FATE AND TRANSPORT POTENTIAL FOR DISSOLVED PENTACHLOROPHENOL AND NAPHTHALENE IN A SHALLOW AQUIFER AT THE OLD MIDLAND PRODUCTS SUPERFUND SITE

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PROBLEM STATEMENT

Residual and pooled dense, non-aqueous phase liquid (DNAPL) creosote in shallow soils and fractured rock at the Old Midland Products Superfund Site, Ola, Arkansas, have contaminated shallow ground water on site. These chemicals were used to preserve wood from damage by bacteria and insects. For the purpose of assisting remedy selection, it is necessary to estimate the fate and transport of contaminants of concern contained in the creosote. The most significant contaminants that pose threats to ground water are pentachlorophenol (PCP) and polycyclic aromatic hydrocarbons (PAHs). To estimate the fate and transport of these contaminants, it was decided to use the computer model (BIOSCREEN ;U.S. EPA, 1997) to determine the migration of the contaminants.

PURPOSE

The purpose of this document is to describe the model variables input and results of a BIOSCREEN simulation of potential fate and transport of PCP by ground-water flow from DNAPL sources in the shallow aquifer laterally, in the direction of the hydraulic gradient.

SCOPE

The scope of this document includes use of the BIOSCREEN Natural Atttenuation Decision Support System, v. 1.4, input of environmental variables from the site, and pertinent variables obtained from the literature. Results are provided in output pages from the BIOSCREEN model and discussed in the Results and Conclusions section.

GENERAL DISCUSSION

The Midland site consists of about 37.75 acres and is located about one-half mile east of Ola, Arkansas. The site contained seven former impoundments and a treatment building in the southern portion of the site where wastes were discharged. Contaminants PCP and PAHs were found in soils and ground water to about 40 feet of depth. Excavation and on site incineration of contaminated soil was completed in 1993. A pump and treat ground-water remedy was emplaced in 1994 to treat shallow ground water from the unweathered, fractured shale aquifer. Slight decreases to increases of contaminants occurred in monitoring wells during the remedy operation. The remedy was halted in 1999 and contaminants were observed to rebound in shut-in recovery wells, so the system was restarted in 2000.

The shallow aquifer is a highly fractured, weathered shale with thicknesses ranging between 10 and 25 feet. This unit overlies a lower aquifer of unweathered shale with fewer, smaller fractures extending to as much as 150 feet bgs. Ground water flow is toward the northwest at about 20 to 40 feet per year.

PCP MODELING

The partition coefficient used for modeling purposes is 31623 L/kg (Howard, 1989). No data of the percent organic carbon in the sediments were collected during the Remedial Investigation, so a conservative value of 0.000014 fraction organic carbon (foc) was assigned to the shallow aquifer along with a bulk density of 1.8 kg/L. These values resulted in a retardation factor of 6.3 for modeling purposes.

Although the PCP is considered recalcitrant in ground-water environments, it can nevertheless degrade to some degree. A conservative estimate of the biodegradation rate (first order decay coefficient) for PCP is reported to be 0.0092/yr, or a half life of 7.5 yr, almost twice as long as the reported value of 4.1 yr (Howard and others, 1991). The estimate was based on the 1998 concentration of PCP of 0.16 mg/L at well 20S, approximately 140 feet downgradient from the source area (fig. 1).

All the variables input to the BIOSCREEN model are provided in figure 2. Simplifying assumptions are listed below.

1. Modeled plume length is 500 ft and aquifer thickness is 40 ft.
2. Porosity is principally fractures where ground-water flow is very slow.
3. Principal direction of flow is northwest, from the impoundment source area to downgradient Effects of withdrawal of ground water are ignored.
4. Fraction of organic carbon for the shallow aquifer is estimated at 1.4×10^{-5}. A partition coefficient of 31,623 L/kg is used for a retardation factor of 6.3.
5. A ground-water flow velocity of 30 ft/yr is used based on the middle of the range of 20-40 ft/yr estimated (U.S. EPA, 1998).
6. Maximum concentration of PCP of 1.4 mg/L is used as the source concentration from a 10,000 kg source in the shallow water-bearing zone.
7. A half-life of 7.5yr for PCP was used for biodegradation (reported first order decay coefficient of 0.092/ yr).

