

Documentation for:

SSA_Analytical.xlsm

Version 3

*Analytical solution to contaminant transport in vadose
zone and saturated zone using Microsoft Excel*

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DOCUMENTATION FOR USING “SSA_Analytical.xlsm”

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Introduction

There are hundreds of sites that pose a risk of groundwater contamination. Contaminants can travel from near surface sources through the unsaturated (vadose zone) and saturated aquifer and end up in groundwater extraction wells or in a surface water body causing adverse ecological and environmental impacts. Groundwater modeling is adopted to evaluate the fate and transport of contaminants in the area using detailed modeling approaches. While rigorous modeling approaches provide a good understanding of the groundwater system being studied, these approaches are often time consuming and also require trained personnel. Since detailed studies are focused on a few sites, the amount of risk posed by several other sites remains unknown.

A source screening module was developed that can be used as a screening tool to classify waste sites based on the risk that these sites pose to the protection of groundwater, in an efficient manner and at the same time generate reliable answers. The module presented here computes contaminant concentrations travelling from a source through vadose and saturated zones to a groundwater receptor well. The module comprises of an analytical solution implemented in Microsoft Excel (referred further in the text as MS Excel, Excel, or Excel file) and was named “SSA_Analytical.xlsm”. Implementing the module in Excel provides transparency to the calculation process and readily plots breakthrough curves. The main advantage of the module is that it provides reasonable answers to evaluate risk posed by contaminated sites very efficiently.

Following sections discuss in detail the conceptual model, formulation, input and output of the module, implementation in Excel, and verification examples.

Source Screening Module

The conceptual model for the source screening analyses is shown schematically in Figure 1. Three sequential calculations are performed as follows.

1. Conversion from soil concentrations to pore water concentrations in the source area;
2. Transport across the vadose zone; and
3. Mixing and transport in the saturated zone to a potential receptor.

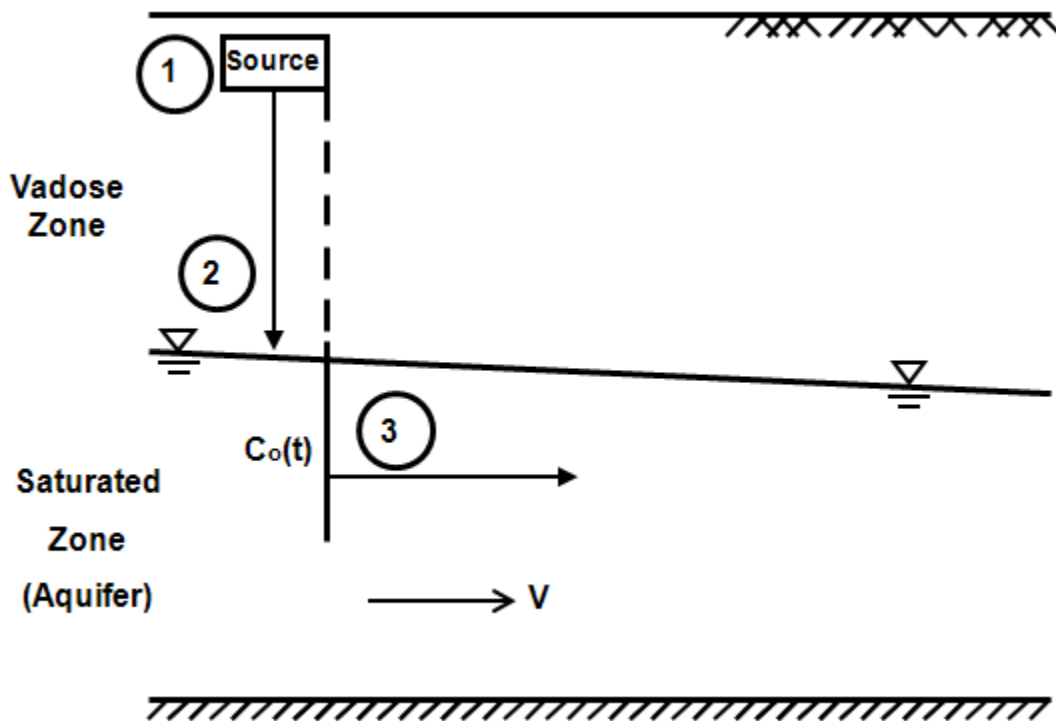


Figure 1. Conceptual model for evaluation of source zone concentrations

Calculations involved in computing source concentration are shown in detail in Appendix A. Appendices B and C discuss the adopted approach, governing equations, and the analytical solution for contaminant transport through the vadose zone and in the saturated zone. Calculations of source concentration, and transport through vadose zone and saturated zone are implemented in the Excel file SSA_Analytical.xlsm.

System Requirements

SSA_Analytical.xlsm was developed with Microsoft Office Excel 2007. This module can also work with previous versions of Microsoft Office (2000, XP, and 2003) by installing Microsoft Office 2007 Compatibility Pack available at the URL

<http://www.microsoft.com/downloads/details.aspx?FamilyId=941b3470-3ae9-4aee-8f43-c6bb74cd1466&displaylang=en>.

Operating system requirements are Windows 2000 Service Pack 4; Windows Server 2003; Windows Vista; Windows Vista Service Pack 1; Windows XP Service Pack 1; Windows XP Service Pack 2; Windows XP Service Pack 3.

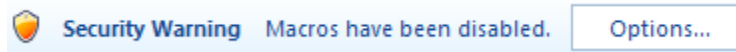
If using Excel 2003, the user must make sure that the following two options are checked before running a simulation. These two options can be seen by clicking on “Tools > Add-Ins...”.

- Analysis ToolPak
- Analysis ToolPak – VBA

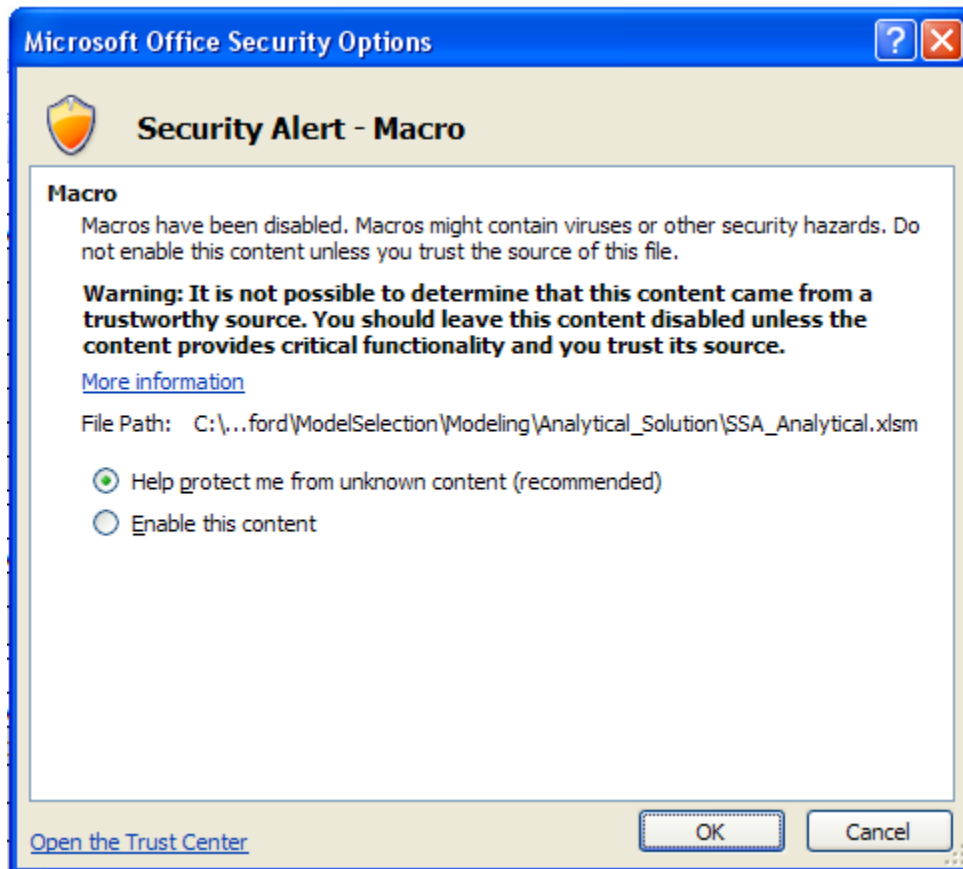
How to Simulate a Scenario

Following is a step by step procedure to perform a simulation.

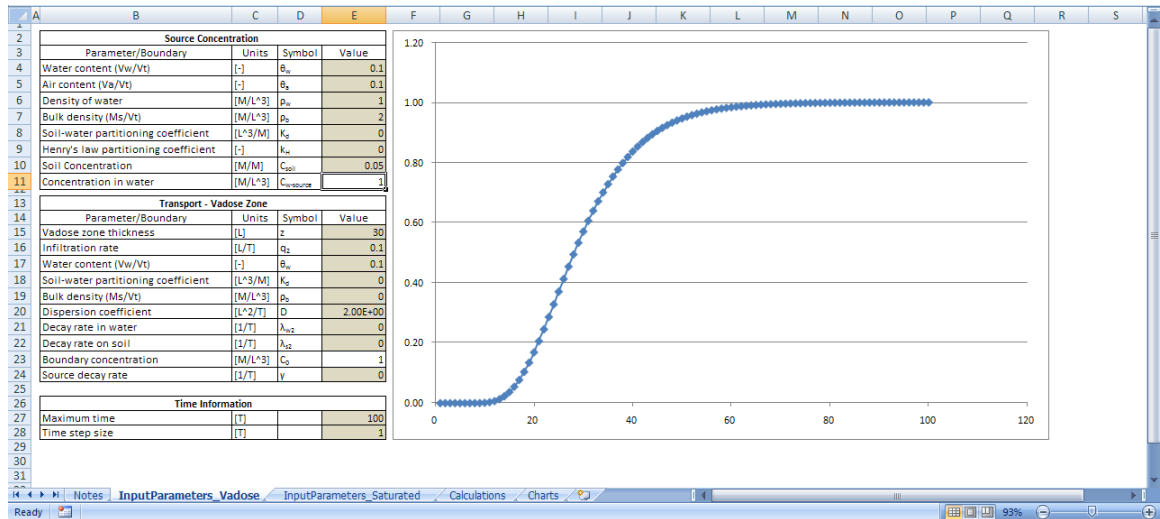
1. Open the Excel file (or workbook) called “SSA_Analytical.xlsm”.
2. On most of the computers, a warning is posted above the worksheet area.



