

APPENDIX B

Part 2

**Contaminant Fate and Transport Modeling
SWMU 62, Sandy Cove Housing 134, 179, and 187 Areas**

BIOSCREEN MODEL DESCRIPTION

This appendix presents results of fate and transport modeling for diesel-range organics (DRO), gasoline-range organics (GRO), and benzene at the Sandy Cove Housing 134, 179, and 187 Areas site using the BIOSCREEN Natural Attenuation Decision Support System Version 1.4 (USEPA, 1996; Newell, et al 1997). Modeling for this portion of the site focused on the area surrounding Housing Unit 134 because of the three source areas it is the farthest downgradient source area based on groundwater flow direction, and therefore the closest to Sweeper Cove. Contaminants in groundwater originating from Area 134 should reach the surface water earlier than those from Areas 179 and 187.

Modeling was conducted for DRO, GRO, and benzene, which have been detected in groundwater samples collected from the site at concentrations exceeding the Alaska DEC groundwater cleanup criteria for groundwater used as a drinking water source (1.5 mg/L for DRO, 1.3 mg/L for GRO, and 0.005 mg/L for benzene). This modeling effort was conducted for the main aquifer beneath the site and does not include the perched groundwater zone or contaminants detected in that zone. It is assumed that the perched zone is laterally discontinuous and does not extend to Sweeper Cove. The discussion presented in this appendix includes a brief description of the BIOSCREEN model, a summary of the limitations of the model, description of the input parameters used during the simulations, and the model output (provided at the end of Part 2). Specific parameters used in the models are summarized in Table 3-29.

B2-1.0 BACKGROUND

BIOSCREEN is a screening model that simulates remediation through natural attenuation of dissolved hydrocarbons at petroleum fuel release sites. The software is used within the Microsoft Excel spreadsheet environment and is based on the Domenico analytical solute transport model. 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.

This model has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions. BIOSCREEN can model in three different ways: 1) solute transport without decay, 2) solute transport with biodegradation modeled as a first-order decay process, and 3) solute transport with biodegradation modeled as an instantaneous biodegradation reaction.

B2-2.0 LIMITATIONS

BIOSCREEN has several limitations. The most important of these are:

- BIOSCREEN is an analytical model and assumes simple groundwater flow conditions.
- BIOSCREEN is a screening tool and only approximates complicated natural processes.
- BIOSCREEN's instantaneous reaction model matches more sophisticated biodegradation models like BIOPLUME II for readily biodegradable contaminants with retardation factors up to 6.0. Contaminants that are considered readily biodegradable include benzene, toluene, ethylbenzene, and total xylenes (BTEX). The instantaneous reaction assumption at sites with retardation factors greater than 6.0 should be performed with caution and verified with a more sophisticated model.
- The instantaneous reaction model type uses utilization factors for BTEX and must be adjusted when other constituents are modeled.

B2-3.0 MODEL STRUCTURE

Descriptions of the input parameters and output display within BIOSCREEN are presented below.

B2-3.1 GENERAL INPUTS

Modeled area widths were selected to show an appropriate scale for the plume width and model type. Modeled lengths were chosen to represent the distance to the closest downgradient surface water body (Sweeper Cove) from the source area. The source of petroleum-related chemicals into the primary groundwater unit beneath the Sandy Cove Housing 134 Area is established at the location where the two drain wells (DW-134-1 and DW-134-2) were installed. The modeled length was chosen to represent the distance to the closest downgradient surface water body from the source area. The chosen modeled length and width for each of the models was 1,700 feet and 750 feet, respectively.

A simulation time of 12 years was used for the initial and calibration simulation runs because it represents the amount of time that has passed since the fuel pipeline sources were repaired at the site (1989) until the date that field data used for model calibration were collected (2001). A final simulation time of 87 years was used to estimate the groundwater concentration that would be expected given that natural attenuation would proceed at the site for an additional 75 years beyond the date used for calibration.

B2-3.2 HYDROGEOLOGIC DATA

Parameters included in hydrogeologic data are seepage velocity, hydraulic conductivity, hydraulic gradient, and effective porosity. The seepage velocity is described as the actual interstitial velocity, equaling the Darcy velocity divided by the effective porosity. If this value is not available, BIOSCREEN calculates the seepage velocity from input values for hydraulic conductivity, hydraulic gradient, and effective porosity.

A hydraulic conductivity of 0.0283 centimeter per second (cm/sec) was used in the initial runs for modeling contaminant fate and transport at the site. The hydraulic conductivity value chosen represents the downtown sand layers, and was obtained from the Final Groundwater Study Report performed for the Naval Air Facility, Adak Island (URS 1995a). A hydraulic gradient of 0.003 foot/foot was calculated using groundwater elevation data for August 29 and 30, 2001. A standard estimate of 0.3 for effective porosity was used in this model. This value was chosen from a standard range of effective porosity values for silt and sand (USEPA, 1996; Newell, et al 1997). This value is representative of typical values for sand.

BIOSCREEN calculated the seepage velocities based on the hydraulic conductivity, effective porosity, and hydraulic gradient inputs. The seepage velocity value calculated was 293 feet per year.

