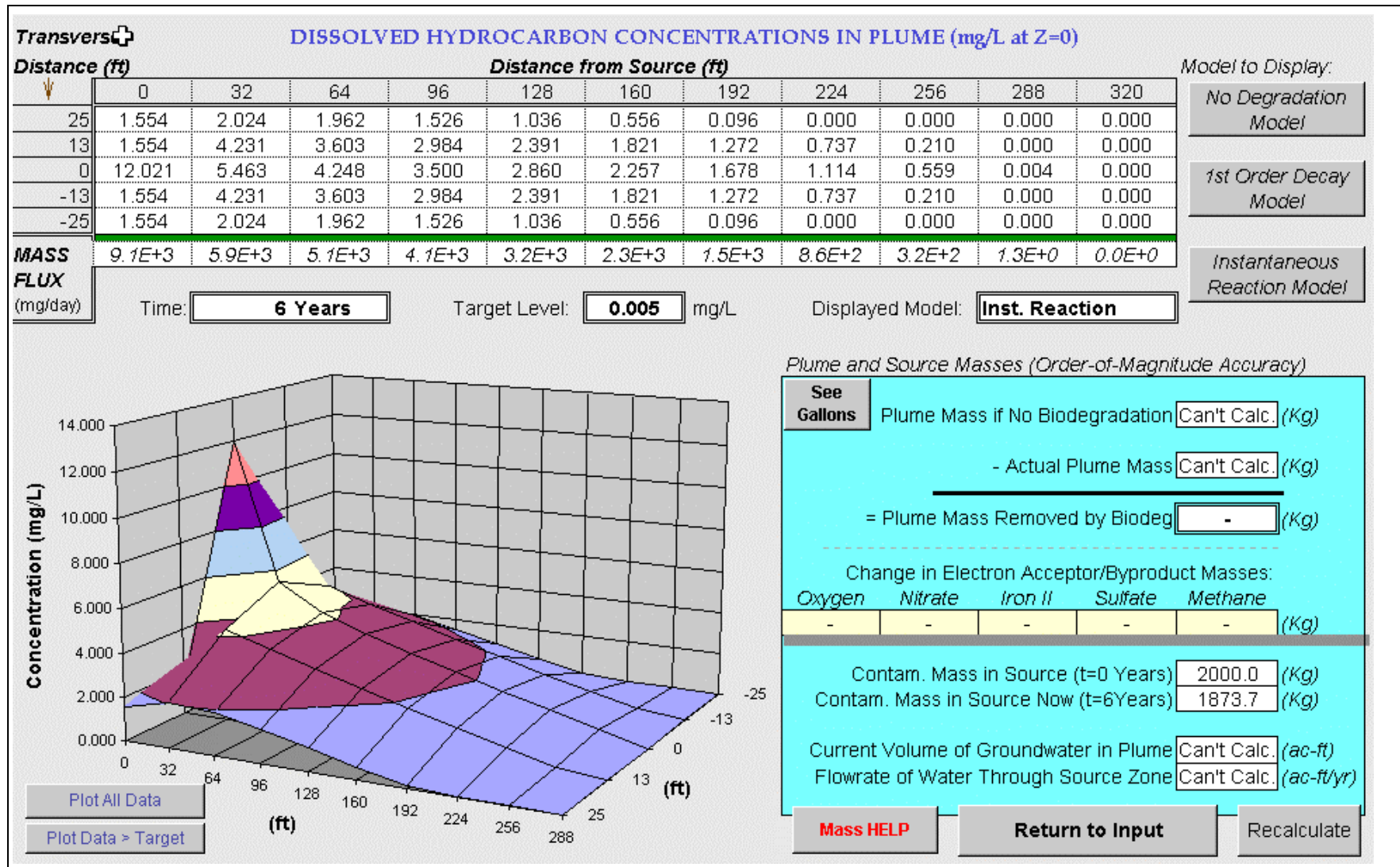


Figure 6. Array Concentration Output. Keesler Air Force Base, Mississippi, with 50 ft. modeled area width.

APPENDIX A.6 BIOSCREEN EXAMPLES**Example 1: SWMU 66, Keesler AFB, Mississippi**

- Input Data
- Fig. 1 Source Map
- BIOSCREEN Modeling Summary
- Fig. 2 BIOSCREEN Input Data
- Fig. 3 BIOSCREEN Centerline Output
- Fig. 4 BIOSCREEN Array Output