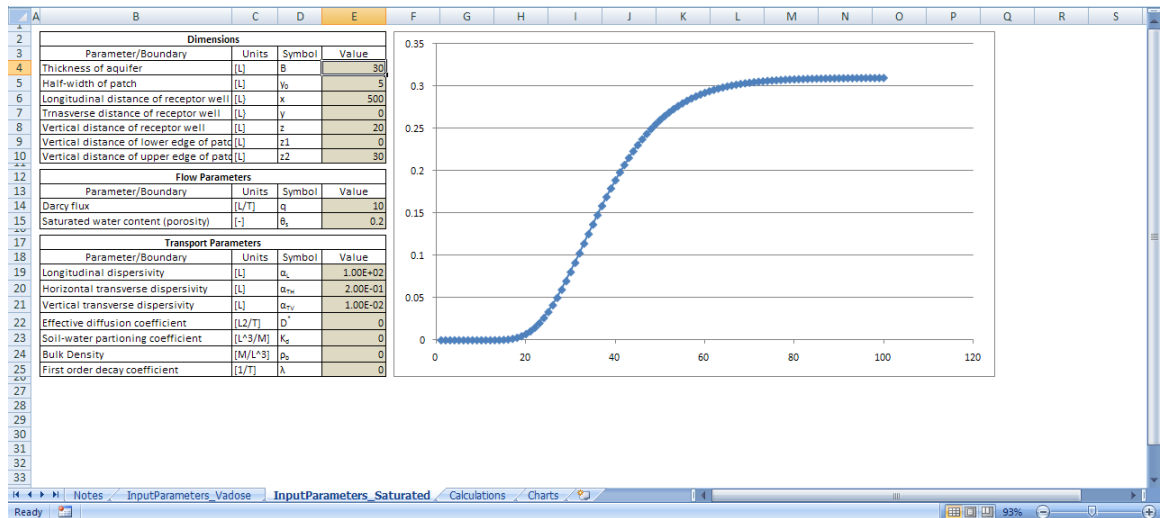
Click on “Options...” and select “Enable this content” and click OK. Selecting this option will enable a macro that runs in the background during a simulation.



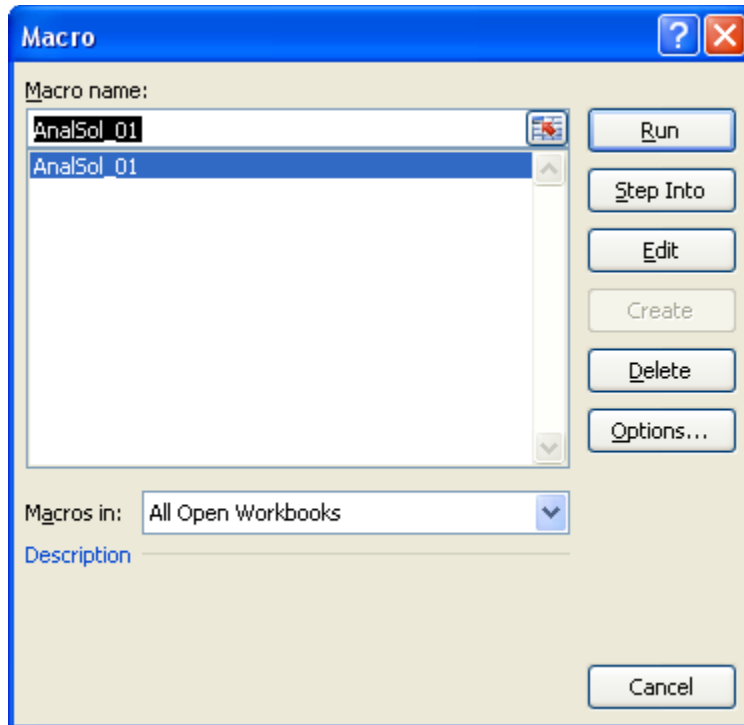
- Provide input for source concentration calculations and vadose zone calculations in the worksheet "InputParameters_Vadose". Input can only be provided in the highlighted cells.



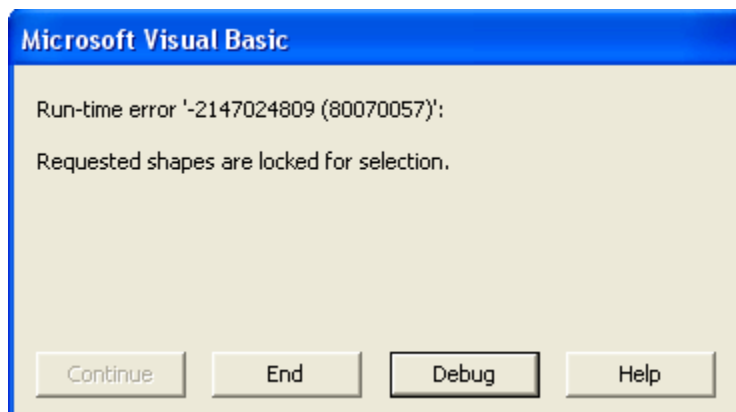
- Provide input for transport calculations through saturated zone in the worksheet "InputParameters_Saturated". Input can only be provided in the highlighted cells.



5. Click on Developer>Macros, select the macro “AnalSol_01” from the list of macros and then click “Run” to run the macro. The same macro can also be run by entering “Ctrl + r” from the keyboard. The Excel file will not be accessible while the macro is running.

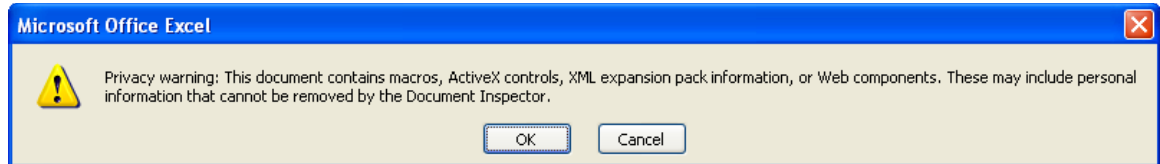


6. If the macro fails for any reason, it will prompt a message similar to the one shown below. Select “End” and contact the developer to identify the problem. If the simulation runs successfully, the user will get back control of the Excel file.



7. Save the Excel file with a different file name. For each scenario start with the Excel file named “SSA_Analytical.xlsm” since this is the name that is hardwired in the macro. If a simulation is performed on a file that is not named “SSA_Analytical.xlsm”, the simulation will not execute.

Click OK on the following warning message that may pop up during a simulation. This is a warning message prompted by MS Excel because of the macro present in the Excel file. The macro is safe and does not pose any threat to the computer. The message below is a general warning prompted by MS Excel.



Various internal error checks are provided in the Excel file. If any checks are violated, the cell violating a constraint or containing an invalid value is highlighted with a red color. An example is shown below.

Longitudinal dispersivity	[L]	α_L	0
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Input

Following is a brief explanation of all the input variables required in source concentration calculations, transport through vadose zone and through saturated zone. Consistent units must be used when entering input variables in the input files.

Source Concentration

Water content (V_w/V_t) or θ_w is a dimensionless parameter and is defined as the volume of water per unit volume of porous medium in the source zone. Water content cannot exceed porosity but can be equal to porosity when the source zone is fully saturated.

Air content (V_a/V_t) or θ_a is a dimensionless parameter and is defined as the volume of air per unit volume of porous medium.

Density of water or ρ_w is the mass of water per unit volume of water. This input is only provided for an alternate method to calculate source concentration based on total concentration. To calculate source concentration based on soil concentration (typically used), this input must be set to zero. If used, typical values are 1 g/cc or 62.4 lb/ft³. Any consistent set of units may be used.

Bulk density (M_s/V_t) or ρ_b is the mass of solids per unit volume of porous medium in the source zone. Units used are typically g/cc or lb/ft³. Any consistent set of units may be used.

Soil-water partitioning coefficient or k_d is sorption partitioning coefficient in the source zone. Any consistent set of units may be used. Typical units are cc/g or ft³/lb.

Henry's law partitioning coefficient or k_H is the Henry's law partitioning coefficient in the source zone. This is a dimensionless parameter.

Soil Concentration or C_{soil} is the measured soil concentration in the source zone expressed as mass of contaminant per unit mass of soil. Any consistent set of units may be used.

Vadose Zone Transport

Vadose zone thickness, z , is the thickness of unsaturated soil column through which transport is computed. Concentrations at the bottom of the soil column are calculated. This thickness should be set equal to the vertical distance of water table from the source. Typical units would be feet or meters. Any consistent set of units may be used.

Infiltration rate, q_2 , is the Darcy velocity of vertical flow from the source to the water table. Typical values are expressed in terms of ft/day or m/day. Any consistent set of units may be used.

Water content (V_w/V_t) or θ_{w2} is the effective water content that participates in the advection process in the vadose zone. Seepage velocity is calculated by dividing the Darcy velocity by this water content. Caution must be exercised when selecting the value of this parameter. For a conservative estimate, this water content may be set equal to residual water content in the vadose zone. For detailed discussion, refer to Appendix B of this document. This is a dimensionless quantity.

Soil-water partitioning coefficient, k_{d2} , is the distribution coefficient in vadose zone. Any consistent set of units may be used. Typical units used are cc/g or ft³/lb.

Bulk density (M_s/V_t), ρ_{b2} , is the mass of solids per unit volume of porous medium in the vadose zone. Any consistent set of units may be used.

Dispersion coefficient, D , is the dispersion coefficient for transport in the vadose zone. Any consistent set of units may be used. Typical units used are ft²/day or m²/day.

Decay rate in water, λ_{w2} and decay rate on soil, λ_{s2} are the first-order transformation rates in pore water and on soil respectively in the vadose zone. Any consistent set of units may be used. Typical units used are day⁻¹.

Time Information

Maximum time, T_{\max} is the total time duration for which breakthrough curves are to be generated in a simulation. Any consistent set of units may be used.

Time step size is the discrete time duration of each time step at which a solution will be computed during a simulation. This parameter is also used to discretize the integral function in the saturated transport calculation with the trapezoidal rule. The smaller the time step size, the higher are the number of steps in which the integration function is evaluated, and better is the accuracy of the solution, but then it also takes more time for computation. Therefore, time step size must be appropriately selected. Any consistent set of units may be used.