PAH (NAPHTHALENE) MODELING

The principal contaminants PAHs were released in the impoundment area as part of the DNAPL contaminants during the life of the facility. The most soluble PAH and, thus, the most transportable in ground water, is naphthalene, which was used as the principal indicator of PAH fate and transport. The partition coefficient used for modeling purposes is 1000 L/kg (Howard, 1989, p. 408). No data of the percent organic carbon in the sediments were collected during the Remedial Investigation, so a conservative value of 2.1×10^{-5}. was assigned to the fractured clay along with a bulk density of 1.8 kg/L. These values resulted in a retardation factor of 1.3 for modeling purposes.

Although the PAH compounds are considered recalcitrant in ground-water environments, they nevertheless degrade to some degree. Biodegradation rate (first order decay coefficient) for naphthalene is reported to be 0.53 yr or a first order decay coefficient of 1.3/yr (Howard and others, 1991, p. 260). A more conservative estimate of 1.2 yr (0.58/yr) was used based on the 1998 concentration of naphthalene of 0.51 mg/L at well 20S, approximately 140 feet downgradient from the source area (fig. 1).

All the variables input to the BIOSCREEN model are provided in figure 2a. Simplifying assumptions are listed below.

1. Plume length is 300 ft and aquifer thickness is 40 ft.
2. Porosity is principally fractures where ground-water flow is very slow.
3. Principal direction of flow toward the northwest
4. Fraction of organic carbon for the fractured shale is 2.1×10^{-5}. A conservative partition coefficient of 1000 L/kg from values reported up to 4100 L/kg.
5. Conservative value of ground-water flow velocity of 30 ft/yr is used.
6. Maximum concentration of naphthalene of 6.3 mg/L is used as the source concentration from a 10,000 kg source in the shallow water-bearing zone.
7. Half-life of 0.53 yr for naphthalene was used.

RESULTS AND CONCLUSIONS

The BIOSCREEN spreadsheet was run for simulations of 50 years to assess the status of the PCP contaminant plume from the source area in the shallow aquifer to downgradient using an approximate flow path from the impoundment area on site to well MW-20S as the flow path, approximately 150 feet from the source area.

Figure 2a shows input variables and model set up for 500 feet of transport. Figure 2b shows the results of PCP transport for 80 years. Concentration of PCP reaches 0.001 mg/L (plume equilibrium) at 500 feet downgradient 100 years from the time of release. The model is most sensitive to the fraction of organic carbon (foc) that affects retardation of the chemical solute. The parameter foc is estimated and should be obtained from field data if any future data collection occurs for this site.

Thus, based on conservative estimates of variables of fate and transport of PCP in the shallow aquifer, a threat of contamination beyond 500 feet downgradient of the impoundment area is not predicted because equilibrium of the plume occurs after 100 years of PCP transport based on current conditions. The action of monitoring the shallow aquifer for PCP that could originate from the source creosote remaining in the shallow soil or the shallow aquifer should be sufficiently protective of the ground-water resource.

The BIOSCREEN spreadsheet was run for 50 years to assess fate and transport of naphthalene from the shallow water-bearing zone to downgradient.

Figure 3a shows input variables and model set up for 50 years of transport. Figure 3b shows the results of naphthalene transport for 15 years. Concentration of naphthalene

reaches approximate equilibrium and 0.001 mg/L at 500 feet in the aquifer downgradient of the source area in about 15 years. Detection of naphthalene (0.001 mg/L) is not observed beyond 500 feet even after 50 years of transport. The risk-based screening level of 0.0062 mg/L would be reached at about 380 feet within 15 years, but would remain at that concentration until the source contaminants are depleted. Transport is relatively insensitive to orders of magnitude variation in foc.