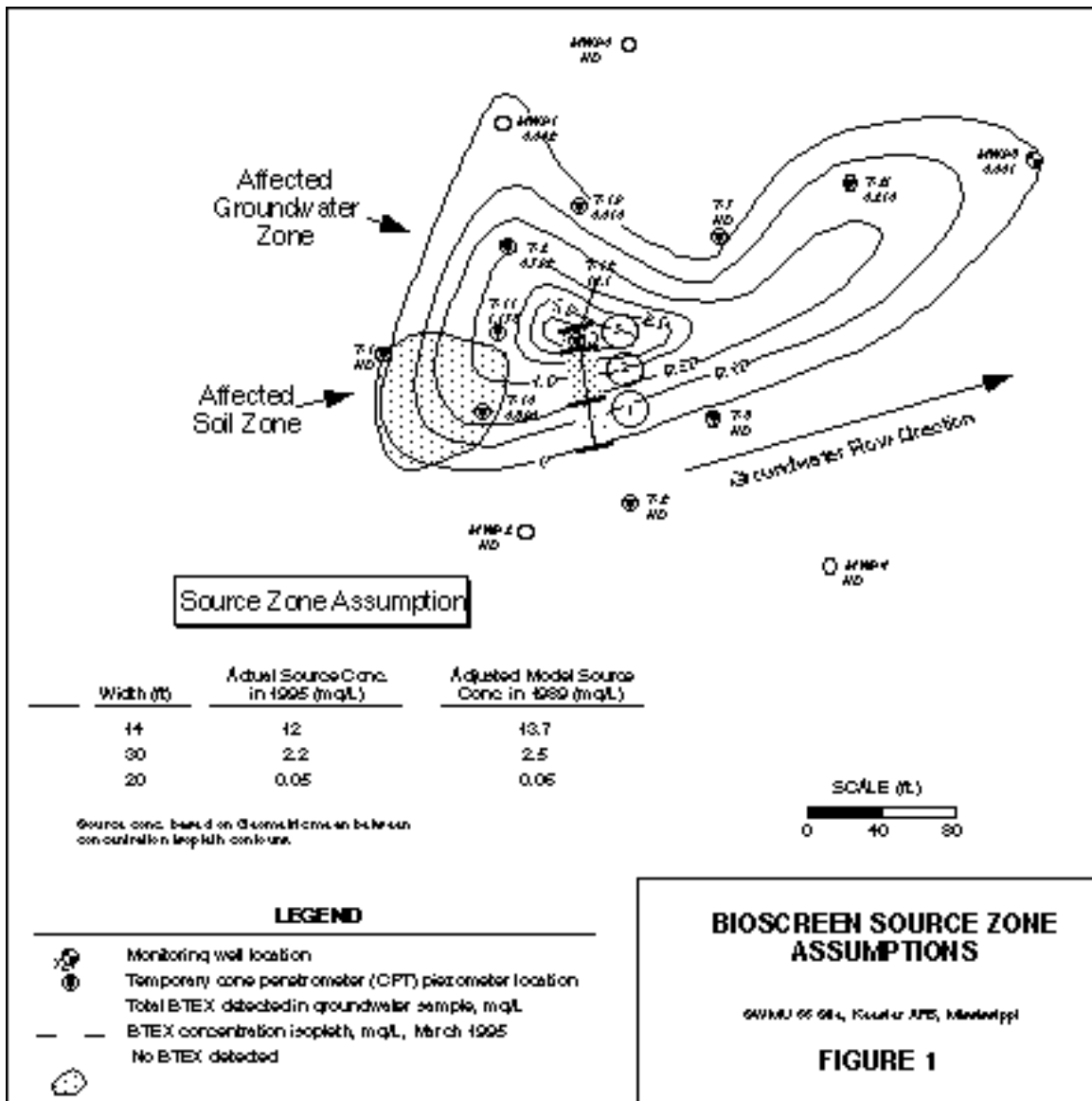
Example 2: UST Site 870, Hill AFB, Utah

- Input Data
- Fig. 5 Source Map
- BIOSCREEN Modeling Summary
- Fig. 6 BIOSCREEN Input Data
- Fig. 7 BIOSCREEN Centerline Output
- Fig. 8 BIOSCREEN Array Output

BIOSCREEN EXAMPLE 1

Keesler Air Force Base, SWMU 66, Mississippi

DATA TYPE	Parameter	Value	Source of Data																								
Hydrogeology	<ul style="list-style-type: none"> Hydraulic Conductivity: Hydraulic Gradient: Porosity: 	1.1 x 10 ⁻² (cm/sec) 0.003 (ft/ft) 0.3	<ul style="list-style-type: none"> Slug-tests results Static water level measurements Estimated 																								
Dispersion	Original: <ul style="list-style-type: none"> Longitudinal Dispersivity: Transverse Dispersivity: Vertical Dispersivity: After Calibration: <ul style="list-style-type: none"> Longitudinal Dispersivity: Transverse Dispersivity: Vertical Dispersivity: 	13.3 (ft) 1.3 (ft) 0 (ft) 32.5 (ft) 3.25 (ft) 0 (ft)	<ul style="list-style-type: none"> Based on estimated plume length of 280 ft and Xu/Eckstein relationship Based on calibration to plume length (Note this is well within the observed range for long. dispersivity; see Fig. A.1 in Appendix A.3. Remember to convert from feet to meters before using the chart). 																								
Adsorption	<ul style="list-style-type: none"> Retardation Factor: Soil Bulk Density ρ_b: foc: Koc: 	1.0 1.7 (kg/L) 0.0057% B: 38 T: 135 E: 95 X: 240	<ul style="list-style-type: none"> Calculated from $R = 1 + K_{oc} \times f_{oc} \times \rho_b / n$ Estimated Lab analysis Literature - use Koc = 38 																								
Biodegradation	Electron Acceptor: Background Conc. (mg/L): Minimum Conc. (mg/L): Change in Conc. (mg/L): Electron Acceptor: Max. Conc. (mg/L): Avg. Conc. (mg/L):	<table border="0"> <tr> <td><u>O₂</u></td> <td><u>NO₃</u></td> <td><u>SO₄</u></td> </tr> <tr> <td>2.05</td> <td>0.7</td> <td>26.2</td> </tr> <tr> <td>- 0.4</td> <td>- 0</td> <td>- 3.8</td> </tr> <tr> <td>1.65</td> <td>0.7</td> <td>22.4</td> </tr> <tr> <td colspan="3"> </td> </tr> <tr> <td><u>Fe</u></td> <td><u>CH₄</u></td> <td></td> </tr> <tr> <td>36.1</td> <td>7.4</td> <td></td> </tr> <tr> <td>16.6</td> <td>6.6</td> <td></td> </tr> </table> <p>Note: Boxed values are BIOSCREEN input values.</p>	<u>O₂</u>	<u>NO₃</u>	<u>SO₄</u>	2.05	0.7	26.2	- 0.4	- 0	- 3.8	1.65	0.7	22.4				<u>Fe</u>	<u>CH₄</u>		36.1	7.4		16.6	6.6		<ul style="list-style-type: none"> Based on March 1995 groundwater sampling program conducted by Groundwater Services, Inc.
<u>O₂</u>	<u>NO₃</u>	<u>SO₄</u>																									
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- 0.4	- 0	- 3.8																									
1.65	0.7	22.4																									
<u>Fe</u>	<u>CH₄</u>																										
36.1	7.4																										
16.6	6.6																										
General	<ul style="list-style-type: none"> Modeled Area Length: Modeled Area Width: Simulation Time: 	320 (ft) 200 (ft) 6 (yrs)	<ul style="list-style-type: none"> Based on area of affected groundwater plume Steady-state flow 																								
Source Data	<ul style="list-style-type: none"> Source Thickness: Source Concentration: 	10 (ft) (See Figure 1)	<ul style="list-style-type: none"> Based on geologic logs and lumped BTEX monitoring data 																								
Actual Data	Distance From Source (ft): BTEX Conc. (mg/L):	<table border="0"> <tr> <td><u>30</u></td> <td><u>60</u></td> <td><u>180</u></td> <td><u>280</u></td> </tr> <tr> <td>5.0</td> <td>1.0</td> <td>0.5</td> <td>0.001</td> </tr> </table>	<u>30</u>	<u>60</u>	<u>180</u>	<u>280</u>	5.0	1.0	0.5	0.001	<ul style="list-style-type: none"> Based on observed concentrations at site 																
<u>30</u>	<u>60</u>	<u>180</u>	<u>280</u>																								
5.0	1.0	0.5	0.001																								
OUTPUT	Centerline Concentration:	See Figure 3																									
	Array Concentration:	See Figure 4																									