Source Depletion

Source depletion option is the option to select a method to calculate source depletion. Based on an option selected, either a source depletion rate, γ is used to simulate source depletion or an arbitrary time-series defining source concentration terms is entered by the user. Source depletion rate γ is set to either γ_1 , or γ_2 , or γ_3 depending on selected options 1, 2, or 3. If option 4 is selected, a user-defined time-series is read and used for computing breakthrough curves. The following options are available:

1. Option 1 – For infinite contaminant source or continuous source the source depletion rate, γ_1 , is set to 0.0.
2. Option 2 – For finite contaminant mass, user defined source depletion rate γ_2 is used. User defined rate, γ_2 is entered by the user as a separate entry. Typical units used are day^{-1} . Any consistent set of units may be used. Two solution options are available with source depletion option 2. These solution options are discussed below later in this section.
3. Option 3 – For finite contaminant mass, source depletion rate γ_3 is calculated based on infiltration rate, total source contaminant mass, source volume, and peak dissolved concentration. Calculation is based on [Rowe, 1991] and is detailed in Appendix A. Two solution options are available with source depletion option 3. These solution options are discussed below later in this section.
4. Option 4 – For a time-varying source concentration defined as discrete points entered as a table containing time versus source concentrations. General solution is applied as discussed in detail in Appendix B of this document.

User defined rate γ_2 , is the source depletion rate entered by the user. Typical units used are day^{-1} . Any consistent set of units may be used. This rate is only used in a simulation if option 2 is selected as the source depletion option.

Depth of source zone is the actual depth of the source zone. Typical units used are meters or feet. Any consistent set of units may be used. This rate is only used in a simulation if option 3 is selected as the source depletion option.

Time versus source concentration (Time, $C_{w\text{-source}}$) table is a user-defined time-varying source term. Units for time and concentration in the table should be consistent with other units defined in the spreadsheet. This input is only required and used if option 4 is selected as the source depletion option.

Solution Option

Solution option is only used when either source depletion option 2 or 3 is selected. Two solution options are available.

1. Option 1 uses a general solution. With this option, the Excel sheet uses the appropriate source depletion rate (γ_2 or γ_3 depending on source depletion option 2 and 3 respectively) and internally calculates a time-series of source concentration and applies the general solution. Time-series is discretized on the time steps as defined in “Time Information” entry (explained above). General solution is discussed in more detail in Appendix B. This is a more robust solution as compared to option 2 except when a very small dispersion coefficient is used. This option will fail when “term3” in the spreadsheet “Calculations” (cell E12) is greater than 708. Excel is limited to determining exponential for terms less than or equal to 708. This option is slower than option 2.
2. Option 2 uses a direct solution. This option yields a faster solution but can fail when condition of applicability is not met. Condition of applicability is checked in case a square root term in the analytical solution is less than zero. This option should be used carefully. Condition of applicability is satisfied if the appropriate source depletion rate (γ_2 or γ_3) is less than or equal to cell E38 of the “InputParameters_Vadose” spreadsheet. If the condition of applicability of a direct solution is not met, the cell E37 of the “InputParameters_Vadose” spreadsheet will turn red. In that case, option 1 should be used.

Solution Level

Solution level determines which aspects of the source screening module will be simulated. The following three levels are available:

1. Solution Level = 1 for source zone calculations only;
2. Solution Level = 2 for source zone and vadose zone calculations; and
3. Solution Level = 3 for source, vadose, and saturated zone calculations.

The user must enter a value between 1 and 3.

Saturated Zone Dimensions

Thickness of aquifer, B , half-width of patch, y_0 , vertical distance of lower edge of patch from the origin, z_1 , and the vertical distance of upper edge of patch from the origin, z_2 , are shown in Figure 2.

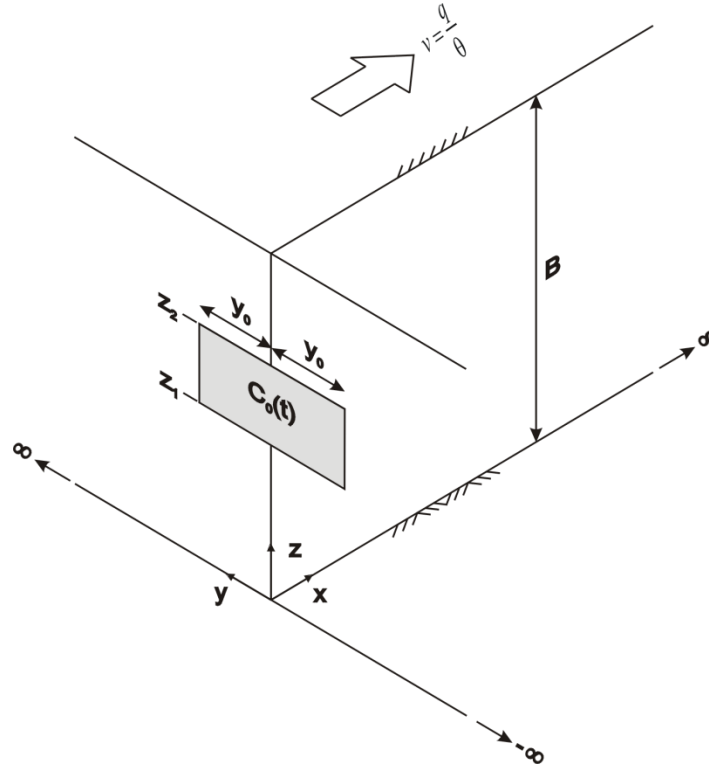


Figure 2. Conceptual model for transport in the aquifer

Longitudinal distance of receptor well, x , transverse distance of receptor well, y , vertical distance of receptor well, z , is the distance of receptor well from the concentration patch along the x , y , and z axis respectively. Distances x , y , and z are calculated from the origin shown in Figure 2. Any consistent set of units may be used.

Saturated Zone Flow and Transport

Darcy flux, q_3 , is the Darcy flux in the aquifer. Any consistent set of units may be used. Darcy flux is typically represented with units of ft/day or m/day.

Saturated water content, θ_{s3} , is the volume of water per unit volume of aquifer in the saturated zone. This parameter is the same as porosity of the aquifer. This is a dimensionless parameter. Any consistent set of units may be used.

Longitudinal dispersivity, α_L , horizontal transverse dispersivity, α_{TH} , and the vertical transverse dispersivity, α_{TV} , are dispersivity values in the longitudinal, transverse horizontal, and transverse vertical directions respectively. Any consistent set of units may be used. Dispersivity is expressed in length units typically feet or meters.

Effective diffusion coefficient, D^* , is the effective molecular diffusion coefficient in the saturated zone. Typical units used are ft^2/day or m^2/day .

Soil-water partitioning coefficient, K_{d3} , is the distribution coefficient in the saturated zone. Typical units used are cc/g or ft^3/lb .

Bulk Density, ρ_{b3} , is the bulk density in the saturated zone. Any consistent set of units may be used. Typical units used are g/cc or lb/ft^3 .

Decay rate in water, λ_{w3} , is the decay coefficient in the saturated zone in the aqueous phase. Typical units are day^{-1} .

Decay rate on soil, λ_{s3} , is the decay coefficient in the saturated zone in the solid phase. Typical units are day^{-1} .

Dilution Factor

Dilution factor option is an option to select a dilution factor, DF, to be applied to saturated zone concentration equation of Appendix C. Dilution factor option, DF, is set to either DF1, DF2, DF3 or DF4, depending on the option selected. Following options are available:

1. Option 1 – User supplied dilution factor, DF1, is used as the dilution factor.
2. Option 2 – Default dilution factor, DF2 set to 20, is used as the dilution factor.
3. Option 3 – Dilution factor, DF3, is calculated based on the volume of infiltrating contaminated water and volume of aquifer water participating in mixing and dilution.
4. Option 4 – Dilution factor, DF4, is used. DF4 is calculated based on depth of penetration, calculated using the Charbeneau (2000) approach described in Appendix C.

User supplied dilution factor, DF1, is the dilution factor applied in saturated zone concentration calculation. DF1 does not have any units and is set greater than one to simulate dilution of vadose zone infiltration with clean aquifer water. DF1 is only used if dilution factor option 1 is selected.

Cross-sectional area of groundwater flow, A_a , is the cross-sectional area through which groundwater moves and participates in the dilution of vadose zone infiltration. A_a is defined in the units of squared length, typically m^2 or ft^2 . Any consistent set of units may be used. This is used only if dilution factor option 3 is selected.

Cross-sectional area of vadose zone flow, A_p , is the cross-sectional area through which vadose zone infiltration takes place. A_p is set equal to the area of the source zone and is defined in the units of squared length, typically m^2 or ft^2 . Any consistent set of units may be used. This is used only if dilution factor option 3 is selected.

Length of source along the flow direction, L is used for calculating DF4. Length of source, L , is defined in the units of length, typically m or ft . Any consistent set of units may be used.

Output

For the three sequential calculations performed in the module, following three outputs are generated.

Source Concentration

Source concentration $C_{w-source}$ is calculated in cell “E11” of the worksheet “InputParameters_Vadose”.

Vadose Zone Transport

Concentration breakthrough curve at the bottom of vadose zone is computed in column “O” of the worksheet “Calculations”. Corresponding time values are output in column “I” in the same spreadsheet. A plot is also generated in two spreadsheets – “InputParameters_Vadose” and “Charts”.

Saturated Zone Transport

Concentration breakthrough curve at the receptor well is computed in column “AE” of the worksheet “Calculations”. Corresponding time values are output in column “I” in the same spreadsheet. A plot is also generated in two spreadsheets – “InputParameters_Saturated” and “Charts”.

Verification Examples

Verification Example 1

The analytical solution for saturated transport used in this module has been implemented as a FORTRAN program called ATRANS (Neville, 2005). ATRANS has been verified against other numerical software like MT3D. SSA_Analytical.xlsm was verified against ATRANS.

Input parameter for the source concentration and vadose zone transport are set as shown in the following tables.

