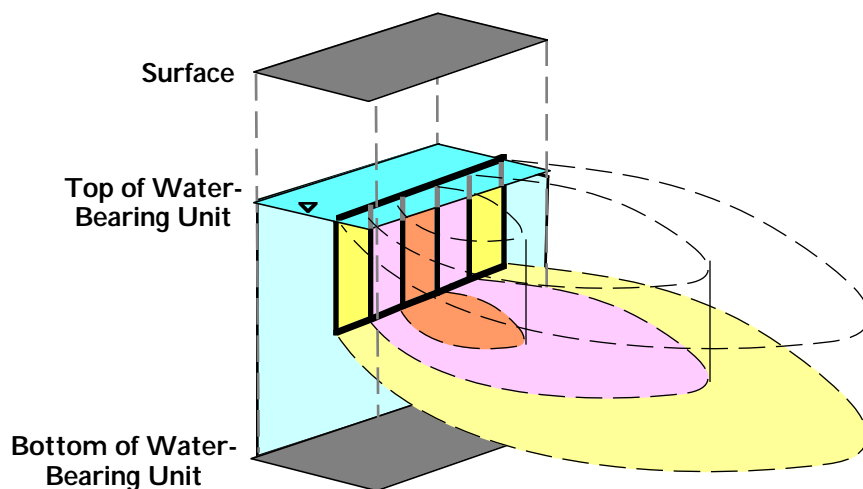

BIOSCREEN

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:

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

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 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 ± 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 Conference, NGWA, 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

$$\% \text{ BTEX} = (63 \text{ mg/L}) \div (93 \text{ mg/L}) = \underline{68 \%}$$

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

$$\% \text{ BTEX} = (112 \text{ mg/L}) \div (126 \text{ mg/L}) = \underline{89 \%}$$

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

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

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% (*note: equals 4.5% of 31.5%*)

% benzenes, alkylbenzenes in complete JP-4 mixture: 18% (*from Stelljes and Watkin, 1993*)

% branched alkanes in all identified compounds:	26%
% branched alkanes in complete JP-4 mixture:	31%
% cycloalkanes in all compounds identified:	7%
% cycloalkanes in complete JP-4 mixture:	16%
% naphthalenes in all compounds identified:	6%
% naphthalenes in complete JP-4 mixture:	3%
% normal alkanes in all compounds identified:	47%
% normal alkanes in complete JP-4 mixture:	32%

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

With 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 a 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.

References for BTEX-Dominated Plumes

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- Wiedemeier, T. H., Wilson, J. T., Kampbell, D. H, Miller, R. N., and Hansen, J.E., 1995. "Technical Protocol for Implementing Intrinsic Remediation With Long-Term Monitoring for Natural Attenuation of Fuel 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>

continued

continued

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).	υ	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)

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

<p>EPA Center for Subsurface Modeling Support (CSMoS) NRMRL/SPRD P.O. Box 1198 Ada, Oklahoma 74821-1198</p>	<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 read and print pdf files.)
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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.