BIOSCREEN Modeling Summary, Keesler Air Force Base, SWMU 66, Mississippi:

- BIOSCREEN was used to try to reproduce the movement of the plume from 1989 (the best guess for when the release occurred) to 1995.
- The soluble mass in soil and NAPL was estimated by integrating BTEX soil concentrations contours mapped as part of the site soil delineation program. An estimated 2000 Kg of BTEX was estimated to be present at the site based on GC/MS analysis of soil samples collected from both the vadose and saturated zone. This value represented a source half-life of 60 years with the instantaneous reaction model (the first value shown in the source half-life box in Figure 2), a relatively long half-life, so the 2000 Kg measured in 1995 was assumed to be representative of 1989 conditions.
- The instantaneous reaction model was used as the primary model to try to reproduce the plume length (~ 280 ft).
- Because a decaying source was used, the source concentration on the input screen (representing concentrations 6 yrs ago) were adjusted so the source concentration on the centerline output screen (representing concentrations now) were equal to 12 mg/L. Because the source decay term is different for the first order decay and instantaneous reaction models, this simulation focused on matching the instantaneous reaction model. The final result was a source concentration of 13.68 mg/L in the center of the source zone (note on the centerline output the source concentration is 12.021 mg/L).
- The initial run of the instantaneous reaction model indicated that the plume was too long. This indicates that there is more mixing of hydrocarbon and electron acceptors at the site than is predicted by the model. Therefore the longitudinal dispersivity was adjusted upwards (more mixing) until BIOSCREEN matched the observed plume length. The final longitudinal dispersivity was 32.5 ft.
- As a check the first-order decay model was used with the BIOSCREEN default value of 2 yrs. This run greatly overestimated the plume length, so the amount of biodegradation was increased by decreasing the solute half-life. A good match of the plume was reached with a solute half-life of 0.15 years. This is within observed ranges reported in the literature (see solute half-life section, page 22).
- As shown in Figure 3, BIOSCREEN matches the observed plume fairly well. The instantaneous model is more accurate near the source while the first order decay model is more accurate near the middle of the plume. Both models reproduce the actual plume length relatively well.
- As shown in Figure 4, the current plume is estimated to contain 7.8 kg of BTEX. BIOSCREEN indicates that the plume under a no-degradation scenario would contain 126.3 kg BTEX. In other words BIOSCREEN indicates that 94% of the BTEX mass that has left the source since 1989 has biodegraded.
- Most of the source mass postulated to be in place in 1989 is still there in 1996 (2000 kg vs. 1837 kg, or 92% left).
- The current plume contains 1.0 ac-ft of contaminated water, with 1.019 acre-ft/yr of water being contaminated as it flows through the source. Because the plume is almost at steady state, 1.019 ac-ft of water become contaminated per year with the same amount being remediated every year due to in-situ biodegradation and other attenuation processes. This indicates that a long-term monitoring approach would probably be more appropriate for this site than active remediation, as the plume is no longer growing in size.

BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence Version 1.3

1. HYDROGEOLOGY

Seepage Velocity* V_s (ft/yr)
↑ or

Hydraulic Conductivity K (cm/sec)
Hydraulic Gradient i (ft/ft)
Porosity n (-)

2. DISPERSION

Longitudinal Dispersivity* α_x (ft)
Transverse Dispersivity* α_y (ft)
Vertical Dispersivity* α_z (ft)
↑ or

Estimated Plume Length L_p (ft)

3. ADSORPTION

Retardation Factor* R (-)
↑ or

Soil Bulk Density ρ (kg/l)
Partition Coefficient K_{oc} (L/kg)
Fraction Organic Carbon f_{oc} (-)

4. BIODEGRADATION

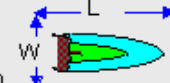
1st Order Decay Coeff* λ (per yr)
↑ or

Solute Half-Life t_{-half} (year)
or Instantaneous Reaction Model

Delta Oxygen* DO (mg/L)
Delta Nitrate* NO_3 (mg/L)
Observed Ferrous Iron* Fe^{2+} (mg/L)
Delta Sulfate* SO_4 (mg/L)
Observed Methane* CH_4 (mg/L)

5. GENERAL

Modeled Area Length* (ft) L
Modeled Area Width* (ft) W
Simulation Time* (yr)



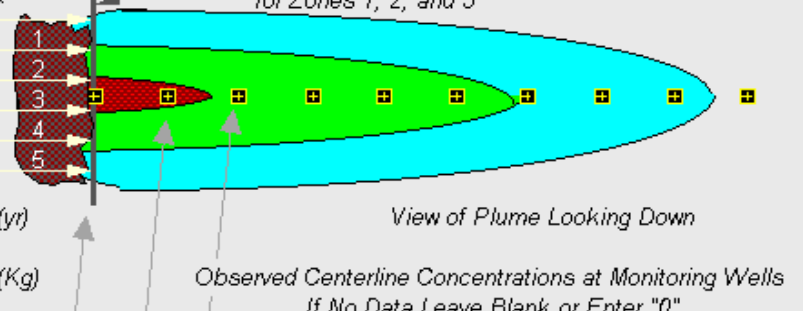
6. SOURCE DATA

Source Thickness in Sat. Zone* (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
28	0.057
30	2.508
14	13.68
30	2.508
28	0.057