Source Concentration			
Parameter/Boundary	Units	Symbol	Value
Water content (Vw/Vt)	[-]	θ_w	0.1
Air content (Va/Vt)	[-]	θ_a	0.1
Density of water	[M/L ³]	ρ_w	0
Bulk density (Ms/Vt)	[M/L ³]	ρ_b	2
Soil-water partitioning coefficient	[L ³ /M]	K_d	0
Henry's law partitioning coefficient	[-]	k_H	0
Soil Concentration	[M/M]	C_{soil}	0.05
Concentration in water	[M/L ³]	$C_{w-source}$	1

Transport - Vadose Zone			
Parameter/Boundary	Units	Symbol	Value
Vadose zone thickness	[L]	z	30
Infiltration rate	[L/T]	q_2	0.1
Water content (Vw/Vt)	[-]	θ_w	0.1
Soil-water partitioning coefficient	[L ³ /M]	K_d	0
Bulk density (Ms/Vt)	[M/L ³]	ρ_b	0
Dispersion coefficient	[L ² /T]	D	2.00E+00
Decay rate in water	[1/T]	λ_{w2}	0
Decay rate on soil	[1/T]	λ_{s2}	0
Boundary concentration	[M/L ³]	C_0	1
Source decay rate	[1/T]	γ	0

Time Information			
Maximum time	[T]		100
Time step size	[T]		1

The resulting breakthrough curve at the bottom of the vadose zone is shown in Figure 3. Concentrations shown in Figure 3 were used as an input to ATRANS to verify the saturated zone solution provided by SSA_Analytical.xlsm. Source zone calculations, vadose zone calculations, and saturated zone calculations are all performed internally within SSA_Analytical.xlsm.

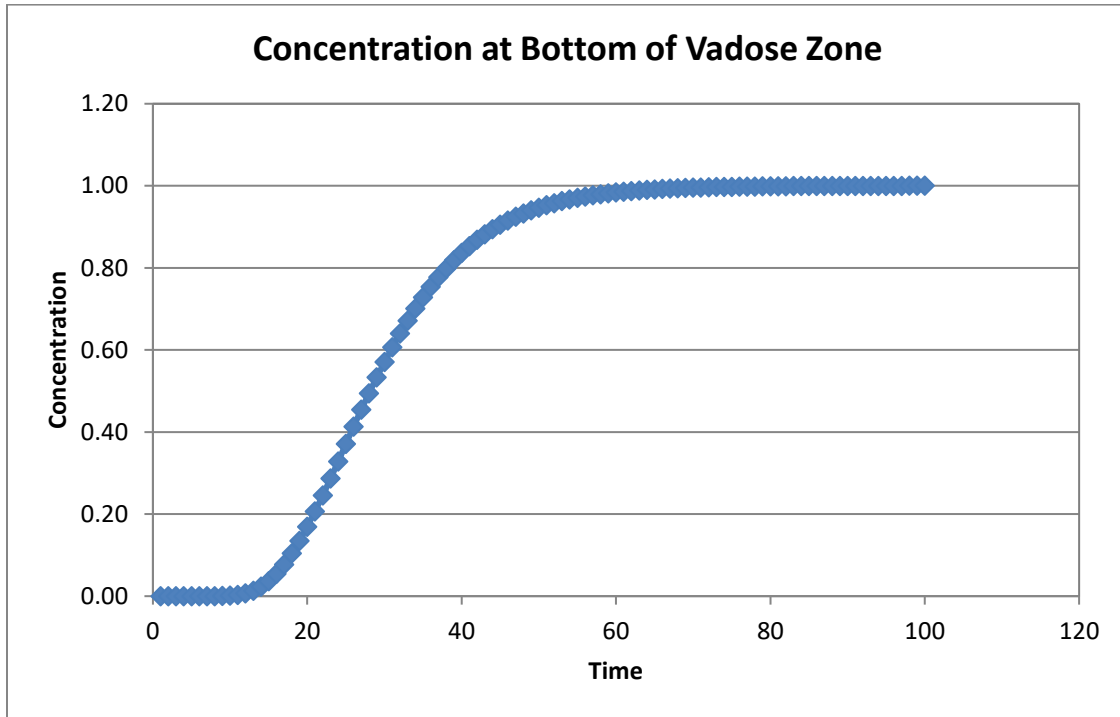


Figure 3. Breakthrough curve at the bottom of vadose zone.

Figure 4 shows the conceptual problem within the saturated zone for the first verification example. Tables below show the input provided in SSA_Analytical.xlsm.

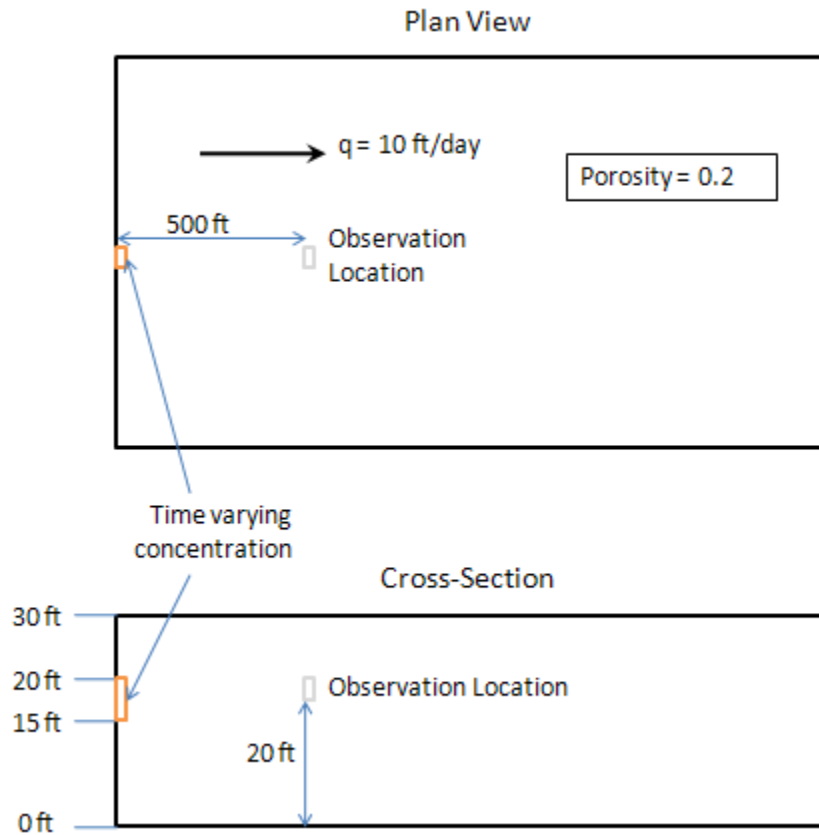


Figure 4. Conceptual problem for verification example 1

Dimensions			
Parameter/Boundary	Units	Symbol	Value
Thickness of aquifer	[L]	B	30
Half-width of patch	[L]	y_0	5
Longitudinal distance of receptor well	[L]	x	500
Transverse distance of receptor well	[L]	y	0
Vertical distance of receptor well	[L]	z	20
Vertical distance of lower edge of patch	[L]	z_1	15
Vertical distance of upper edge of patch	[L]	z_2	20

Flow Parameters			
Parameter/Boundary	Units	Symbol	Value
Darcy flux	[L/T]	q	10
Saturated water content (porosity)	[-]	θ_s	0.2

Transport Parameters			
Parameter/Boundary	Units	Symbol	Value
Longitudinal dispersivity	[L]	α_L	2.00E+00

Horizontal transverse dispersivity	[L]	α_{TH}	1.00E+00
Vertical transverse dispersivity	[L]	α_{TV}	1.00E+00
Effective diffusion coefficient	[L ² /T]	D^*	0
Soil-water partitioning coefficient	[L ³ /M]	K_d	0
Bulk Density	[M/L ³]	ρ_b	0
Decay rate in water	[1/T]	λ_{w3}	0
Decay rate on soil	[1/T]	λ_{s3}	0

Breakthrough curves generated for verification example 1 are shown in Figure 5. Concentrations generated using the program ATRANS are also shown. The two breakthrough curves are noted to be in good agreement.

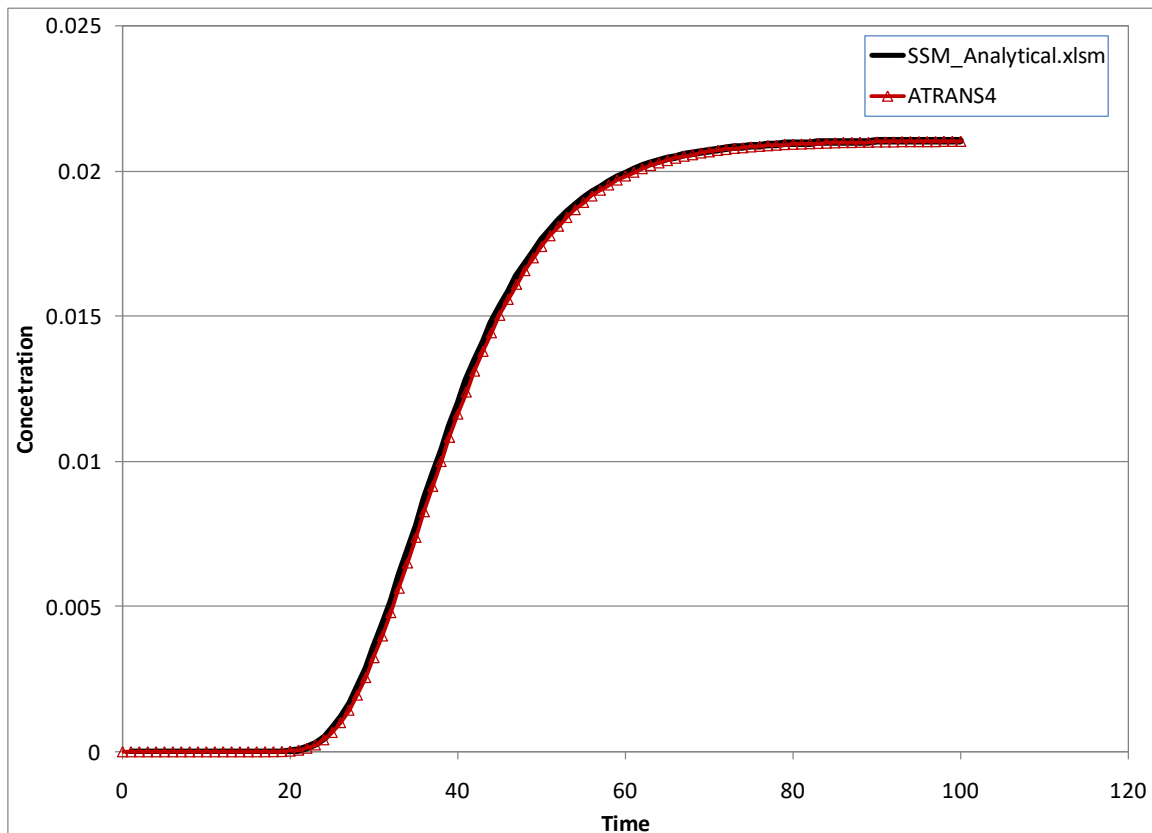


Figure 5. Breakthrough curve at receptor well 500 ft from the source for verification example 1

Verification Example 2

This example is based on example 1 and examines the effect of retardation on the breakthrough curve. A soil-water partitioning coefficient value of 0.117647 cc/g was used with a bulk density of 1.7 g/cc. Porosity of 0.2 results in a retardation factor of 2. Breakthrough curves for verification example 2 are shown in Figure 6. It can be noted that retardation factor slows the timing of the occurrence of the peak without changing the peak concentration attained by the breakthrough curve. The results are in good agreement with the results obtained using ATRANS.

