Natural Attenuation

BIOSCREEN Natural Attenuation Decision Support System – Version 1.4

BIOSCREEN is a screening level model developed by the U.S. Environmental Protection Agency and the U.S. Air Force. The model simulates remediation through natural attenuation of dissolved petroleum hydrocarbons. The model is an analytical solution, and therefore, the geology must be homogeneous (may be anisotropic) and the flow of groundwater must be constant in magnitude and direction. The model is programmed in Microsoft® Excel spreadsheet environment. The model approximates a solution using the Domenico solute transport model in a three-dimensional porous media for a single chemical. BIOSCREEN has the ability to simulate advection, dispersion, adsorption, and first order decay (aerobic and anaerobic).

BIOSCREEN includes three different model types:

1) Solute transport without decay (conventional approach).
2) Solute transport with biodegradation modeled as first order decay process (simple, lumped-parameter approach). The solute degradation rate is proportional to the solute concentration.
3) Solute transport with biodegradation modeled as an "instantaneous" biodegradation reaction (approach used by BIOPLUME models).

1st order decay - rate of loss of mass at any given time is directly proportional to the mass present at that time. Use of the first order decay coefficient is modified to fit the representative field data for calibration. Uncertainties in parameters (e.g., dispersion, sorption, biodegradation) are "lumped" together in a "single" calibration parameter.

Suggested uses for BIOSCREEN:

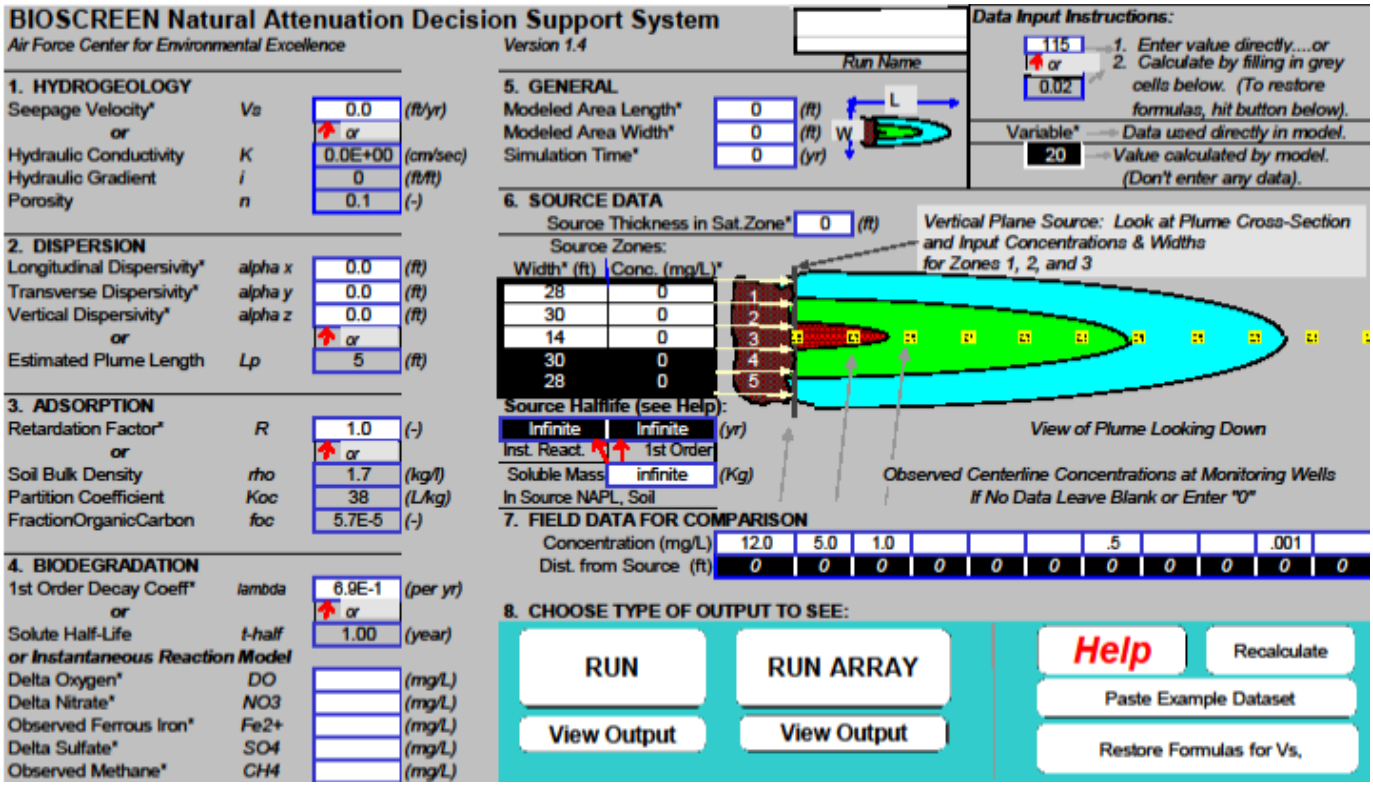
1) How far will the dissolved contaminate plume extend if no engineered controls or further source zone reduction measures are implemented?
2) How long will the plume persist until natural attenuation processes cause it to dissipate?