Source Decay (see Help):
Source Half-life* (yr)
Soluble Mass (Kg)
In NAPL, Soil (Kg)



7. FIELD DATA FOR COMPARISON

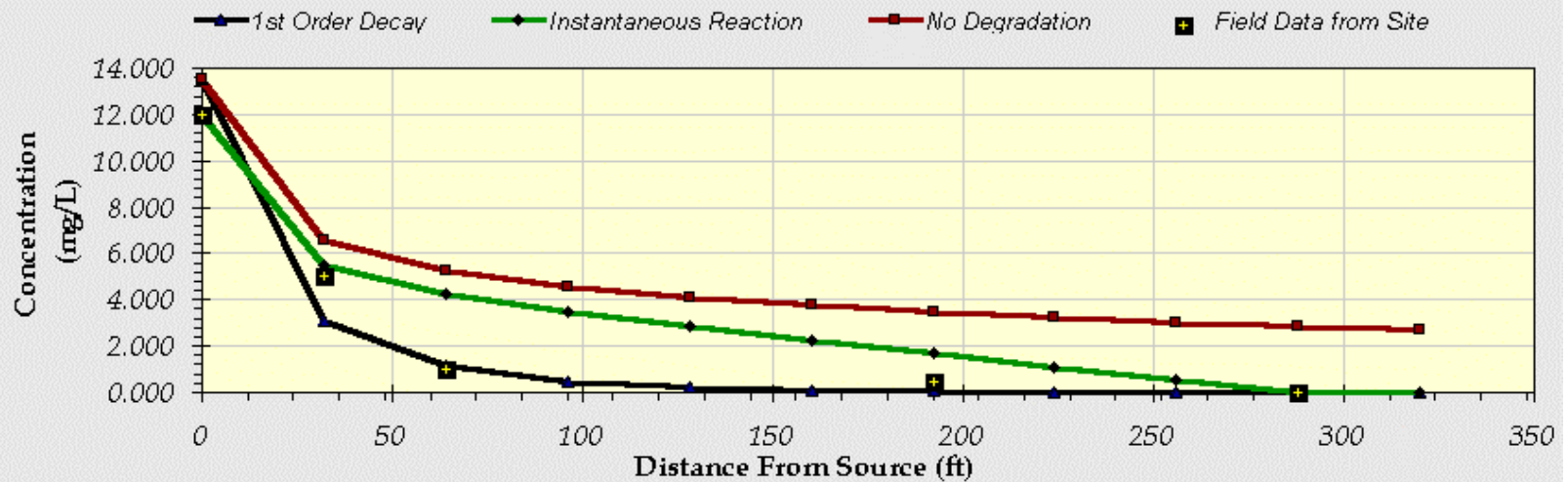
Concentration (mg/L)	12.0	5.0	1.0				.5		.001		
Dist. from Source (ft)	0	32	64	96	128	160	192	224	256	288	320

8. CHOOSE TYPE OF OUTPUT TO SEE:

Figure 2. BIOSCREEN Input Screen. Keesler Air Force Base, Mississippi.

DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

TYPE OF MODEL	Distance from Source (ft)										
	0	32	64	96	128	160	192	224	256	288	320
No Degradation	13.544	6.575	5.280	4.581	4.107	3.754	3.474	3.241	3.040	2.861	2.697
1st Order Decay	13.544	3.117	1.186	0.488	0.208	0.090	0.040	0.018	0.008	0.004	0.002
Inst. Reaction	12.021	5.463	4.248	3.500	2.860	2.257	1.678	1.114	0.559	0.004	0.000
Field Data from Site	12.000	5.000	1.000				0.500			0.001	



Calculate Animation

Time:
6 Years

Return to Input

Recalculate This Sheet

Figure 3. Centerline Output. Keesler Air Force Base, Mississippi.