Thus, little or no threat of contamination beyond about 500 feet from the impoundment area is likely to occur. The action of monitoring the shallow aquifer for the PAH contaminants that could originate from the source creosote remaining in the impoundment area should be sufficiently protective of this aquifer downgradient.

REFERENCES

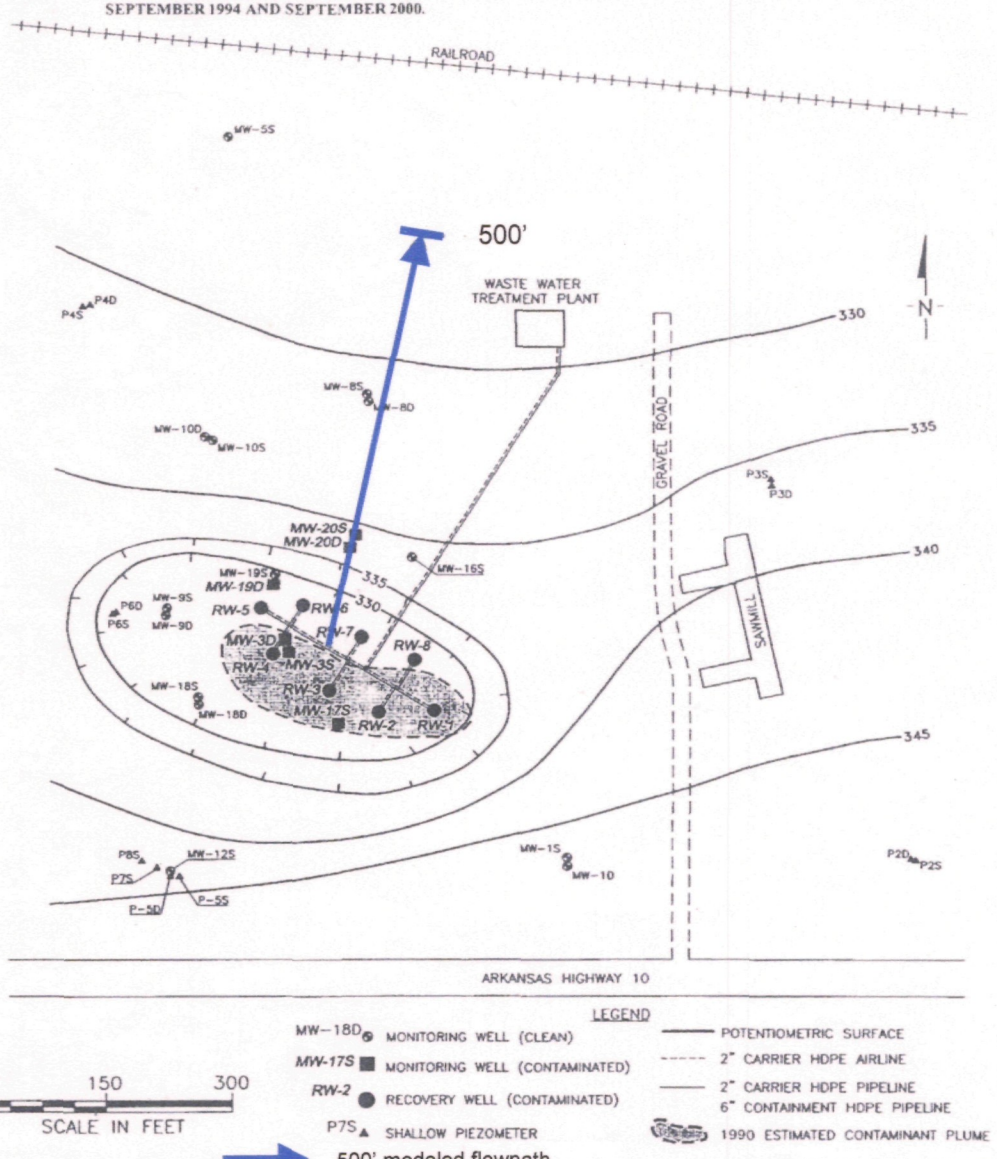
Howard, P.H., 1989. Handbook of environmental fate and exposure data, Lewis Publishers, vol. 1, 574 p.

Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., and Michalenko, E.M., 1991. Handbook of Environmental Degradation Rates, Lewis Publishers, 725 p.

U.S. Environmental Protection Agency, 1997. BIOSCREEN–Natural attenuation decision support system, Version 1.4. EPA/600/r-96/087.

Figure 1
Old Midland Superfund Site

SITE LAYOUT SHOWING THE POTENTIOMETRIC SURFACE FROM SEPTEMBER 2000, 1990 ESTIMATED CONTAMINANT PLUME, AND WELLS WITH AND WITHOUT CONTAMINATION BETWEEN SEPTEMBER 1994 AND SEPTEMBER 2000.



NOTE: Potentiometric surface taken from the September 2000 O&M Report, IT Corporation. 1990 estimated contaminant plume taken from the Old Midland Products Remedial Action, Vol. III, IT Corporation, 1990. Well sampling data taken from September 1994 through September 2000 O&M Reports, IT Corporation.

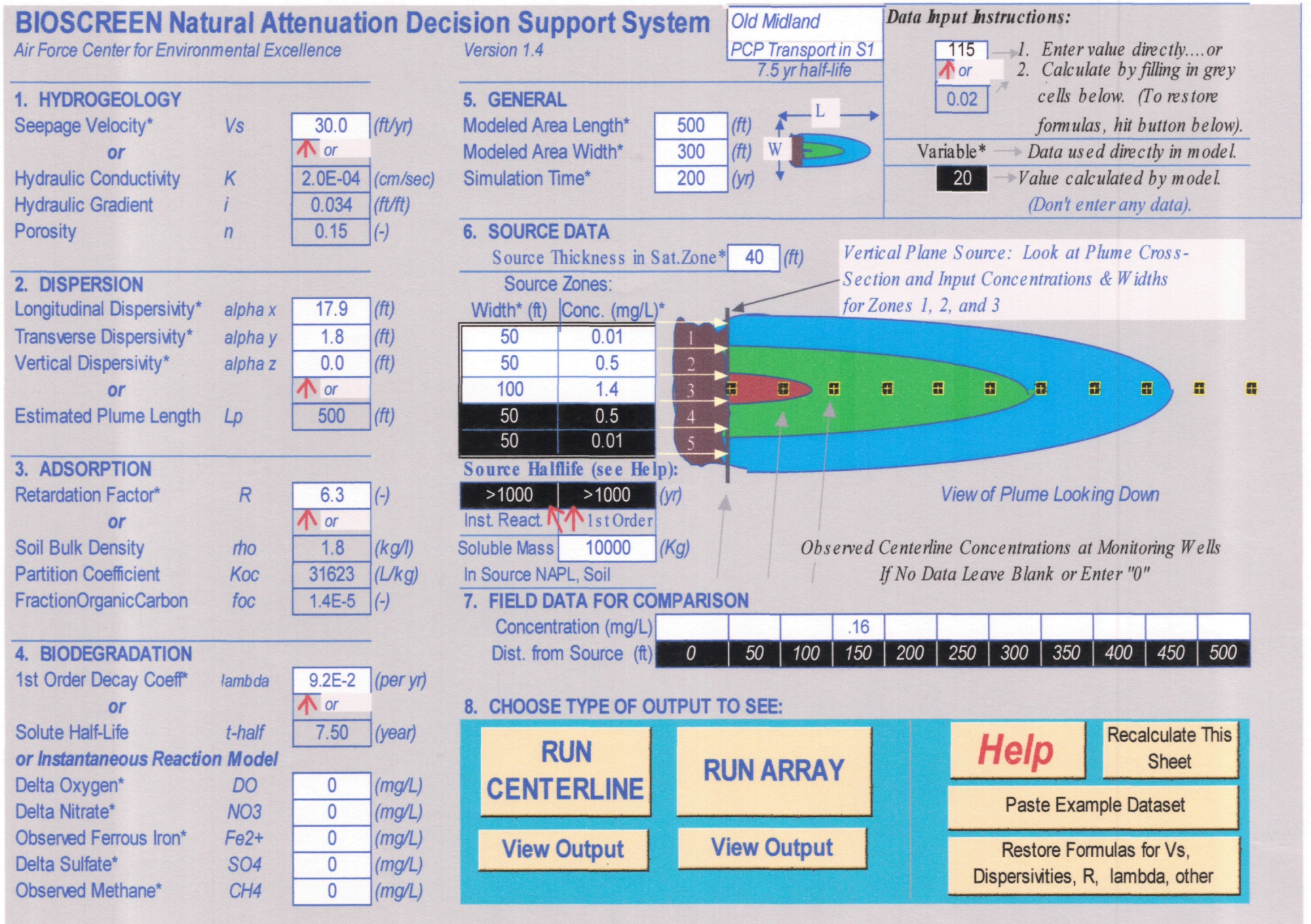
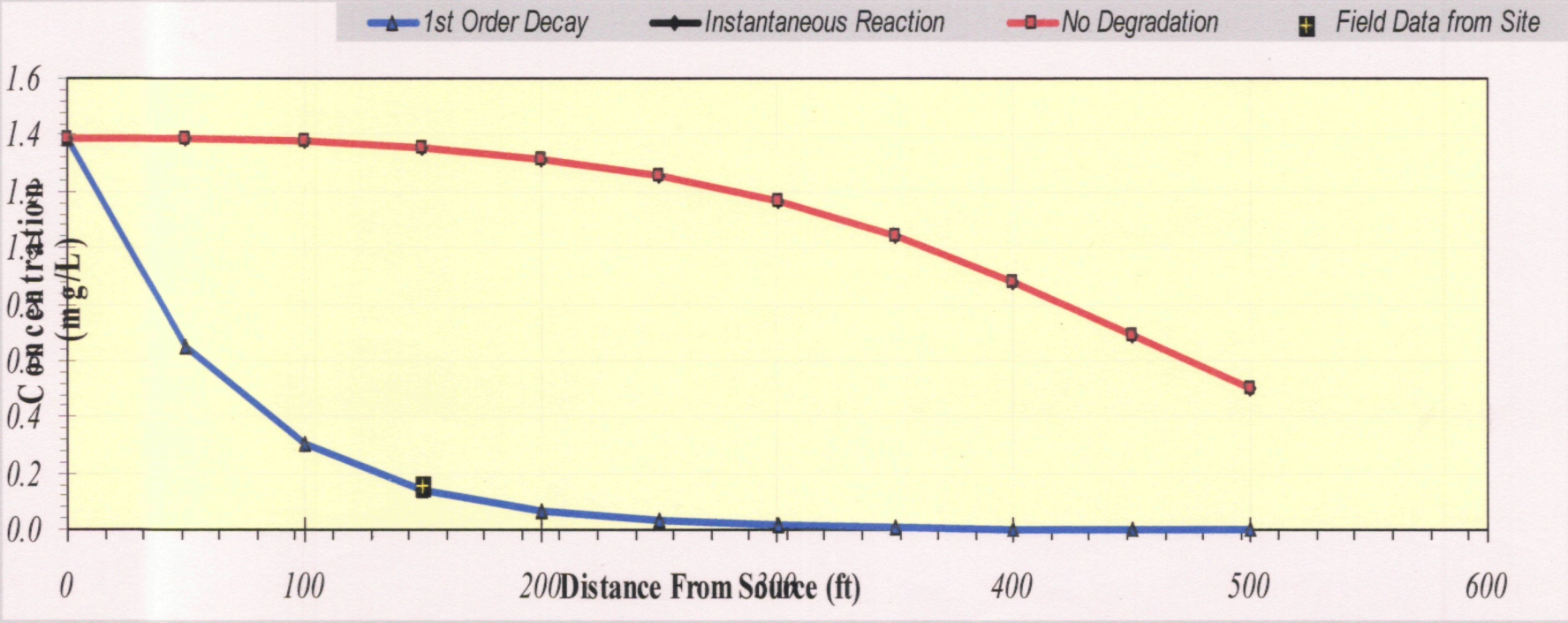


Figure 2a.