The following limitations are present in the model:

1) BIOSCREEN assumes simple groundwater flow conditions as an analytical model.
   a) Do not use in pumping systems
   b) Do not use where vertical gradients affect contaminant transport
2) BIOSCREEN as a screening tool only approximates more complicated processes that occur in the field
   a) Should not be used where detailed results are required. Requires the use of more complicated modeling efforts.

BIOSCREEN data input:

Input Parameters – the inputs are inter-related to each other. Need to begin evaluating collection of site parameters early in the site characterization phases. The better the input parameter data the more "accurate" the model.



1. Hydrogeology

   Seepage velocity – $V_s = Ki/\phi$ (ft/yr)

   Actual interstitial groundwater velocity, equaling Darcy velocity divided by effective porosity. The Domenico model and BIOSCREEN are not formatted to simulate the effects of chemical diffusion. Therefore, care should be utilized when applying to contaminant transport in low-flow hydrogeologic regimes.

   or

   Hydraulic conductivity – K (cm/sec) - **HORIZONTAL**
   Hydraulic gradient – i (ft/ft)
   Effective porosity – ϕ (unitless) – measured (best) or estimated.

Sources: Field data (Best); Freeze and Cherry, Driscoll, Fetter, Todd, etc.

Please verify all input parameters – DO THEY MAKE SENSE

2. Dispersion
   Refers to the process whereby a plume will spread out in longitudinal, horizontal, and vertically (x, y, z). Due to the difficulty in measuring actual values, selection of dispersivity is a difficult process.

   Longitudinal – alpha x (ft)
   Transverse – alpha y (ft)
   Vertical - alpha z (ft) or

   Plume length (ft)

Estimated length of the existing or hypothetical groundwater plume being modeled. Plume length is a key parameter as it is used to estimate dispersivity terms.

If modeler choses to use Xu and Eckstein (1995) formula for estimating/calculating the longitudinal dispersion, modeler must be cautioned to use consistent units. The formula given in this paper is in meters. BIOSCREEN manual contains the appropriate conversion.

$3.28 \times 0.83[\log_{10} (L_p)/3.28)]^{2.414}$

3. Adsorption

   Retardation Factor - R (unitless) – Retardation is the rate at which dissolved contaminants migrating through a water-bearing zone can be reduced by sorption to the sediment matrix.

   or

   Soil Bulk Density - rho (kg/l)
   Partition Coefficient – K_{oc} (L/kg) – chemical specific
   Fraction of Organic Carbon – f_{oc} (unitless) – Fraction of the soil matrix comprised of natural organic carbon. Greater content of carbon equates to greater adsorption capacity of matrix. Default value of 0.001 is often used.