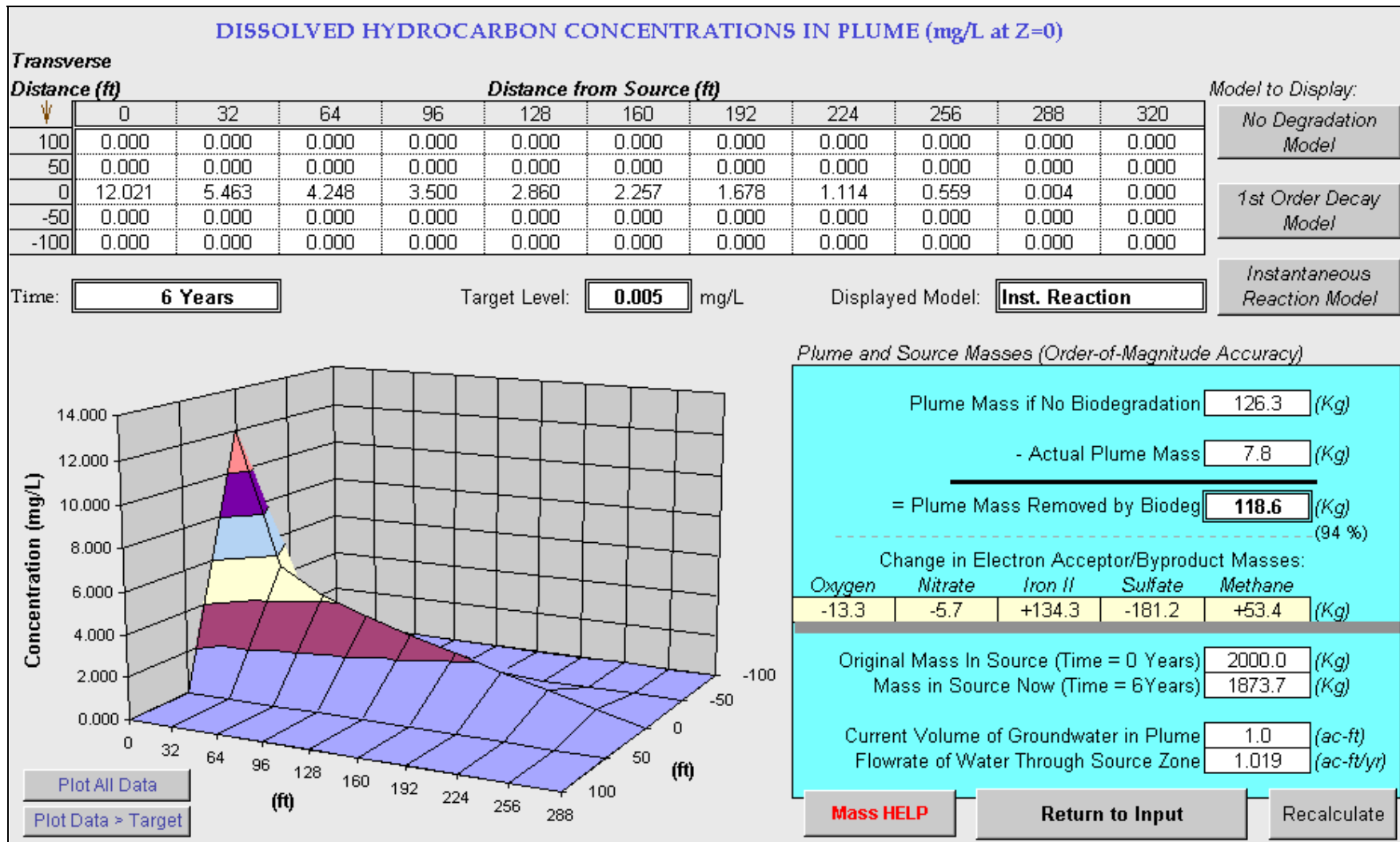
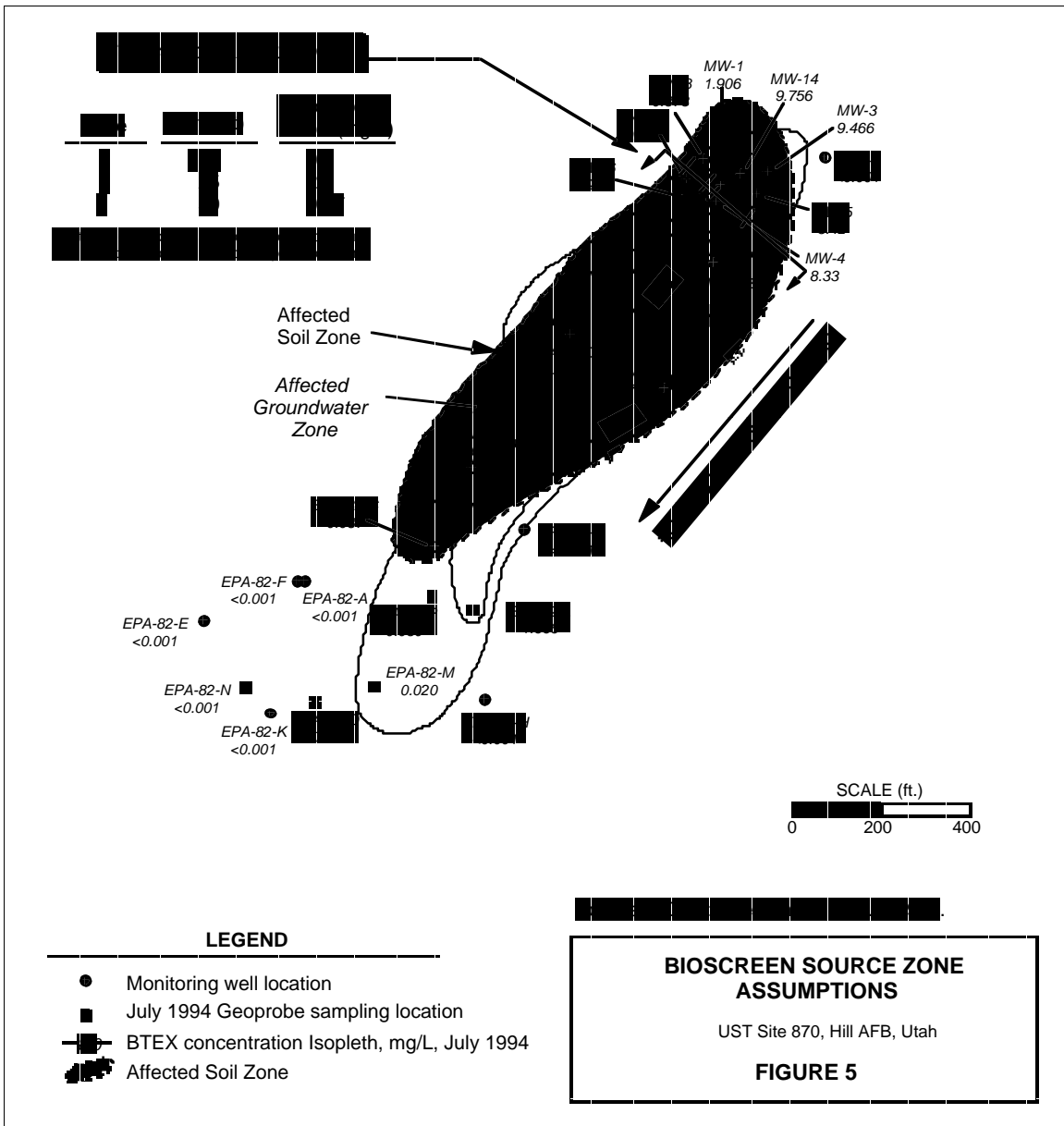


Figure 4. Array Concentration Output. Keesler Air Force Base, Mississippi.