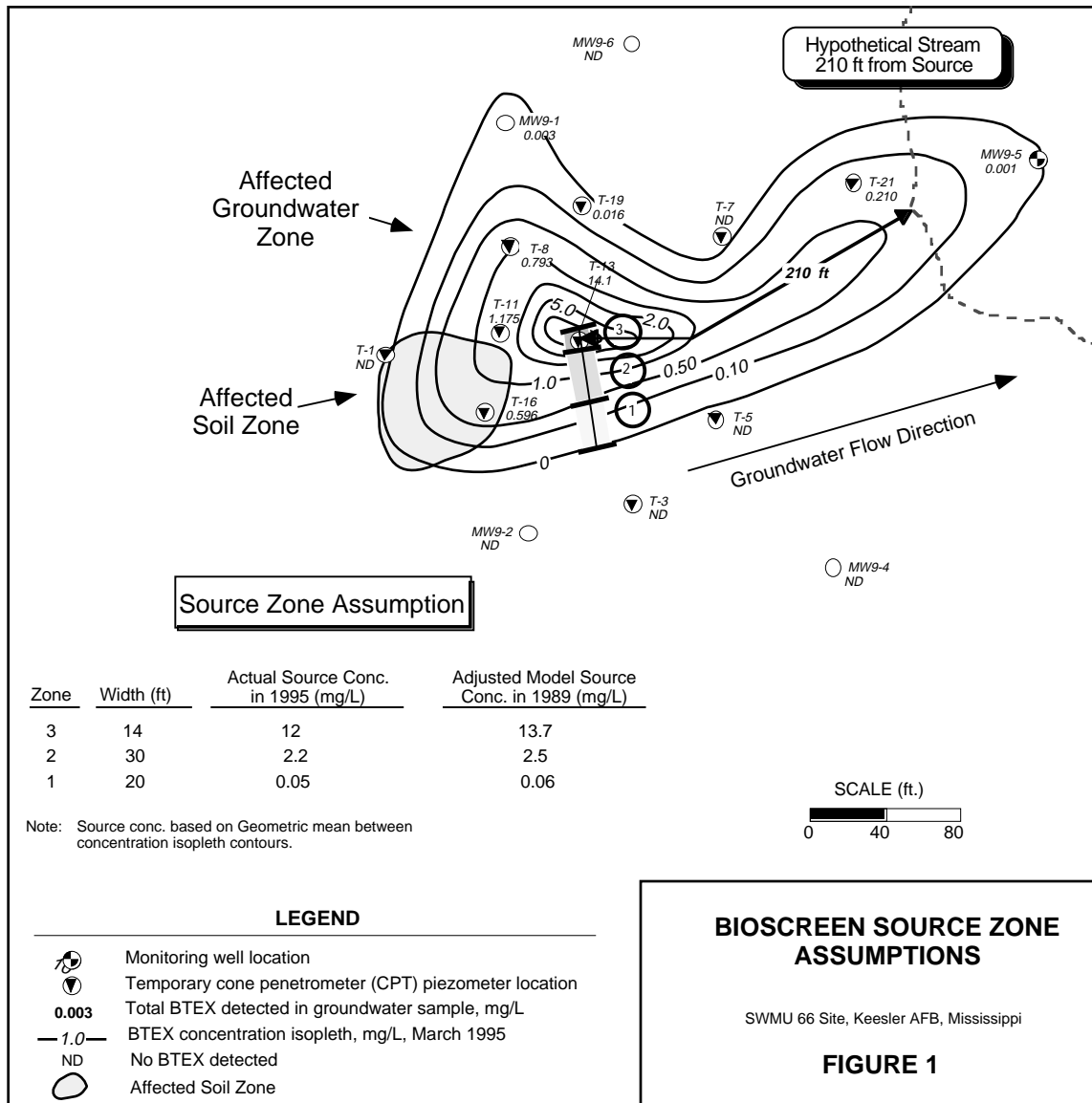
APPENDIX 1. BIOSCREEN Version 1.4 EXAMPLE**Example 1: SWMU 66, Keesler AFB, Mississippi**

- 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 $R = 1 + Koc \times foc \times \rho_b / n$ 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																												
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	<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* Vs (ft/yr)
 or (cm/sec)

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 (ft)

Estimated Plume Length L_p (ft)

3. ADSORPTION

Retardation Factor* R (-)
 or (kg/l)

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* 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) 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 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

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).

View of Plume Looking Down

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

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.)