Retardation will also represent the slow diffusion of contaminants from lower permeability matrix back into the higher permeability matrix – Concentration gradient

4. Biodegradation

   1st Order Decay – lambda (per year) – BIOSCREEN assumes the rate of biodegradation depends only on the concentration of the constituents and the rate coefficient.

   or

   Solute half-life – t-half (year) – Time for dissolved constituents concentrations to decay by one-half as contaminants migrate.

   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 Parameters

   Modeled Area Length (ft) – sets up distances in the field data entry.
   Modeled Area Width (ft)
   Simulation Time (yr)

6. Source Data

   Source Thickness (ft) – Equates to the smear zone or source zone created from the historical maximum and minimum of groundwater fluctuations.
   Source Zone
   Mass – reduce during current and future conditions iterations

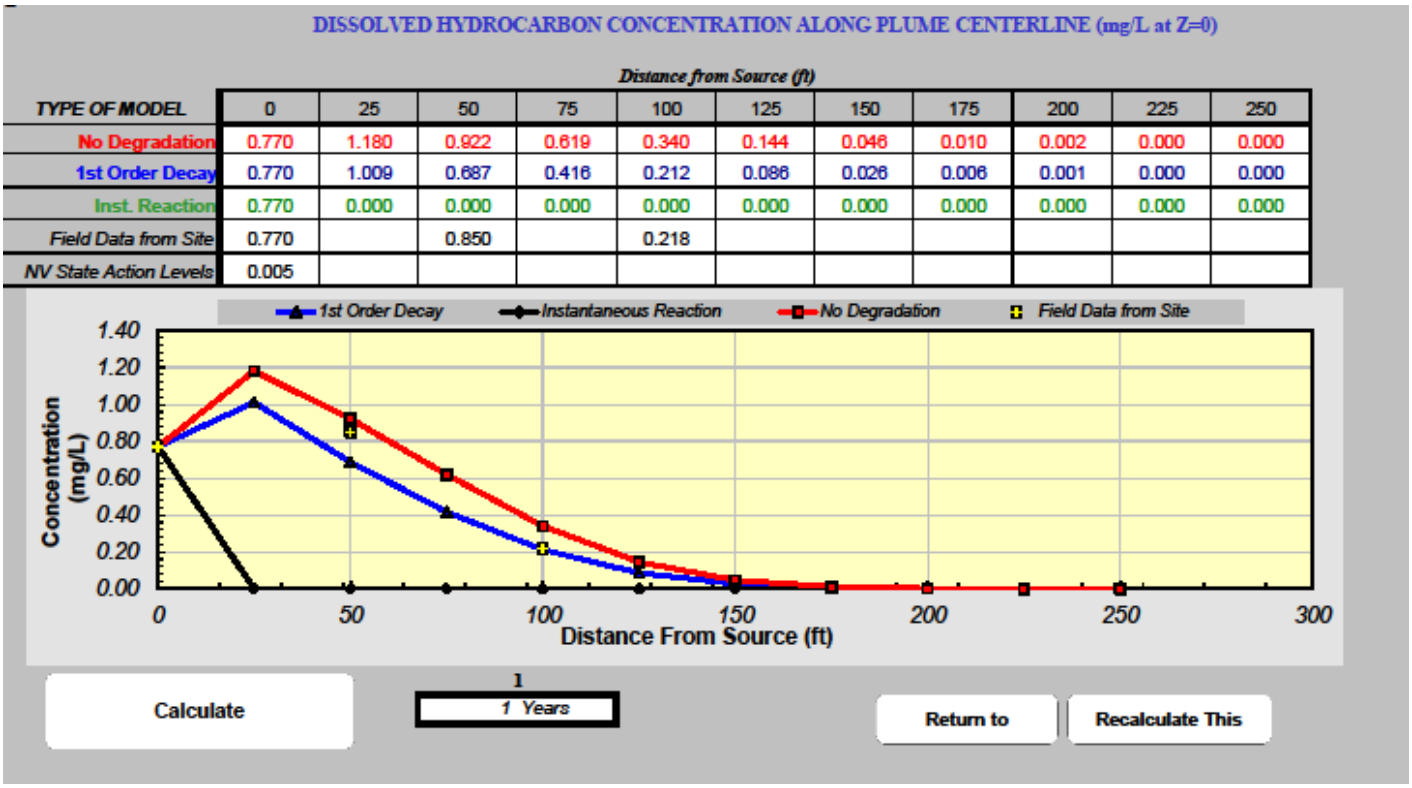
7. Field Data

   Actual field data – this is what you are calibrating to (i.e., calibration, current conditions).