EXAMPLE 2

Hill Air Force Base, UST Site 870, Utah

DATA TYPE	Parameter	Value	Source																												
Hydrogeology	<ul style="list-style-type: none"> Hydraulic Conductivity: Hydraulic Gradient: Porosity: 	8.05 x 10 ⁻³ (cm/sec) 0.048 (ft/ft) 0.25	<ul style="list-style-type: none"> Slug-tests results Static water level measurements Estimated 																												
Dispersion	Original <ul style="list-style-type: none"> Longitudinal Dispersivity: Transverse Dispersivity: Vertical Dispersivity: 	28.5 (ft) 2.85 (ft) 0 (ft)	<ul style="list-style-type: none"> Based on estimated plume length of 1450 ft and Xu's dispersivity formula Note: No calibration was necessary to match the observed plume length. 																												
Adsorption	<ul style="list-style-type: none"> Retardation Factor: Soil Bulk Density ρb: foc: Koc: 	1.3 1.7 (kg/L) 0.08% B: 38 T: 135 E: 95 X: 240	<ul style="list-style-type: none"> Calculated from R = 1+Koc x foc x ρb/n Estimated Lab analysis Literature - use Koc = 38 																												
Biodegradation	Electron Acceptor: Background Conc. (mg/L): Minimum Conc. (mg/L): Change in Conc. (mg/L): Electron Acceptor: Max. Conc. (mg/L): Avg. Conc. (mg/L):	<table border="0"> <tr> <td></td> <td style="text-align: center;"><u>O₂</u></td> <td style="text-align: center;"><u>NO₃</u></td> <td style="text-align: center;"><u>SO₄</u></td> </tr> <tr> <td></td> <td style="text-align: center;">6.0</td> <td style="text-align: center;">17.0</td> <td style="text-align: center;">100</td> </tr> <tr> <td></td> <td style="text-align: center;">- 0.22</td> <td style="text-align: center;">- 0</td> <td style="text-align: center;">- 0</td> </tr> <tr> <td></td> <td style="text-align: center;">5.78</td> <td style="text-align: center;">17.0</td> <td style="text-align: center;">100</td> </tr> <tr> <td></td> <td></td> <td style="text-align: center;"><u>Fe</u></td> <td style="text-align: center;"><u>CH₄</u></td> </tr> <tr> <td></td> <td></td> <td style="text-align: center;">50.5</td> <td style="text-align: center;">2.04</td> </tr> <tr> <td></td> <td></td> <td style="text-align: center;">11.3</td> <td style="text-align: center;">0.414</td> </tr> </table> <p>Note: Boxed values are BIOSCREEN input values.</p>		<u>O₂</u>	<u>NO₃</u>	<u>SO₄</u>		6.0	17.0	100		- 0.22	- 0	- 0		5.78	17.0	100			<u>Fe</u>	<u>CH₄</u>			50.5	2.04			11.3	0.414	<ul style="list-style-type: none"> Based on July 1994 groundwater sampling program conducted by Parsons Engineering Science, Inc.
	<u>O₂</u>	<u>NO₃</u>	<u>SO₄</u>																												
	6.0	17.0	100																												
	- 0.22	- 0	- 0																												
	5.78	17.0	100																												
		<u>Fe</u>	<u>CH₄</u>																												
		50.5	2.04																												
		11.3	0.414																												
General	<ul style="list-style-type: none"> Modeled Area Length: Modeled Area Width: Simulation Time: 	1450 (ft) 320 (ft) 5 (yrs)	<ul style="list-style-type: none"> Based on area of affected groundwater plume Steady-state flow 																												
Source Data	<ul style="list-style-type: none"> Source Thickness: Source Concentration: 	10 (ft) (See Figure 5)	<ul style="list-style-type: none"> Based on geologic logs and lumped BTEX monitoring data 																												
Actual Data	Distance from Source (ft): BTEX Conc. (mg/L):	<table border="0"> <tr> <td style="text-align: center;"><u>340</u></td> <td style="text-align: center;"><u>1080</u></td> <td style="text-align: center;"><u>1350</u></td> <td style="text-align: center;"><u>1420</u></td> </tr> <tr> <td style="text-align: center;">8.0</td> <td style="text-align: center;">1.0</td> <td style="text-align: center;">0.02</td> <td style="text-align: center;">0.005</td> </tr> </table>	<u>340</u>	<u>1080</u>	<u>1350</u>	<u>1420</u>	8.0	1.0	0.02	0.005	<ul style="list-style-type: none"> Based on observed concentration contour at site (see Figure 5) 																				
<u>340</u>	<u>1080</u>	<u>1350</u>	<u>1420</u>																												
8.0	1.0	0.02	0.005																												
OUTPUT	Centerline Concentration:	See Figure 7																													
	Array Concentration:	See Figure 8																													



BIOSCREEN Modeling Summary Hill Air Force Base, UST Site 870, Utah:

- BIOSCREEN was used to try to reproduce the movement of the plume.
- An infinite source was assumed to simplify the modeling scenario because no estimates of the source mass were available from soil sampling data. The source was assumed to be in the high concentration zone of the plume area (see Figure 5). Note that the zone of affected soil was quite large; however much of the affected soil zone downgradient of the source was relatively low concentration.

Two modeling approaches could be applied: 1) assuming the source zone is just downgradient of the affected soil area (near well EPA-82-C) and ignoring the area upgradient of the this point, and 2) modeling most of the plume with source near MW-1. Alternative 1 is theoretically more accurate, as BIOSCREEN cannot account for the contributions from any affected soil zone downgradient of the source. At the case of Hill AFB, however, it was assumed that the contributions from this downgradient affected soil were relatively minor and that the main process of interest was the length of the plume from the high-concentration source zone. Therefore Alternative 2 was modeled, with the note that the middle of the actual plume may actually have higher concentrations than would be expected due to the contaminants in the downgradient affected soil zone.