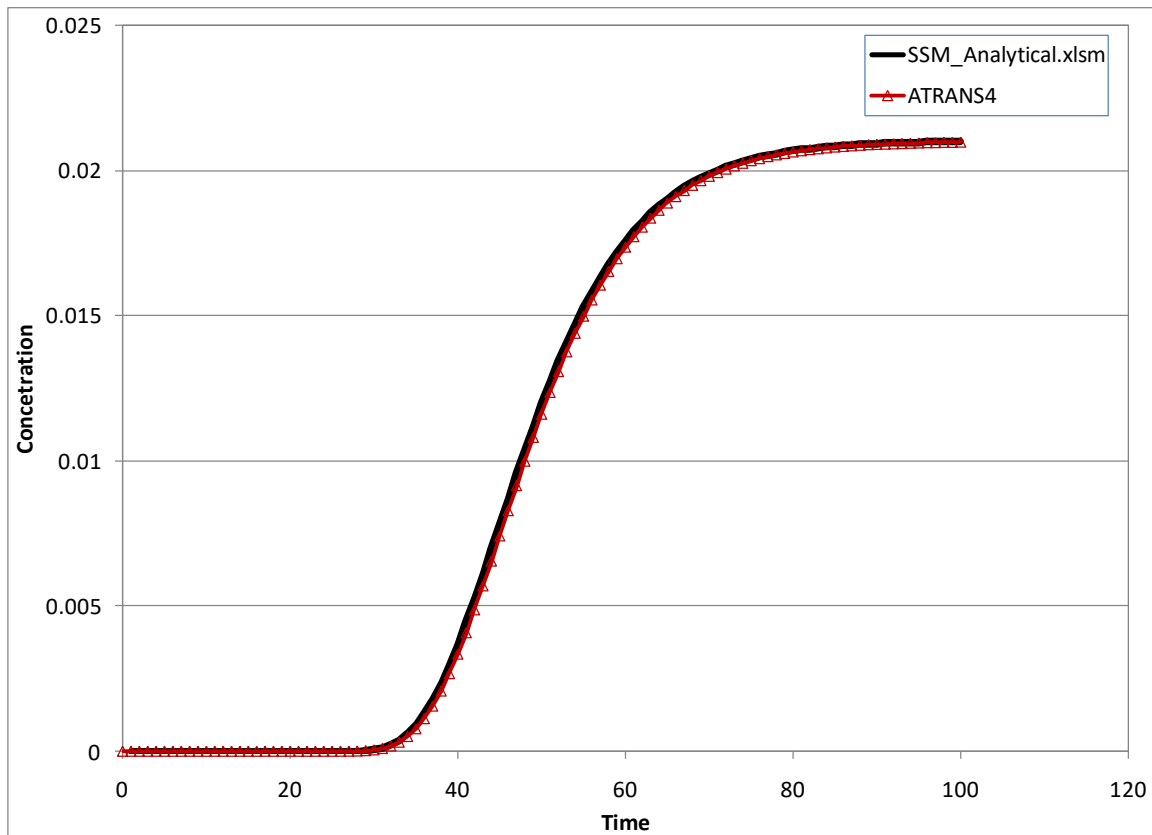


Figure 6. Breakthrough curve at receptor well 500 ft from the source for verification example 2

Verification Example 3

This example is based on example 2 and illustrates the effect of first-order decay rate constant. A first-order decay rate of 0.01 day^{-1} was used in this example. It is assumed that the solute undergoes a first-order reaction at the same rates in the dissolved (water) and sorbed phases (solids). Breakthrough curves for verification example 3 are shown in Figure 7. It can be noted that applying decay reduces the value of peak concentration but does not change the timing of arrival of the contaminant at the receptor well. Results show good agreement with results obtained by ATRANS.

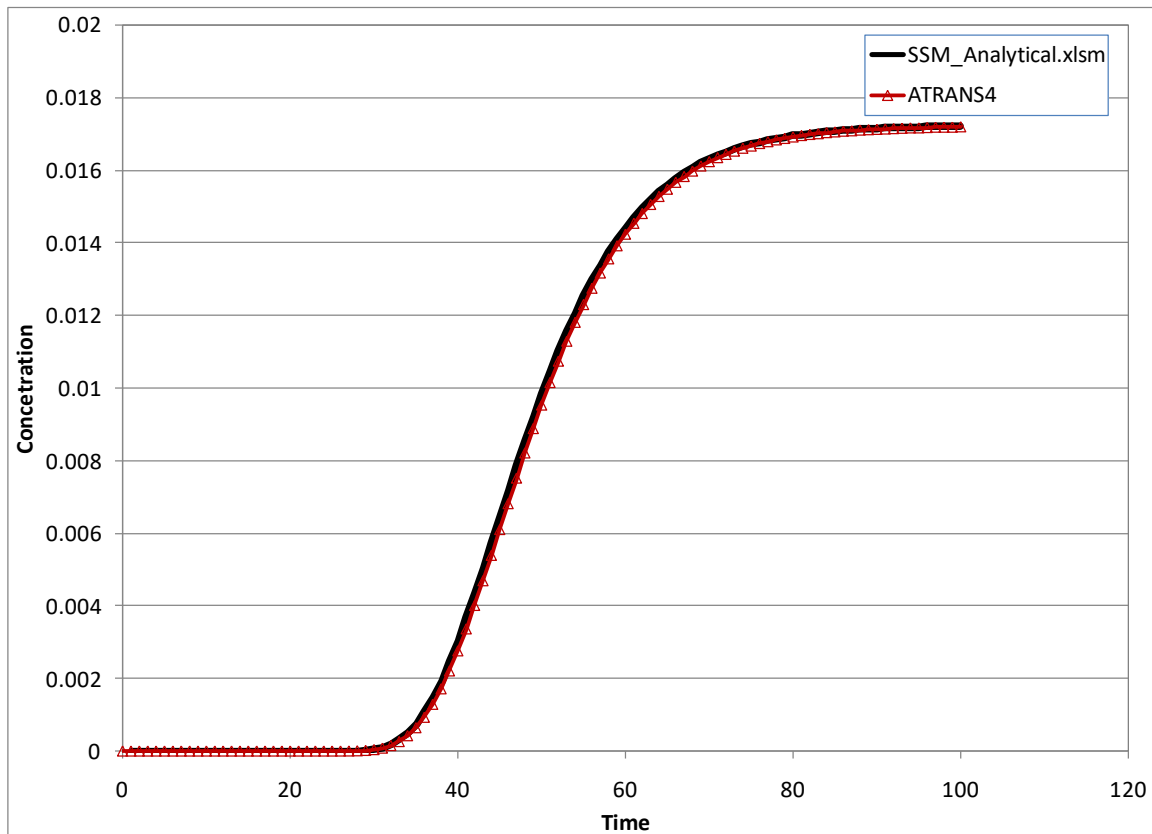


Figure 7. Breakthrough curve at receptor well 500 ft from the source for verification example 3

Verification Example 4

This example demonstrates depleting source concentration representing a finite contaminant source. Source depletion rate as calculated with Rowe (1972) is used in this example. Following input is used.

Source Concentration			
Parameter/Boundary	Units	Symbol	Value
Water content (Vw/Vt)	[-]	θ_w	0.1
Air content (Va/Vt)	[-]	θ_a	0.1
Density of water	[M/L ³]	ρ_w	0
Bulk density (Ms/Vt)	[M/L ³]	ρ_b	2
Soil-water partitioning coefficient	[L ³ /M]	K_d	0
Henry's law partitioning coefficient	[-]	K_H	0
Soil Concentration	[M/M]	C_{soil}	0.05
Concentration in water	[M/L ³]	$C_{w-source}$	1

Transport - Vadose Zone			
Parameter/Boundary	Units	Symbol	Value
Vadose zone thickness	[L]	z	30
Infiltration rate	[L/T]	q_2	0.1
Water content (Vw/Vt)	[-]	θ_{w2}	0.1
Soil-water partitioning coefficient	[L ³ /M]	K_{d2}	0
Bulk density (Ms/Vt)	[M/L ³]	ρ_{b2}	0
Dispersion coefficient	[L ² /T]	D	1.00E-01
Decay rate in water	[1/T]	λ_{w2}	0
Decay rate on soil	[1/T]	λ_{s2}	0
Boundary concentration	[M/L ³]	C_0	1
Source depletion rate	[1/T]	γ	0.2

Time Information			
Maximum time	[T]		100
Time step size	[T]		0.02

Source Depletion			
Source depletion input	Units	Symbol	Value
Option	[-]		3
Source depletion rate	[1/T]	γ	0.2
Rate for constant concentration	[1/T]	γ_1	0
User defined rate	[1/T]	γ_2	0
Depth of source zone	[L]	H	5
Calculated rate (Rowe)	[1/T]	γ_3	0.2
Condition of applicability	[1/T]		2.5

Saturated Zone Patch Dimensions			
Parameter/Boundary	Units	Symbol	Value
Thickness of aquifer	[L]	B	30
Half-width of patch	[L]	y_0	10000
Longitudinal distance of receptor well	[L]	x	500
Transverse distance of receptor well	[L]	y	0
Vertical distance of receptor well	[L]	z	15
Vertical distance of lower edge of patch	[L]	z_1	0
Vertical distance of upper edge of patch	[L]	z_2	30

Saturated Zone Flow Parameters			
Parameter/Boundary	Units	Symbol	Value
Darcy flux	[L/T]	q_3	10
Saturated water content (porosity)	[-]	θ_{s3}	0.2

Saturated Zone Transport Parameters			
Parameter/Boundary	Units	Symbol	Value
Longitudinal dispersivity	[L]	α_L	1.00E-03
Horizontal transverse dispersivity	[L]	α_{TH}	1.00E-03
Vertical transverse dispersivity	[L]	α_{TV}	1.00E-03
Effective diffusion coefficient	[L ² /T]	D^*	0
Soil-water partitioning coefficient	[L ³ /M]	K_{d3}	0
Bulk Density	[M/L ³]	ρ_{b3}	0
Decay rate in water	[1/T]	λ_{w3}	0
Decay rate on soil	[1/T]	λ_{s3}	0

Dilution Factor			
Dilution factor input	Units	Symbol	Value
Option	[-]		1
Dilution factor	[-]		1.00
User supplied dilution factor	[-]	DF1	1
Default dilution factor	[-]	DF2	20
Cross-sectional area of groundwater flow	[L ²]	A_a	5
Groundwater flow volume	[L ³ /T]	Q_a	50
Cross-sectional area of vadose zone flow	[L ²]	A_p	30
Vadose zone flow volume	[L ³ /T]	Q_p	3
Calculated dilution factor	[-]	DF3	17.67

Figure 8 shows the source concentration, breakthrough curve at the bottom of vadose zone, and breakthrough curve at a location 500 m down-gradient of the source. Peak concentration in the source is 1 [unit] at the beginning of the simulation which depletes with time. Peak concentration of 0.46 [units] is seen at the bottom of vadose zone at 32 time units and peak concentration of 0.46 [units] is seen at a location 500 m down-gradient of the source location at 42 days. It can also be noted that the breakthrough curve at the bottom of the vadose zone agrees with the results obtained using a program called OneD. OneD is a program that implements the vadose zone analytical solution in Fortran mentioned in Appendix B.