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

TYPE OF MODEL	Distance from Source (ft) 0	50	100	150	200	250	300	350	400	450	500
No Degradation	1.386	1.387	1.379	1.354	1.313	1.253	1.165	1.041	0.880	0.693	0.500
1st Order Decay	1.386	0.647	0.300	0.138	0.063	0.029	0.013	0.006	0.003	0.001	0.001
Inst. Reaction	1.386	1.387	1.379	1.354	1.313	1.253	1.165	1.041	0.880	0.693	0.500
Field Data from Site				0.160							



Replay Animation | Next Timestep | Prev Timestep

Time: 100 Years

Return to Input | Recalculate This Sheet

Figure 2b.

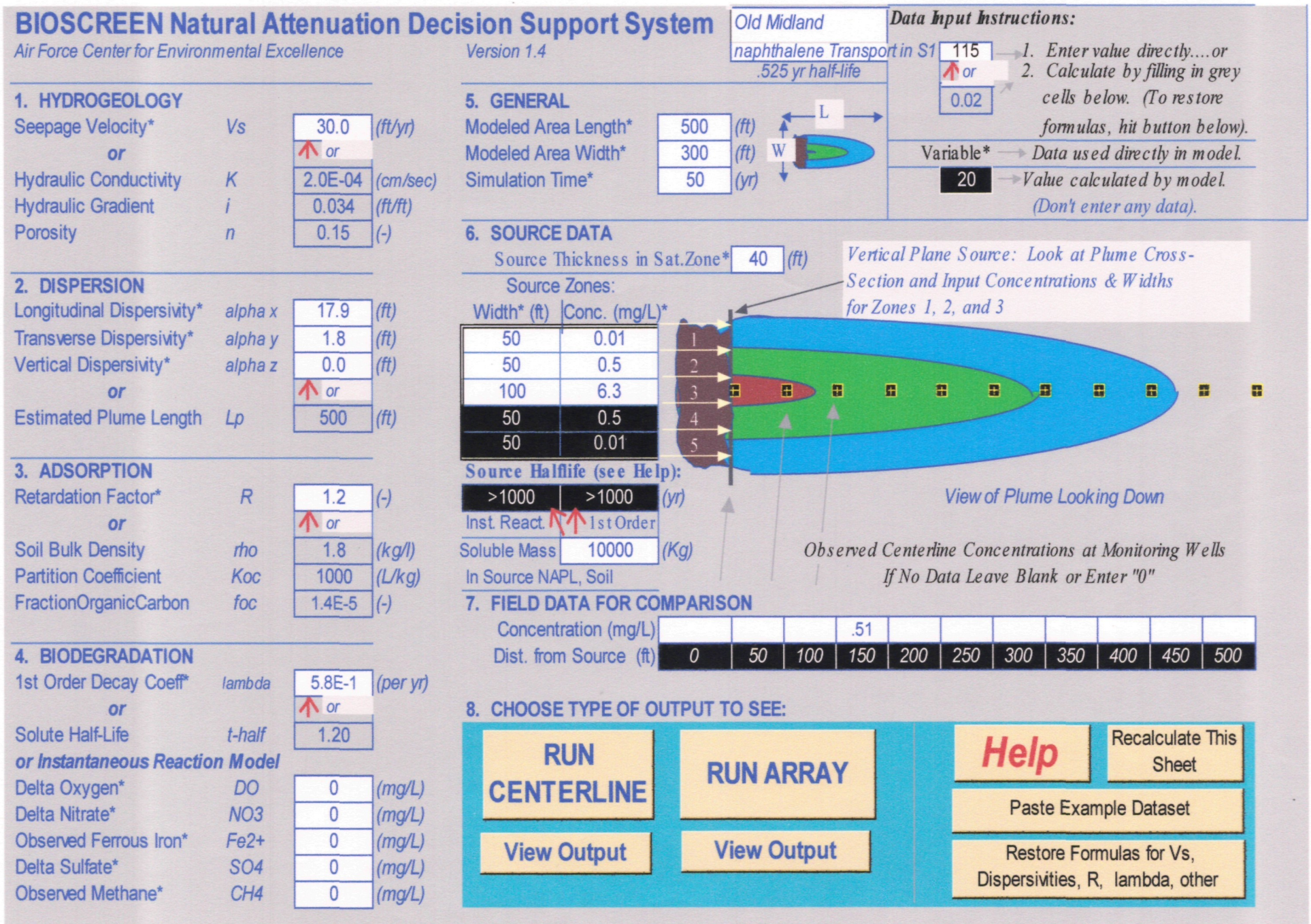

BIOSCREEN Natural Attenuation Decision Support System
Air Force Center for Environmental Excellence
Version 1.4
Old Midland
naphthalene Transport in S1
.525 yr half-life
Data Input Instructions:
1. Enter value directly....or
2. Calculate by filling in grey cells below. (To restore formulas, hit button below).
Variable* → Data used directly in model.
20 → Value calculated by model. (Don't enter any data).
1. HYDROGEOLOGY
Seepage Velocity* Vs 30.0 (ft/yr)
or
Hydraulic Conductivity K 2.0E-04 (cm/sec)
Hydraulic Gradient i 0.034 (ft/ft)
Porosity n 0.15 (-)
2. DISPERSION
Longitudinal Dispersivity* alpha x 17.9 (ft)
Transverse Dispersivity* alpha y 1.8 (ft)
Vertical Dispersivity* alpha z 0.0 (ft)
or
Estimated Plume Length Lp 500 (ft)
3. ADSORPTION
Retardation Factor* R 1.2 (-)
or
Soil Bulk Density rho 1.8 (kg/l)
Partition Coefficient Koc 1000 (L/kg)