- The instantaneous reaction model was used as the primary model to try to reproduce the plume length (~ 280 ft) as shown in Figure 7.
- The initial run of the instantaneous reaction model reproduced the existing plume without any need for calibration of dispersivity.
- As a check the first-order decay model was used with the BIOSCREEN default value of 2 yrs. This run greatly overestimated the plume length, so the amount of biodegradation was increased by decreasing the solute half-life. A half-life value of 0.1 years was required to match the plume length, although the match in the middle in the plume was much poorer.
- As shown in Figure 7, BIOSCREEN matches the observed plume fairly well. The instantaneous model is more accurate near the source while the first order decay model is more accurate near the middle of the plume. Both models reproduce the actual plume length relatively well.
- As shown in Figure 8, the model was unable to calculate the mass balances. A quick evaluation shows the reason: with a seepage velocity of 1609 ft/yr and a 5 year simulation time, the undegraded plume should be over 8000 ft long. Because the mass balance is based on a comparison of a complete undegraded plume vs. a degraded plume, a model area length of 8000 ft would be required for BIOSCREEN to complete the mass balance calculation. Therefore two runs would be needed to complete the simulation: 1) a run with a modeled length of 1450 feet to calibrate and evaluate the match to existing data, and 2) a run with a modeled length of 8000 ft to do the mass balance. The results of the second run (change of model area length from 1450 ft to 8000 ft) indicate that over 99% of the mass that has left the source has biodegraded by the time groundwater has traveled 1450 ft.

Because the plume is no longer moving, a long-term monitoring approach is probably more appropriate for this site than active remediation.

BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence Hill AFB
Version 1.3 UST Site 870
Run Name

1. HYDROGEOLOGY

Seepage Velocity* V_s (ft/yr)
↑ or

Hydraulic Conductivity K (cm/sec)
Hydraulic Gradient i (ft/ft)
Porosity n (-)

2. DISPERSION

Longitudinal Dispersivity* α_x (ft)
Transverse Dispersivity* α_y (ft)
Vertical Dispersivity* α_z (ft)
↑ or

Estimated Plume Length L_p (ft)

3. ADSORPTION

Retardation Factor* R (-)
↑ or

Soil Bulk Density ρ (kg/l)
Partition Coefficient K_{oc} (L/kg)
Fraction Organic Carbon f_{oc} (-)

4. BIODEGRADATION

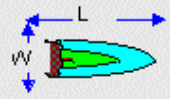
1st Order Decay Coeff* λ (per yr)
↑ or

Solute Half-Life t_{half} (year)
or Instantaneous Reaction Model

Delta Oxygen* DO (mg/L)
Delta Nitrate* NO_3 (mg/L)
Observed Ferrous Iron* Fe^{2+} (mg/L)
Delta Sulfate* SO_4 (mg/L)
Observed Methane* CH_4 (mg/L)

5. GENERAL

Modeled Area Length* (ft) L
Modeled Area Width* (ft) w
Simulation Time* (yr)



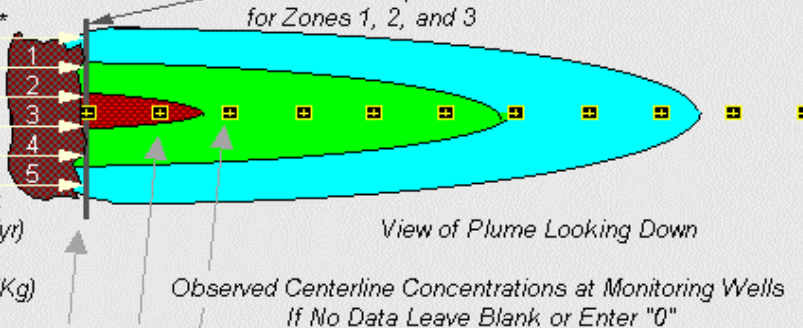
6. SOURCE DATA

Source Thickness in Sat. Zone* (ft)

Source Zones:

Width* (ft)	Conc. (mg/L)*
50	0.07
25	2.8
100	9
25	2.8
50	0.07

Source Decay (see Help):
Source Half-life* (yr)
Soluble Mass (Kg)
In NAPL, Soil (Kg)



View of Plume Looking Down
Observed Centerline Concentrations at Monitoring Wells
If No Data Leave Blank or Enter "0"

7. FIELD DATA FOR COMPARISON

Concentration (mg/L)	9.0	8.0					1.0	.02	.005		
Dist. from Source (ft)	0	145	290	435	580	725	870	1015	1160	1305	1450