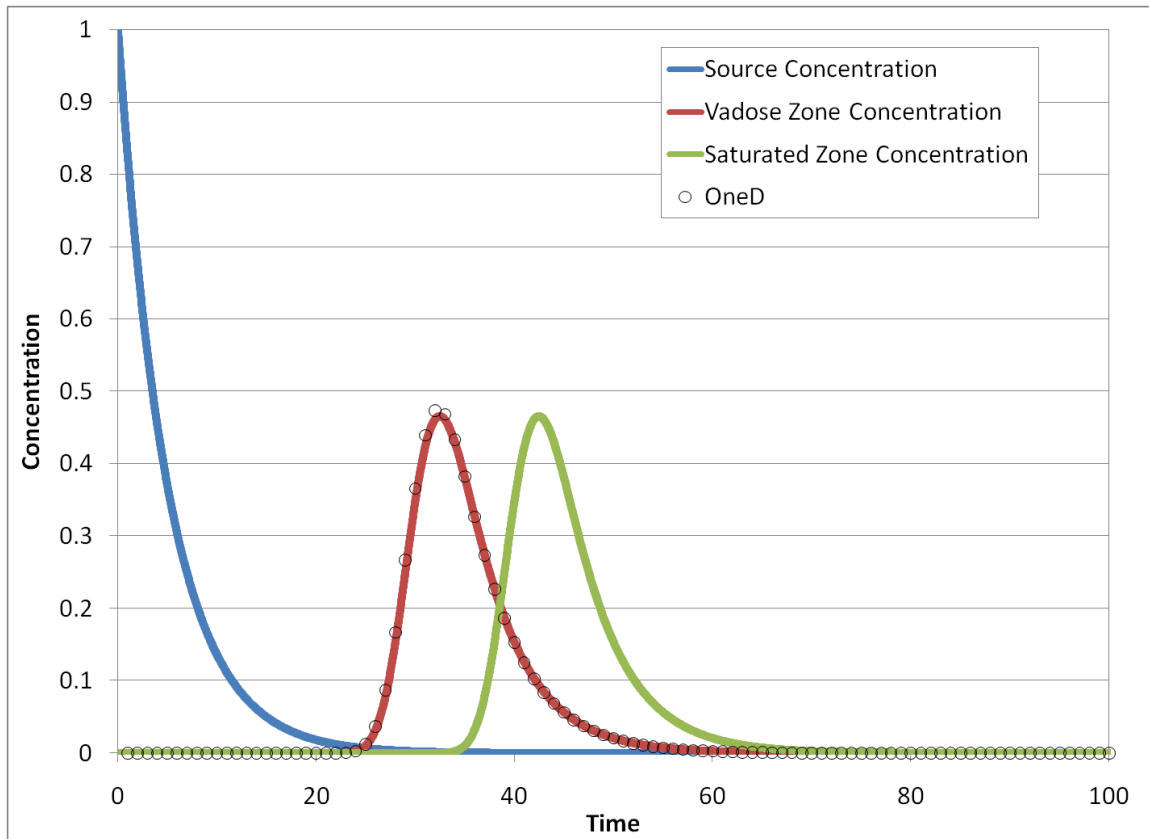


Figure 8. Source concentration depletion and breakthrough curves at bottom of vadose zone and at receptor well 500 ft from the source for verification example 4

Appendix A

Calculation of dissolved concentration in source area (flash calculations)

Concentrations in a source area in the vadose zone are typically reported in terms of the *soil* concentration, defined on a mass/mass basis:

$$C_{soil} = \frac{\text{Total mass of species}}{\text{Mass of solids}}$$

With respect to a receptor in the underlying aquifer, the concentration that is of interest is the dissolved concentration, defined on a mass/volume basis:

$$C_{w-source} = \frac{\text{Mass of species dissolved}}{\text{Volume of water}}$$

The first step in the analysis is a conversion from the soil concentration to the equivalent dissolved concentration in the pore water in the vadose zone. For the conversion calculation the material in the source area is idealized as a three-phase porous medium, as shown schematically in Figure A1.

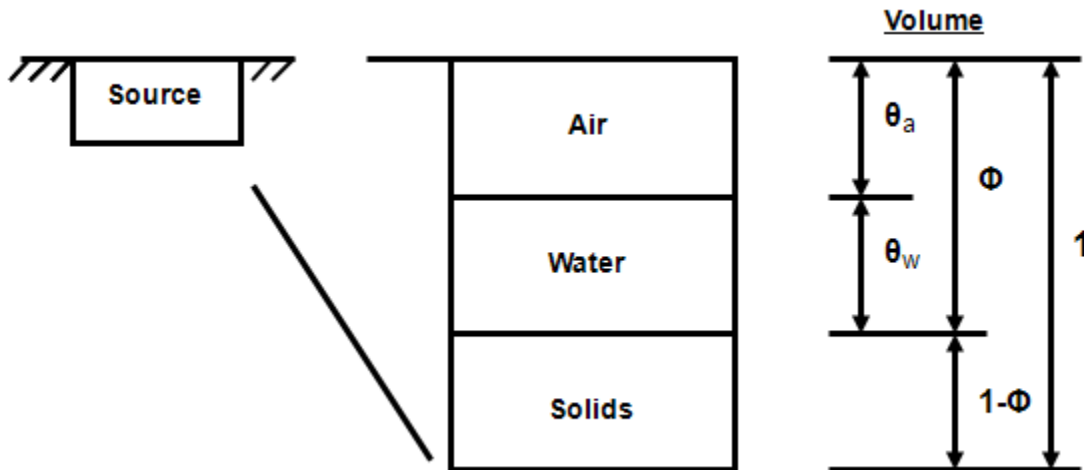


Figure A1. Idealization of the material in the source area

Equilibrium (instantaneous and reversible) partitioning is assumed between the species in the three phases. Calculations following from this assumption are sometimes referred to as “flash calculations”. The total mass of the species in the source area is partitioned between the water (dissolved), solids (sorbed), and vapor (air) phases.

The sorbed-phase concentration is defined as:

$$\bar{C}_{s-source} = \frac{\text{Mass of species sorbed}}{\text{Mass of solids}}$$

Assuming equilibrium sorption governed by a linear isotherm:

$$\bar{C}_{s-source} = K_d C_{w-source}$$

Here $K_{d-source}$ is the sorption partitioning coefficient in the source zone.

The concentration in the air phase of the vadose zone is defined as:

$$C_{a-source} = \frac{\text{Mass of species in air phase}}{\text{Volume of air phase}}$$

Assuming equilibrium between the concentrations in the pore water and pore air:

$$C_{a-source} = K_H C_{w-source}$$

Here K_H is the Henry's Law partitioning coefficient in the source zone.

The total mass of species per unit volume of porous medium is given by the sum of the masses in each phase:

$$M_T = \theta_{w-source} C_{w-source} + \theta_{a-source} C_{a-source} + \rho_b \bar{C}_{s-source}$$

Here θ_w is the moisture content (volume of water per unit volume of porous medium), θ_a is the air content (volume of air per unit volume of porous medium), and ρ_b is the bulk dry density of the porous medium (mass of solids per unit volume of porous medium).

Substituting for $C_{a-source}$ and $\bar{C}_{s-source}$ yields:

$$M_T = \theta_w C_{w-source} + \theta_a K_H C_{w-source} + \rho_b K_d C_{w-source} = C_{w-source} (\theta_w + \theta_a K_H + \rho_b K_d)$$

The mass of the solids per unit volume of porous medium is simply ρ_b ; therefore, the soil concentration is given by:

$$C_{soil} = \frac{M_T}{M_{soil}} = \frac{C_{w-source} (\theta_w + \theta_a K_H + \rho_b K_d)}{\rho_b}$$

Rearranging yields the final expression for the dissolved concentration in terms of the soil concentration:

$$C_{w-source} = C_{soil} \frac{\rho_b}{(\theta_w + \theta_a K_H + \rho_b K_d)}$$

An alternative measure of concentration is the *total* concentration, defined as:

$$C_{total} = \frac{\text{Mass of species}}{\text{Mass of porous medium}}$$

The mass of the air is negligible, so the total mass of the porous medium is given by:

$$M_{PM} = \theta_w \rho_w + \rho_b$$

The total concentration is therefore given by:

$$C_{total} = \frac{M_T}{M_{PM}} = \frac{C_{w-source} (\theta_w + \theta_a K_H + \rho_b K_d)}{\theta_w \rho_w + \rho_b}$$

Rearranging yields the final expression for the dissolved concentration in terms of the total concentration:

$$C_{w-source} = C_{total} \frac{\theta_w \rho_w + \rho_b}{(\theta_w + \theta_a K_H + \rho_b K_d)}$$

Appendix B

Transport of dissolved species across the vadose zone

Approach

The conceptual model for transport across the vadose zone is shown schematically in Figure B1. The analysis considers one-dimensional flow across the vadose zone, with one-dimensional dispersion, equilibrium sorption, and first-order transformation reactions. The source represents infiltration through the source zone for which the dissolved concentration is calculated in the first part of the analysis.