Important to calibrate the model to field conditions that are present prior to any remediation being conducted at the site. This removes any potential variation any data.

Run Center Line – (Many times). Modifications to input parameters including time will need to be adjusted in order to approximate the field data. It is recommended to change only one parameter at a time, so that the modeler can inherently observe the results of that parameter on the model (positive or negative effect – next parameter). Once calibrated, the modeler can then use the model to simulate flow conditions for length of the dissolved plume, time to a given receptor, etc.

Change to current conditions (category 7) and continue iterations using input parameters categories 5 and 6 only.

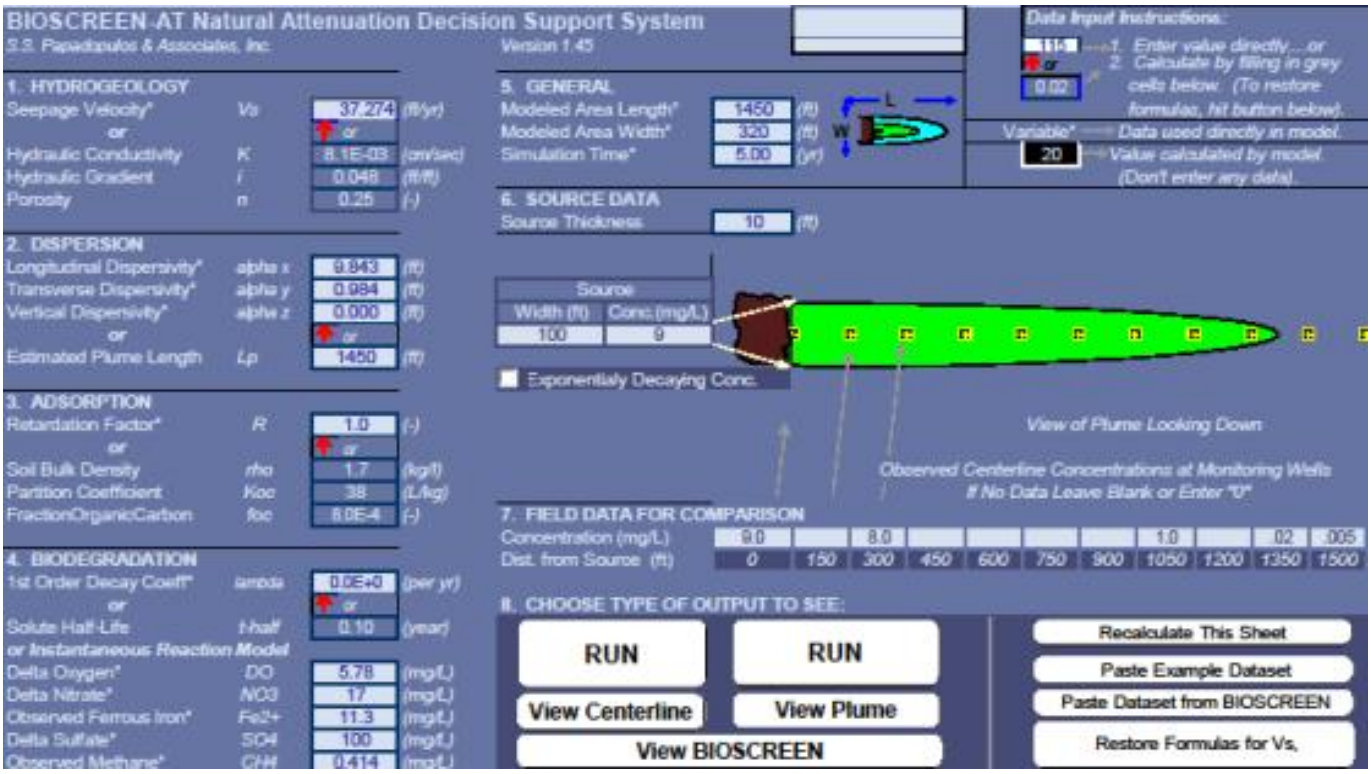


Note that the "calibrated" model curves should fit the field data relatively well.