8. CHOOSE TYPE OF OUTPUT TO SEE:

RUN CENTERLINE

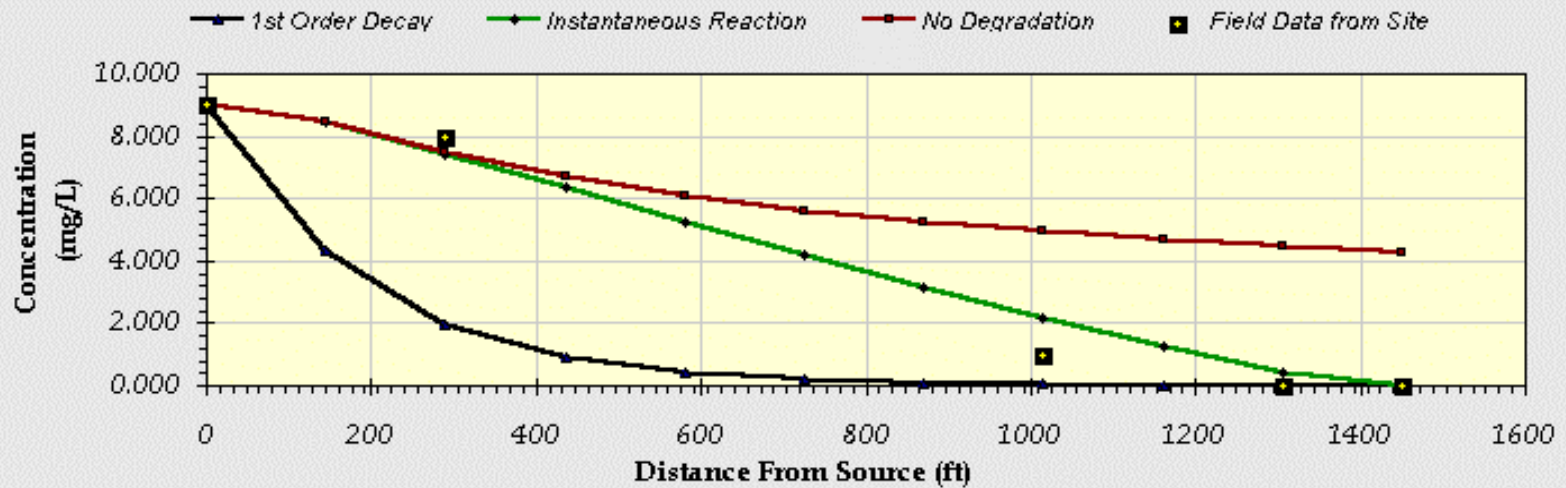
RUN ARRAY

Help

Figure 6. BIOSCREEN Input Screen. Hill Air Force Base, Utah.

DISSOLVED HYDROCARBON CONCENTRATION ALONG PLUME CENTERLINE (mg/L at Z=0)

TYPE OF MODEL	Distance from Source (ft)										
	0	145	290	435	580	725	870	1015	1160	1305	1450
No Degradation	9.000	8.467	7.466	6.684	6.089	5.624	5.250	4.940	4.679	4.455	4.260
1st Order Decay	9.000	4.348	1.969	0.905	0.424	0.201	0.096	0.047	0.023	0.011	0.005
Inst. Reaction	9.000	8.466	7.407	6.350	5.268	4.192	3.152	2.168	1.245	0.385	0.000
Field Data from Site	9.000		8.000					1.000		0.020	0.005



Calculate Animation

Time:
5 Years

Return to Input

Recalculate This Sheet

Figure 7. Centerline Output. Hill Air Force Base, Utah.

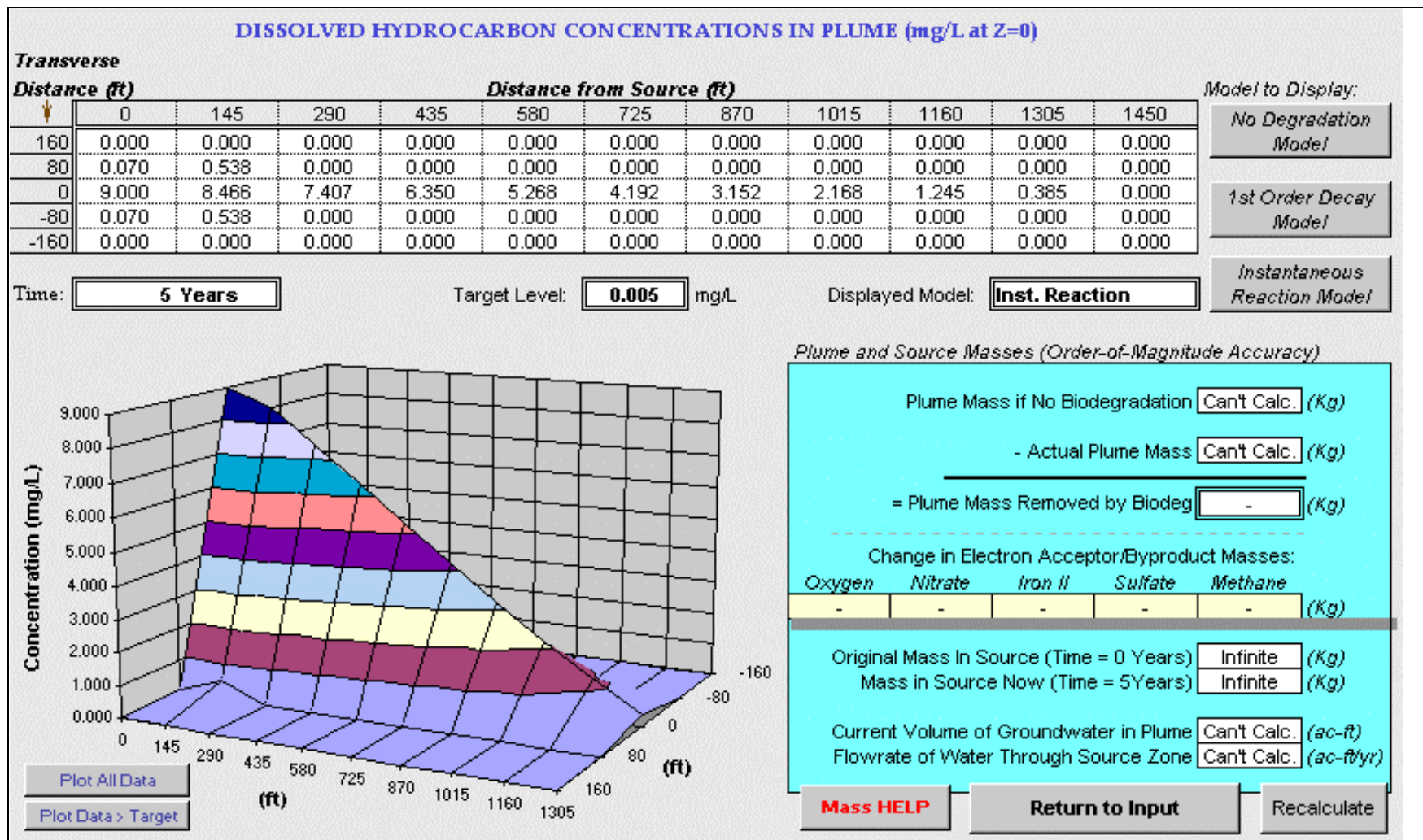


Figure 8. Array Concentration Output. Hill Air Force Base, Utah.