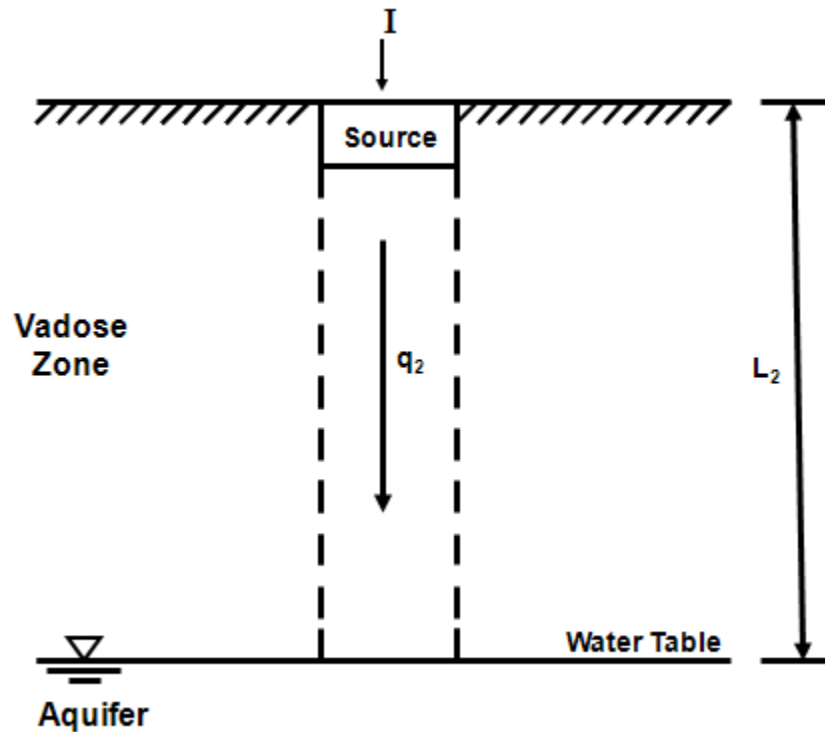


Figure B1. Conceptual model for transport across the vadose zone

Analysis

The governing equation for transport across the vadose zone is:

$$\frac{\partial}{\partial t}(\theta_w C_2 + \rho_b \bar{C}_2) = -\frac{\partial}{\partial z}(q_2 C_2) + \frac{\partial}{\partial z}\left(\theta_w D_2 \frac{\partial C_2}{\partial z}\right) - \theta_w \lambda_{w2} C_2 - \rho_b \lambda_{s2} \bar{C}_2$$

where:

C_2 = dissolved concentration in the vadose zone [M solute/ L³ water];

\bar{C}_2 = sorbed concentration in the vadose zone [M solute/ M solids];

z = spatial coordinates [L];

t = time [T].

θ_w = water content in the vadose zone [L³ water/ L³ porous medium];

ρ_b = bulk density [M solids/ L³ porous medium];

q_2 = Darcy flux across the vadose zone [L/ T];

D = dispersion coefficient for transport in the vadose zone [L²/ T];

λ_{w2} = first-order transformation rate in the pore water in the vadose zone [T⁻¹]; and

λ_{s2} = first-order transformation rate in the sorbed phase in the vadose zone [T⁻¹].

The Darcy flux across the vadose zone, q_2 , is equal to the rate at which infiltration of precipitation recharges the water table. There is a physical limit on the rate of infiltration - the infiltration rate cannot exceed the saturated hydraulic conductivity of the materials in the vadose zone. If the anticipated infiltration rate, that is, the difference between precipitation and evapotranspiration, exceeds the saturated hydraulic conductivity, water will pond at the surface and evaporate instead of infiltrating.

Assuming equilibrium partitioning between the dissolved and sorbed phases:

$$\bar{C}_2 = K_d C_2$$

We define the retardation factor as:

$$R_2 = 1 + \frac{\rho_b}{\theta_w} K_d$$

We do not presume that the first-order transformation reactions proceed at the same rates in the dissolved and sorbed phases. By considering an “effective” transformation rate, a general approach can be accommodated:

$$\lambda_{2E} = \frac{1}{R_2} \left(\lambda_{w2} + \frac{\rho_b \lambda_{s2} K_d}{\theta_w} \right)$$

Substituting into the governing equation yields:

$$\frac{\partial C_2}{\partial t} = -v'_2 \frac{\partial C_2}{\partial z} + D'_2 \frac{\partial^2 C_2}{\partial z^2} - \lambda_{2E} C_2$$

The parameters appearing in the final form of the governing equation are:

$$v'_2 = \frac{q_2}{\theta_w R_2}$$

$$D'_2 = \frac{D_2}{R_2}$$

At this point we must address the treatment of the moisture content in the vadose zone. As shown schematically in Figure B2, the moisture content varies across the thickness of the vadose zone.

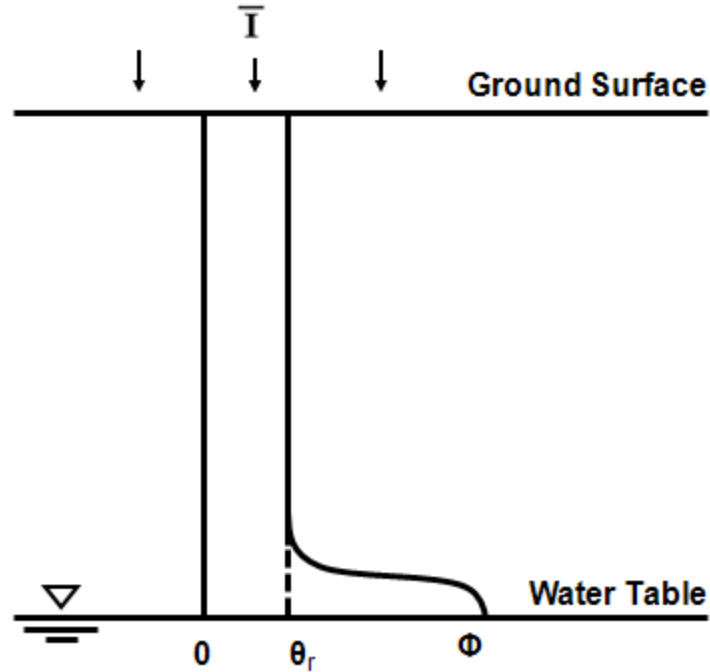


Figure B2. Conceptual distribution of moisture across the vadose zone

For an analytical approach to be tractable, the moisture content must be constant. We expect that averaged through time, the pore water is at the residual moisture content, θ_r , across much of the thickness of the vadose zone. The simplest approach is to assign the

residual moisture content as the single value of the moisture content across the full thickness of the vadose zone. This approach is conservative in that it leads to the highest rate of migration across the vadose zone. However, this approach may not be physically realistic. If the residual moisture content is interpreted as representing water that is immobilized by capillary forces, then this conceptual model would imply that there is no advection across the vadose. It may therefore be more appropriate to assign a single value for the moisture content of the vadose zone as some value that is higher than the residual.

The initial and boundary conditions are:

$$C_2(x, y, z, 0) = 0$$

$$C_2(0, t) = C_0(t)$$

$$C_2(\infty, t) = 0$$

General solution

When the concentration in the source is represented as a general function of time,

$C_{w-source}(t)$, the inner boundary condition is written as:

$$C_2(0, t) = C_{w-source}(t)$$

the general solution is:

$$C_2(z, t) = \frac{z}{2\sqrt{\pi D'_2}} \text{EXP} \left\{ \frac{v'_2 z}{2D'_2} \right\} \int_0^t C_{w-source}(\tau) \frac{1}{(t-\tau)^{3/2}} \text{EXP} \left\{ - \left(\frac{v'^2_2}{4D'_2} + \lambda_{2E} \right) (t-\tau) - \frac{z^2}{4D'_2(t-\tau)} \right\} d\tau$$

Solution for a constant source concentration

The most conservative assessment will correspond to the case in which the source is assumed to contain an inexhaustible mass such that the source concentration is effectively constant through time (Figure B3):

$$C_2(0, t) = C_0$$

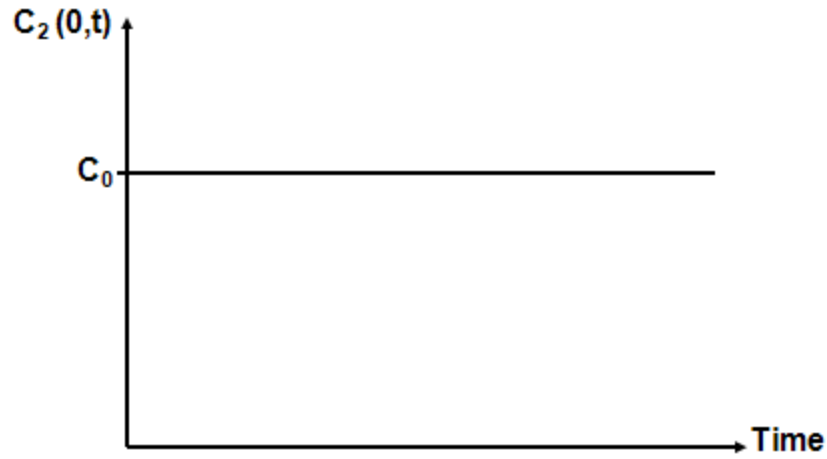


Figure B3. Concentration boundary for an infinite source

For a constant source, the solution is generalized from Ogata and Banks (1961) for sorption and decay:

$$C_2(z,t) = \frac{C_0}{2} \left[\begin{aligned} & \text{EXP} \left\{ \frac{v'_2 z}{2D'_2} + \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\} \text{ERFC} \left\{ \frac{z}{2\sqrt{D'_2 t}} + \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \sqrt{t} \right\} \\ & + \text{EXP} \left\{ \frac{v'_2 z}{2D'_2} - \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\} \text{ERFC} \left\{ \frac{z}{2\sqrt{D'_2 t}} - \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \sqrt{t} \right\} \end{aligned} \right]$$