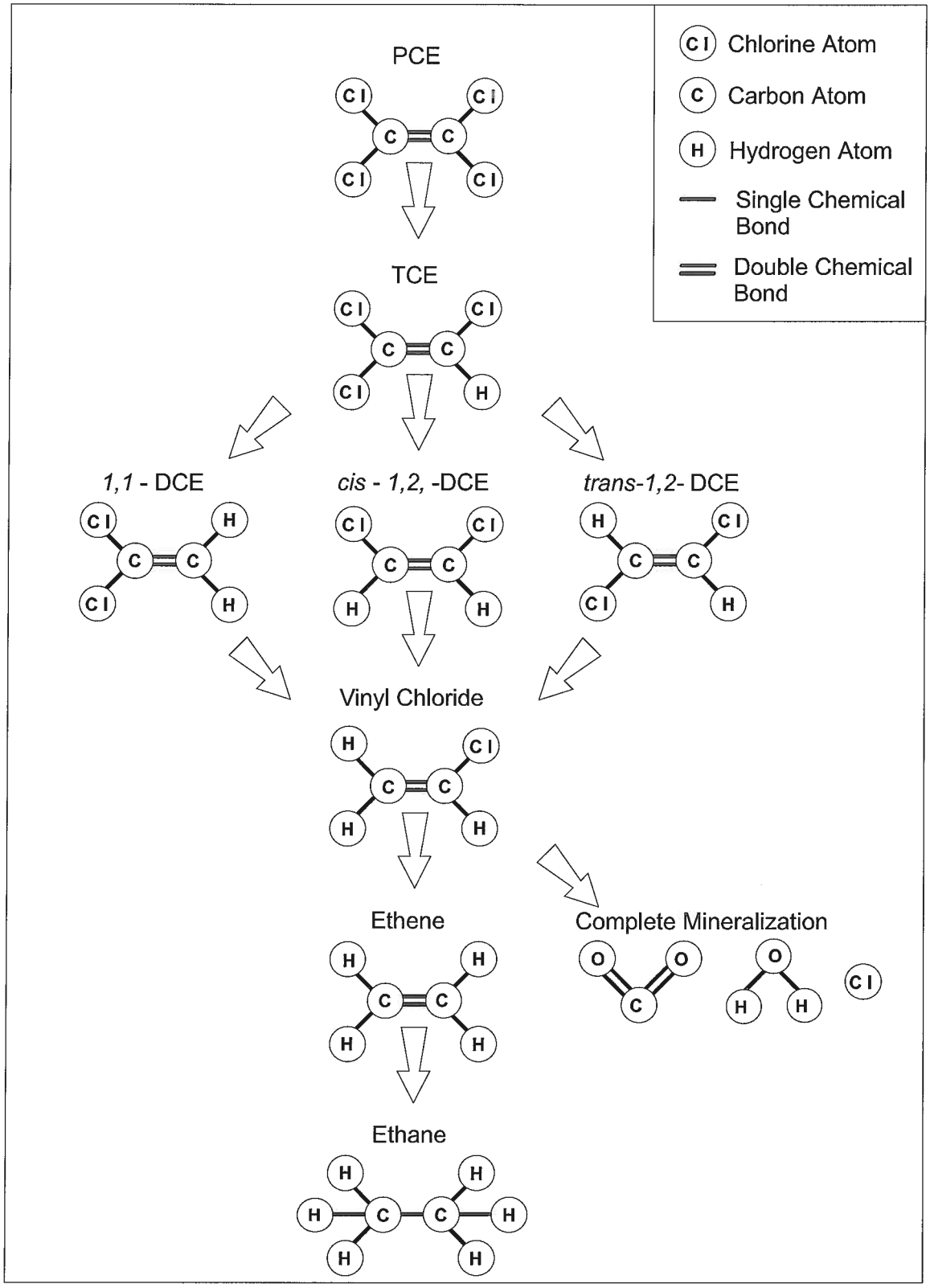
BIOSCREEN - AT

- BIOSCREEN left out an integral which only approximates the solution
- BIOSCREEN - AT uses the complete integral and therefore, provides a more exact solution.
- For low flow environment, such as Las Vegas, BIOSCREEN is sufficient.

EPA has acknowledge the error in the BIOSCREEN model. However, at this time, EPA has not modified the use of BIOSCREEN. Using BIOSCREEN – AT, the modeler can quickly see a comparison between the two model version results.


BIOSCREEN-AT Natural Attenuation Decision Support System
S.S. Papadopulos & Associates, Inc.
Version 1.45
1. HYDROGEOLOGY
Seepage Velocity*
Vs
37.274
(ft/yr)
or
Hydraulic Conductivity
K
8.1E-03
(cm/sec)
Hydraulic Gradient
i
0.048
(ft/ft)
Porosity
n
0.25
(-)
2. DISPERSION
Longitudinal Dispersivity*
alpha x
9.843
(ft)
Transverse Dispersivity*
alpha y
0.984
(ft)
Vertical Dispersivity*
alpha z
0.000
(ft)
or
Estimated Plume Length
Lp
1450
(ft)
3. ADSORPTION
Retardation Factor*
R
1.0
(-)
or
Soil Bulk Density
rho
1.7
(kg/l)
Partition Coefficient
Koc
38
(L/kg)
FractionOrganicCarbon
foc
6.0E-4
(-)
4. BIODEGRADATION
1st Order Decay Coeff*
lambda
0.0E+0
(per yr)
or
Solute Half-Life
t-half
0.10
(year)