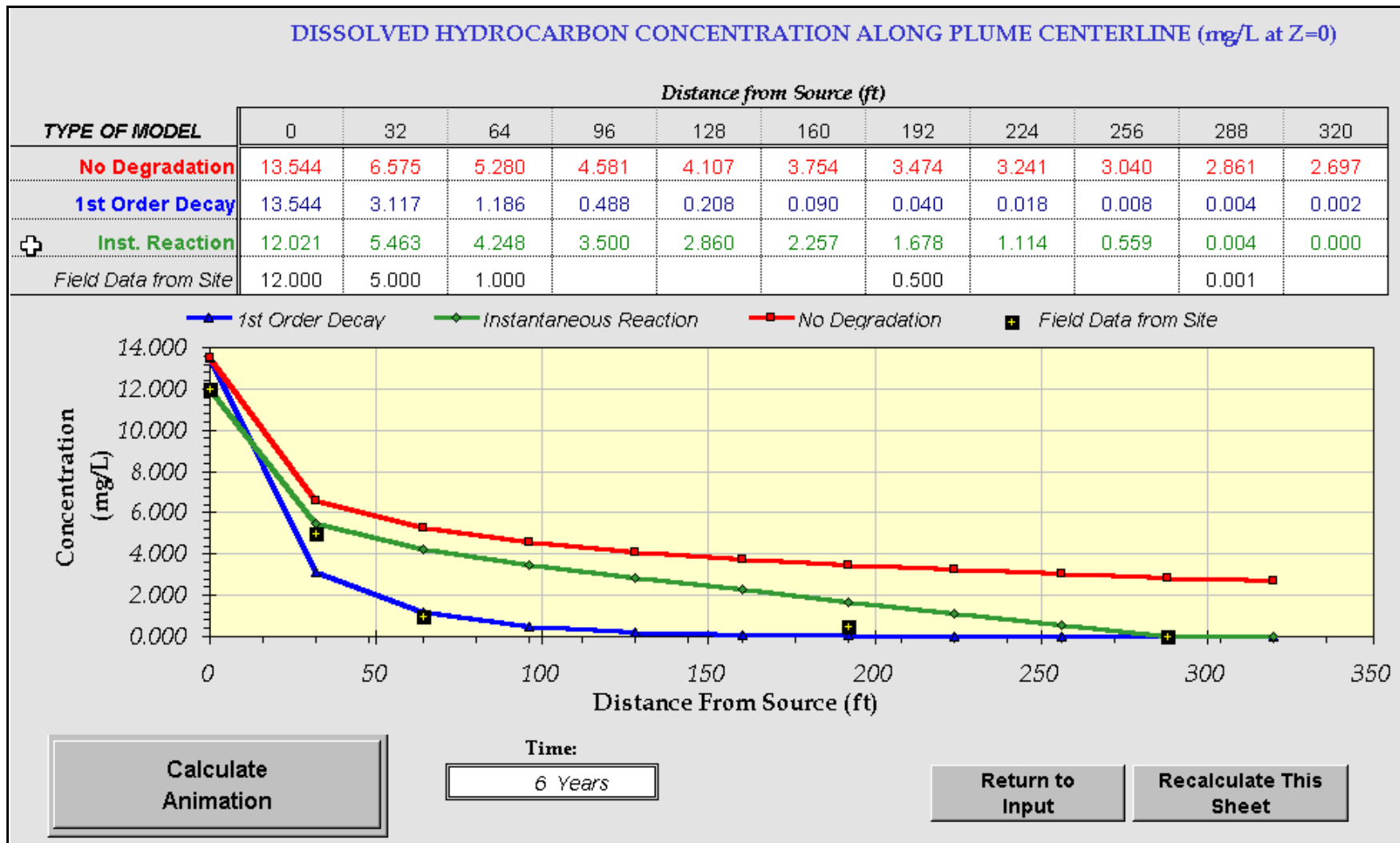


Figure 3. Centerline Output. Keesler Air Force Base, Mississippi.