FractionOrganicCarbon foc 1.4E-5 (-)
4. BIODEGRADATION
1st Order Decay Coeff* lambda 5.8E-1 (per yr)
or
Solute Half-Life t-half 1.20
or Instantaneous Reaction Model
Delta Oxygen* DO 0 (mg/L)
Delta Nitrate* NO3 0 (mg/L)
Observed Ferrous Iron* Fe2+ 0 (mg/L)
Delta Sulfate* SO4 0 (mg/L)
Observed Methane* CH4 0 (mg/L)
5. GENERAL
Modeled Area Length* 500 (ft)
Modeled Area Width* 300 (ft)
Simulation Time* 50 (yr)
L
W
115
or
0.02
6. SOURCE DATA
Source Thickness in Sat.Zone* 40 (ft)
Source Zones:
Width* (ft) Conc. (mg/L)*
50 0.01
50 0.5
100 6.3
50 0.5
50 0.01
1
2
3
4
5
Source Halflife (see Help):
>1000 >1000 (yr)
Inst. React. 1st Order
Soluble Mass 10000 (Kg)
In Source NAPL, Soil
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"
7. FIELD DATA FOR COMPARISON
Concentration (mg/L) .51
Dist. from Source (ft) 0 50 100 150 200 250 300 350 400 450 500
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 3a.

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

	Distance from Source (ft)										
TYPE OF MODEL	0	50	100	150	200	250	300	350	400	450	500
No Degradation	6.267	6.257	6.181	5.962	5.586	5.022	4.254	3.324	2.347	1.471	0.808
1st Order Decay	6.267	2.655	1.117	0.463	0.190	0.078	0.032	0.013	0.005	0.002	0.001
Inst. Reaction	6.267	6.257	6.181	5.962	5.586	5.022	4.254	3.324	2.347	1.471	0.808
Field Data from Site				0.510							

Replay Animation | Next Timestep | Prev Timestep

Time: 15 Years

Return to Input | Recalculate This Sheet

Figure 3b.