or Instantaneous Reaction Model
Delta Oxygen*
DO
5.78
(mg/L)
Delta Nitrate*
NO3
17
(mg/L)
Observed Ferrous Iron*
Fe2+
11.3
(mg/L)
Delta Sulfate*
SO4
100
(mg/L)
Observed Methane*
CH4
0.414
(mg/L)
5. GENERAL
Modeled Area Length*
1450
(ft)
Modeled Area Width*
320
(ft)
Simulation Time*
5.00
(yr)
L
W
Data Input Instructions:
1. Enter value directly ... or
2. Calculate by filling in grey cells below. (To restore formulas, hit button below).
0.02
Variable* ---- Data used directly in model.
20 ---- Value calculated by model. (Don't enter any data).
6. SOURCE DATA
Source Thickness
10
(ft)
Source
Width (ft)
Conc.(mg/L)
100
9
Exponentialy Decaying Conc.
View of Plume Looking Down
Observed Centerline Concentrations at Monitoring Wells
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
150
300
450
600
750
900
1050
1200
1350
1500
II. CHOOSE TYPE OF OUTPUT TO SEE:
RUN
RUN
View Centerline
View Plume
View BIOSCREEN
Recalculate This Sheet
Paste Example Dataset
Paste Dataset from BIOSCREEN
Restore Formulas for Vs,

BIOCHLOR


Cl Chlorine Atom
C Carbon Atom
H Hydrogen Atom
Single Chemical Bond
Double Chemical Bond
PCE
TCE
1,1 - DCE
cis - 1,2, -DCE
trans-1,2- DCE
Vinyl Chloride
Ethene
Ethane
Complete Mineralization
O
O
C
O
H
H
Cl