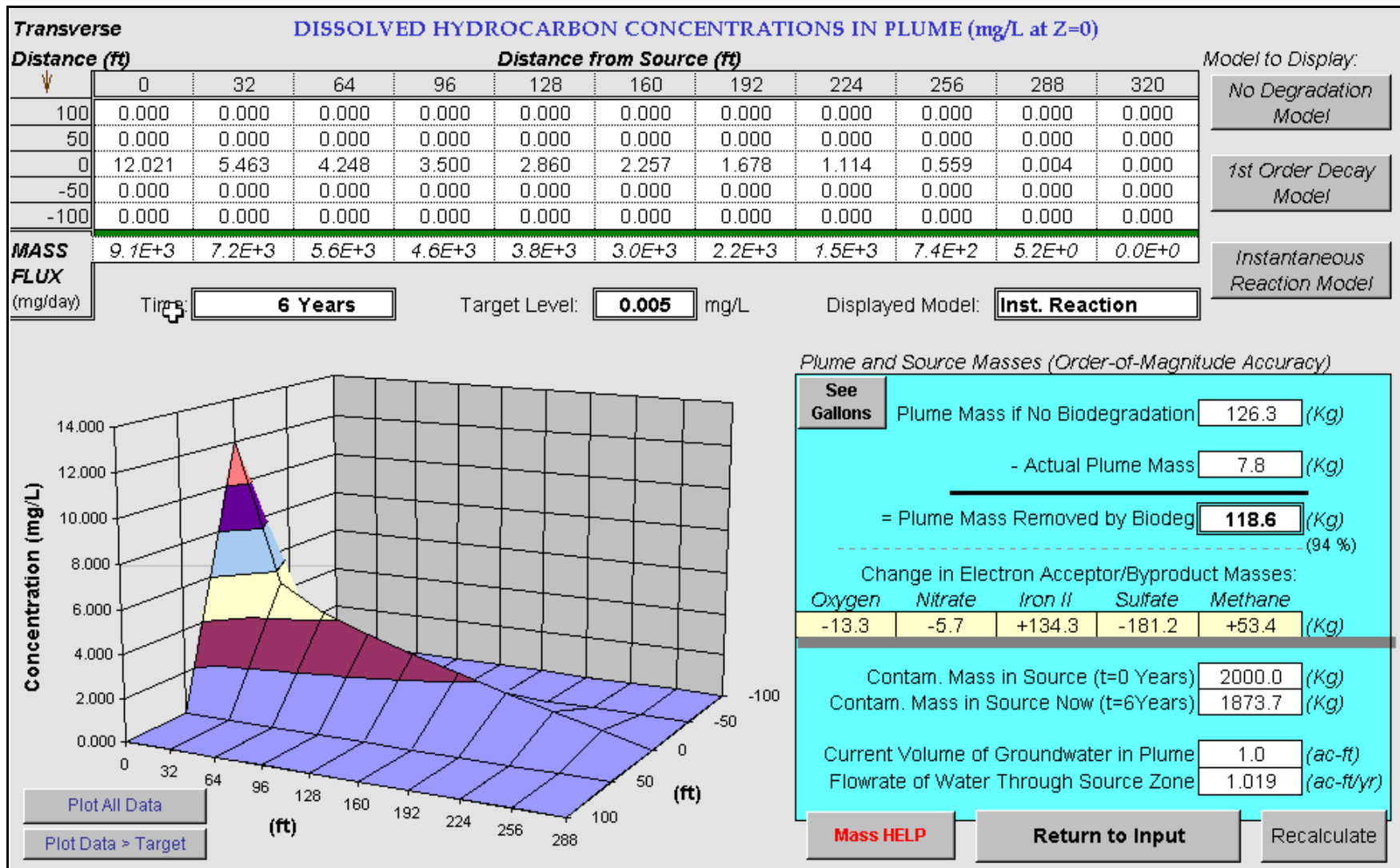


Figure 4. Array Concentration Output. Keesler Air Force Base, Mississippi.

BIOSCREEN Natural Attenuation Decision Support System

Air Force Center for Environmental Excellence

Version 1.4

Keesler AFB
SWMU 66
Run Name

Data Input Instructions:

→ 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).

1. HYDROGEOLOGY

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

Hydraulic Conductivity K (cm/sec)

Hydraulic Gradient i (ft/ft)

Porosity n (-)

2. DISPERSION

Longitudinal Dispersivity* alpha x (ft)

Transverse Dispersivity* alpha y (ft)

Vertical Dispersivity* alpha z (ft)
 or (ft)

Estimated Plume Length Lp (ft)

3. ADSORPTION

Retardation Factor* R (-)
 or (kg/l)

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 (year)

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)

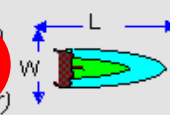
Observed Methane* CH4 (mg/L)

5. GENERAL

Modeled Area Length (ft)

Modeled Area Width (ft)

Simulation Time* (yr)