B2-3.3 DISPERSIVITY

Contaminant dispersivity is addressed in the model in three dimensions: longitudinal dispersivity, transverse dispersivity, and vertical dispersivity. Each can be entered directly or calculated by BIOSCREEN from the estimated plume length.

A 300-foot plume length was input to calculate the longitudinal, transverse, and vertical dispersivities for this site for the DRO, GRO, and benzene models. This plume length value was selected because it is the distance from the DRO source area (near the two drain wells DW-134-1 and DW-134-2) to the estimated downgradient extent where concentrations of petroleum-related

chemicals in groundwater have exceeded cleanup criteria (Figure 3-10). This downgradient extent is established as the midpoint between MW-134-1 and 03-155.

B2-3.4 ADSORPTION DATA

The contaminant adsorption parameters included in the BIOSCREEN model are retardation factor, soil bulk density, organic carbon partition coefficient (K_{oc}), and fraction organic carbon (f_{oc}). The retardation factor may be entered directly or BIOSCREEN will calculate the retardation factor from the remaining parameters.

The soil bulk density may be measured in the laboratory, however in most cases estimated values such as 1.7 or 1.8 kilograms per liter (kg/L) are used. Because bulk density values have not been measured for this site, a typical value for soil bulk density of 1.8 kg/L was used.

The organic carbon partition coefficient (K_{oc}) is chemical specific and relates soil organic carbon to the aqueous phase. The values of 5,010 L/kg for DRO, 1,260 L/kg for GRO, and 58.9 L/kg for benzene as specified in Alaska DEC guidance were used in the initial simulations (ADEC 2002). Because the models calibrated to the site data with this level of adsorption, no adjustment to the K_{oc} values were necessary.

Fraction organic carbon (f_{oc}) is the portion of the aquifer soil matrix comprised of natural organic carbon in uncontaminated areas. If possible, this value should be measured in the laboratory on a sample representing the uncontaminated zone of the aquifer. Because a site-specific value is not known, a default value of 0.0005 was used in the initial simulation runs. For the models to fit site data, the initial simulations required adjustment of the f_{oc} value. The adjusted f_{oc} values used in the GRO and benzene models for the final simulations were 0.001 and 0.0007, respectively. No adjustment to the f_{oc} value was necessary for the DRO model.

B2-3.5 BIODEGRADATION DATA

Biodegradation input parameters are dependent upon the type of degradation model specified for the simulation: no degradation, first-order decay, or instantaneous reaction.

If the first-order decay model is specified, the solute degradation rate is proportional to the solute concentration. The first-order decay coefficient describes the decay process for dissolved constituents. This value can be entered directly or calculated by BIOSCREEN if the dissolved plume solute half-life is input. The decay coefficient and solute half-life are chemical specific values that may be obtained from literature. This model does not account for site-specific degradation information or assume any biodegradation of dissolved constituents in the source

zone. That is, the model assumes that biodegradation starts immediately downgradient of the source, and not in the source zone itself.

If the instantaneous reaction model is specified, then BIOSCREEN requires multiple chemical specific data that comprise the total biodegradation capacity of the groundwater as it flows through the source zone and contaminant plume. The biodegradation capacity parameters include delta oxygen, delta nitrate, observed ferrous iron, delta sulfate, and observed methane. The BIOSCREEN model authors do not recommend use of the instantaneous reaction model for contaminants that possess a retardation factor greater than 6.0 (AFCEE 1996). The instantaneous reaction model assumes BTEX is the contaminant in calculation of the biodegradation capacity. This assumption is appropriate for use at sites where gasoline-range petroleum hydrocarbons are the contaminant source. The first-order decay model is recommended for use at sites where diesel-range petroleum hydrocarbons are the contaminant source.

Three types of biodegradation (no degradation, first-order decay, and instantaneous reaction) were evaluated in this modeling effort. It should be noted that the representativeness of the input parameters used in the instantaneous reaction model is uncertain. Typically, delta values for oxygen, nitrate, and sulfate are obtained by subtracting the minimum concentration measured in a well located within the dissolved plume from the concentration measured in an upgradient background well. Average site-specific parameter values collected from several wells located within the dissolved petroleum plume or from downgradient areas not impacted by petroleum hydrocarbons (Table 3-30) were used in these models to estimate the change in parameter values. The following natural attenuation parameters were used in the instantaneous reaction model for the Sandy Cove Housing 102 Area: 7.35 mg/L for delta oxygen, 0.007 mg/L for delta nitrate, 3.87 mg/L for observed ferrous iron, 0 mg/L for delta sulfate, and 1.95 mg/L for observed methane. Natural attenuation parameter monitoring conducted at the New Housing Fuel Leak site is discussed in Section 3.6.3.