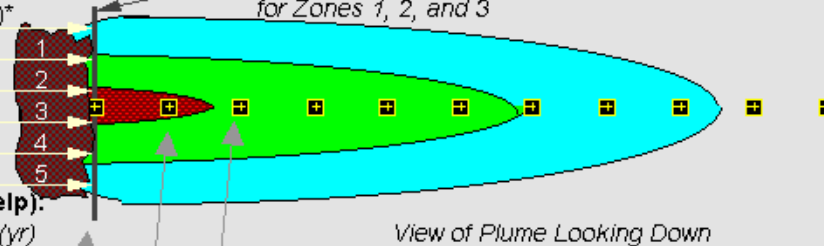
6. SOURCE DATA

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

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3



View of Plume Looking Down

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

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

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

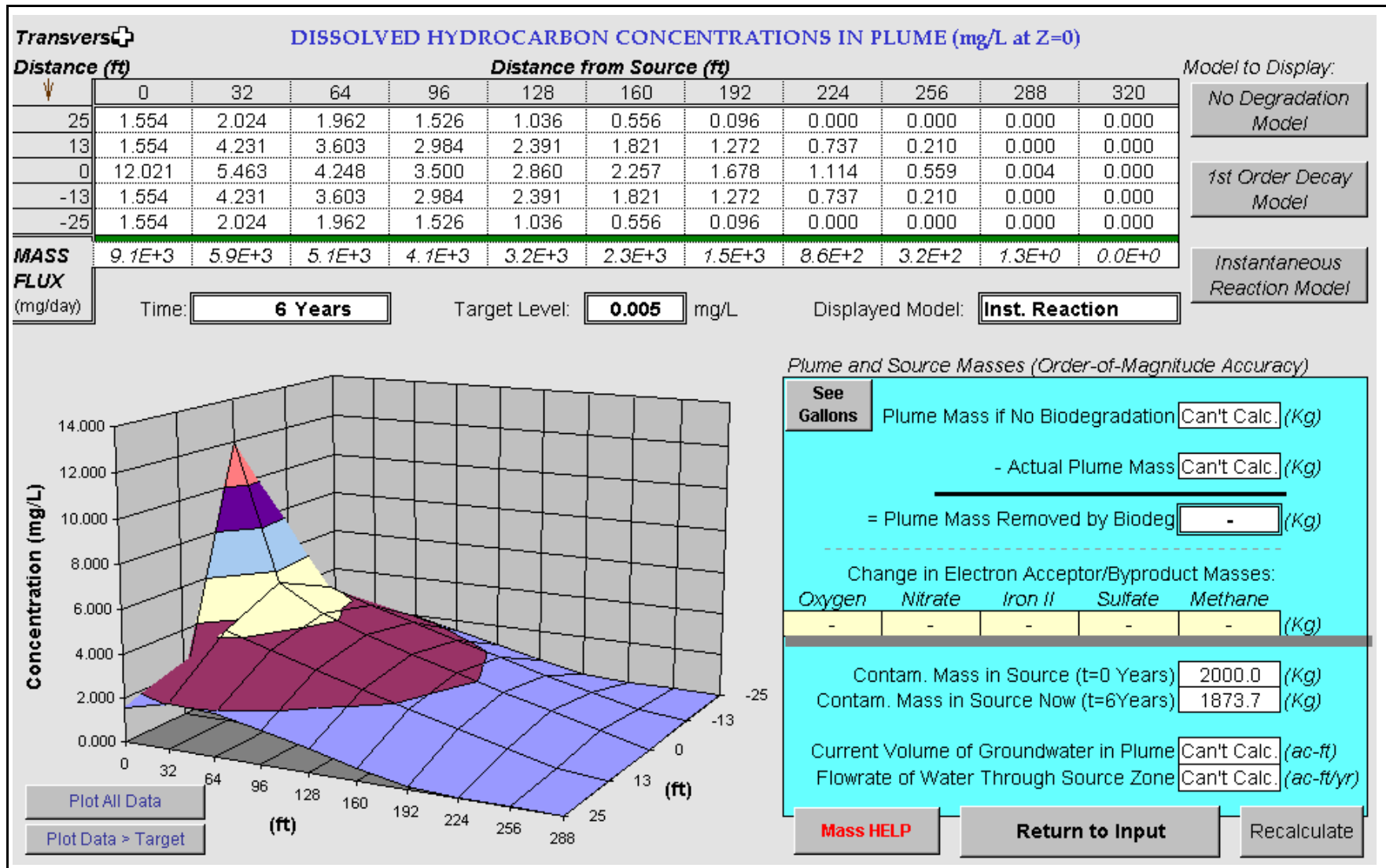


Figure 6. Array Concentration Output. Keesler Air Force Base, Mississippi, with 50 ft. modeled area width.