Degradation rates (as first-order decay coefficients) were used in each model in place of unavailable solute half-life values. A value of 0.37 per year for DRO, 0.34 per year for GRO, and 0.41 per year for benzene were input for each initial run. The value for benzene has been recommended by EPA (USEPA 1995). Because published rates could not be found for DRO and GRO, surrogate values were used (URSG 1997). The degradation rate chosen for DRO is the average of published degradation rates for xylenes, naphthalene, and phenanthrene. These three chemicals match the carbon ranges of weathered JP-5, as measured by DRO, and therefore are estimated to represent the degradation rate of DRO. Likewise, the degradation rate chosen for GRO is the published degradation rate for cyclohexane, which is estimated to represent JP-5 as measured by GRO. The coefficients did not require adjustments during model calibration to fit the model outputs to the existing site data.

B2-3.6 SOURCE DATA

The Domenico analytical solute transport model used by BIOSCREEN assumes a vertical plane source of constant concentration. This section describes the dimensions of this vertical source plane.

Source Thickness in Saturated Zone

The thickness in the saturated zone can be determined by evaluating groundwater data from wells near the source zone screened at different depths. If this data is not available, the thickness could be estimated by using the amount of water table fluctuation that has occurred since the time of release. Otherwise, an assumption of 10 feet would probably be appropriate for many petroleum release sites. A saturated zone source thickness of 8 feet was assumed for this site based on available information such as the amount of water table fluctuation in source area soil.

Source Zone Width

BIOSCREEN allows up to five source zones with different concentrations to account for spatial variations in the source area. The width of each zone is entered directly into the model. Conservative estimates of one source zone at a width of 156 feet for DRO, GRO, and benzene were used in the model simulations for this site.

Source Zone Concentration

The concentrations that correspond to each source zone width are entered directly into the model. The source zone concentration selected for DRO (27 mg/L) is the concentration reported for the groundwater sample collected from MW-134-10 on July 3, 1993. The source zone concentrations selected for GRO (4.9 mg/L) and benzene (0.25 mg/L) are the concentrations reported for the groundwater sample collected from HMW-134-2 on November 10, 1997. These values were selected because they are the maximum DRO, GRO, and benzene concentrations that were detected in the primary groundwater unit in the vicinity of Housing Unit 134.

Source Zone Half-Life

A value for source zone half-life is automatically calculated by the model based on the user's best estimate for the mass of dissolvable organics available in the source zone (i.e., soluble organic constituents sorbed on the soil, residual NAPLs, and free-phase NAPLs).

Soluble Mass in Source

The best estimate of dissolvable organics in the source zone normally is obtained by adding the mass of dissolvable organics on soils, free-phase NAPLs, and residual NAPLs. The estimate can come from an estimate of the total mass of spilled fuel (converted to dissolvable mass), a calculation using contaminated soil concentrations and the volume of soil at that concentration, and a calculation using free-phase NAPL densities and concentrations and the volume that the NAPL occupies.

Soluble mass in soil was calculated for DRO using the maximum detected concentration (12,000 mg/kg) measured in soil in Sandy Cove Housing Area 134 between 1989 and 1997 that exceeded Alaska DEC cleanup criteria for DRO. The source zone concentration selected for DRO, which exceeded Alaska DEC cleanup criteria, is the concentration reported for the soil sample collected from soil boring 03-609 on February 17, 1997 (see Plate 1). The resulting calculated soluble mass was 99,174 kg (Table 3-29). The DRO model did not require adjustment to the soluble mass value for the model to fit site data.

Because no detected concentrations for GRO in soil were above reporting limits, soluble mass in soil for GRO was calculated using the cleanup criteria of 260 mg/kg. Soluble mass in soil for GRO using average and maximum concentrations were not calculated. The resulting calculated mass was 2,149 kg (Table 3-29). The GRO model did not require adjustment to the soluble mass value for the model to fit site data.

Because no detected concentrations for benzene in soil were above reporting limits, soluble mass in soil for benzene was calculated using the cleanup value of 0.02 mg/kg. Soluble mass in soil for benzene using average and maximum concentrations were not calculated. The resulting calculated mass was 0.17 kg (Table 3-29). Because the benzene model could not be calibrated to the site data using initial input parameters, the soluble mass was adjusted during model calibration to better fit the existing site data. The adjusted value used in the final benzene simulation was 3.0 kg.

B2-3.7 FIELD DATA FOR COMPARISON

The field data parameters are concentrations of the dissolved organics in wells near the centerline of the plume. The data is presented in Table 3-29 and displayed with model results in the Centerline Output sheets (provided at the end of Part 2).

DRO, GRO, and benzene concentration data reported for groundwater samples collected on September 2, 2001 were input to calibrate the instantaneous reaction model results (Table 3-29). A calibration period of 12 years was used to simulate the period from source removal to collection of calibration data (1989 to 2001). Adjustments to f_{oc} or soluble mass in soil values were necessary to calibrate the GRO and benzene models to site data. No adjustments to the DRO model were necessary.

B2-3.8 CENTERLINE OUTPUT

This screen shows the average concentration at the top of the saturated zone along the centerline of the plume. The concentrations at distances away from the source are displayed in graph and table format for each model type run for this site (no degradation, first-order decay, and instantaneous reaction).

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Appendix B
Revision No.: 0
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Page B-9

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