Solution for a leaching source

If the source area contains a finite amount of mass, the leaching of the source will give rise to a dissolved concentration that declines through time (Figure B4). The decline follows a negative exponential function:

$$C_2(0,t) = C_0 \text{EXP}\{-\gamma t\}$$

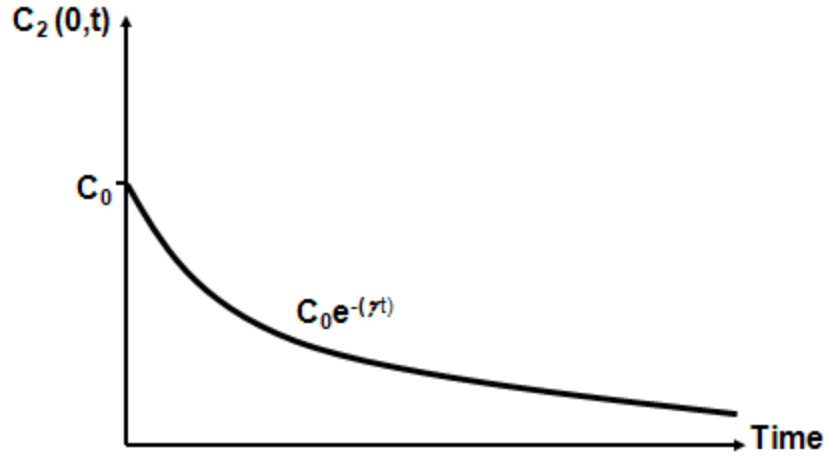


Figure B4. Concentration boundary for a finite source

Here C_0 represents the initial dissolved concentration in the source, and the parameter γ represents the source decay rate. Following the analysis of Rowe (1991), the source decay rate is:

$$\gamma = \frac{q_2}{H_r}$$

The parameter H_r is defined as:

$$H_r = \frac{M_0}{C_0 L W}$$

where M_0 is the initial total mass in the source, and L and W are the length and width of the source. In other words, M_0/LW represents the mass of the source per unit area.

For a concentration in the source area that declines through time following a negative exponential function, the transport across the vadose zone can be simulated with the following analytical solution:

$$C_2(z,t) = \frac{C_0}{2} \text{EXP}\{-\gamma t\} \left[\text{EXP}\left\{ \frac{v'_2 z}{2D'_2} + \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + (\lambda_E - \gamma) \right)^{1/2} \right\} \text{ERFC}\left\{ \frac{z}{2\sqrt{D'_2}t} + \left[\left(\frac{(v'_2)^2}{4D'} + (\lambda_E - \gamma) \right) t \right]^{1/2} \right\} \right. \\ \left. + \text{EXP}\left\{ \frac{v'_2 z}{2D'_2} - \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + (\lambda_E - \gamma) \right)^{1/2} \right\} \text{ERFC}\left\{ \frac{z}{2\sqrt{D'_2}t} - \left[\left(\frac{(v'_2)^2}{4D'} + (\lambda_E - \gamma) \right) t \right]^{1/2} \right\} \right]$$

The case of a constant source concentration corresponds to $\gamma = 0.0$

This solution for an exponentially decaying source is not entirely robust. It is important to note that the solution will fail under the following conditions:

$$\frac{v'^2}{4D'_2} + (\lambda_E - \gamma) < 0$$

Therefore, the condition for applicability of the solution is:

$$\gamma < \frac{v'^2}{4D'_2} + \lambda_E$$

The condition of applicability represents a constraint on the rate at which mass can be leached from the source.

More complex source concentration histories

We can conceive of particular source concentration histories that are more complex than the two cases discussed previously. Two possibilities are shown in Figure B5.

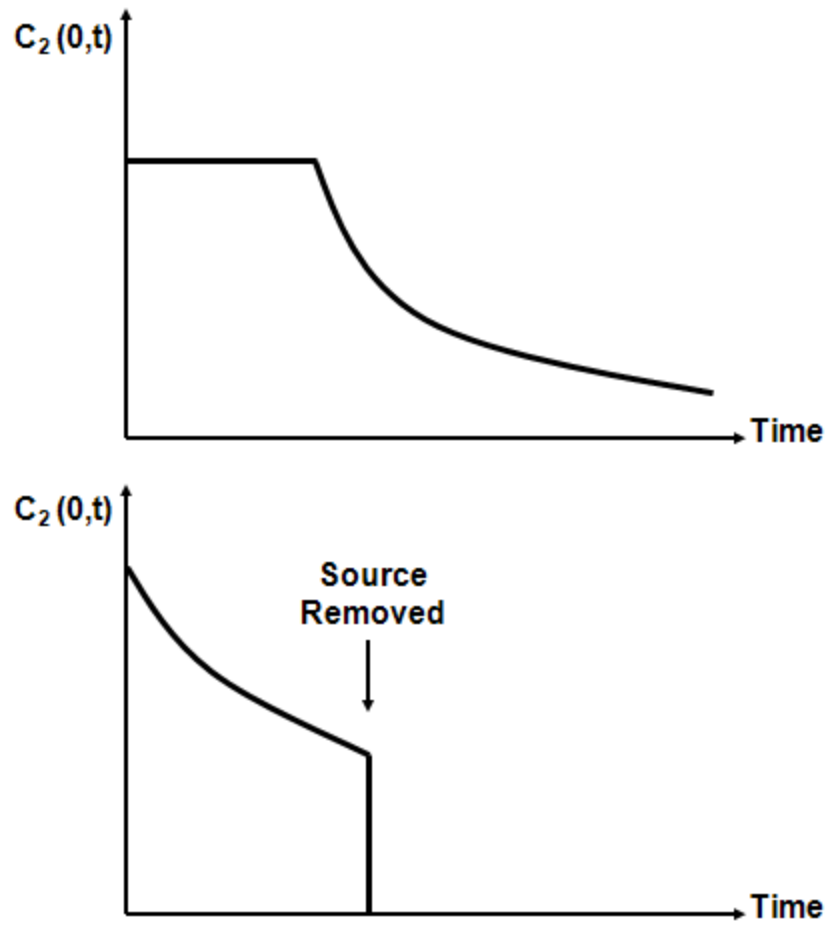


Figure B5. Time varying concentration boundary for a finite source

For more complex source histories, we recommend specifying the source history as a set of discrete points. This is illustrated below in Figure B6.

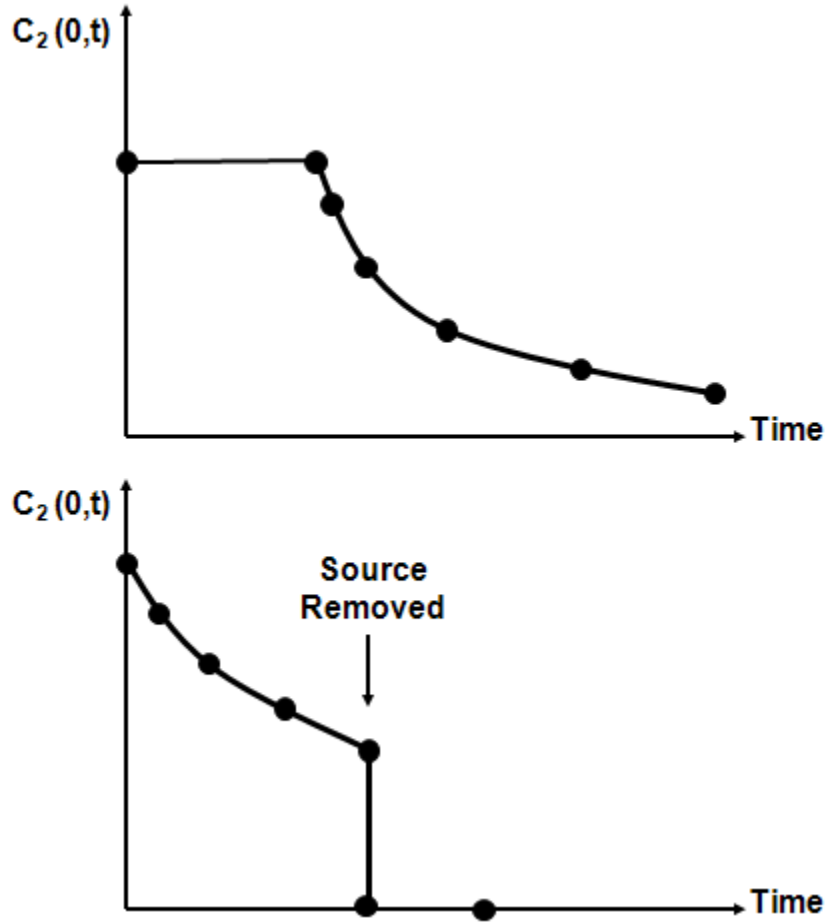


Figure B6. Time varying concentration boundary defined as discrete points for a finite source

Following the approach adopted in the ATRANS model, the concentration at any point in the vadose zone is calculated by superposition of discrete steps ΔC_i that start at time ts_i :

$$C_2(z,t) = \sum_{i=1}^{NP(t)} \frac{\Delta C_i}{2} \left[\begin{aligned} &EXP \left\{ \frac{v'_2 z}{2D'_2} + \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\} ERFC \left\{ \frac{z}{2\sqrt{D'_2}(t-ts_i)} + \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \sqrt{(t-ts_i)} \right\} \\ &+ EXP \left\{ \frac{v'_2 z}{2D'_2} - \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\} ERFC \left\{ \frac{z}{2\sqrt{D'_2}(t-ts_i)} - \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \sqrt{(t-ts_i)} \right\} \end{aligned} \right]$$

Implementation of the analytical solution

For source screening analysis, the analytical solution was implemented in Excel 2007 and was called “SSA_Analytical.xlsm”. Standard formulae available in Excel were used. For robustness of the solution over a wide range of possible input values, the complementary error function $erfc(y)$ was evaluated using an asymptotic expansion for all values of y greater than or equal to 3.4 and values of y less than 14, where y is a positive real number (Abramowitz and Stegun, 1972). The asymptotic expansion is evaluated only up to two terms and is given by the relation:

$$erfc(y) = \left(\frac{e^{-y^2}}{y\sqrt{\pi}} \right) \left(1 - \frac{1}{2y^2} \right)$$

Here, y is a positive number for which complimentary error function is evaluated. For negative values of y , following symmetry relation is applied.

$$erfc(-y) = 2 - erfc(y)$$

Product of terms $exp(x)$ and $erfc(y)$ was determined to be zero if the value of the term $erfc(y)$ was determined to be zero. This provision provides robustness to the solution when values of x and y are extreme and the term $exp(x)$ cannot be determined within reasonable limits.

Time-varying concentration boundary was implemented using user-defined discrete points. Discrete points used for defining source concentration are independent of the time for which simulation is performed. Vadose zone solution at desired time values is obtained by piecewise linear interpolation as shown in Figure B7.

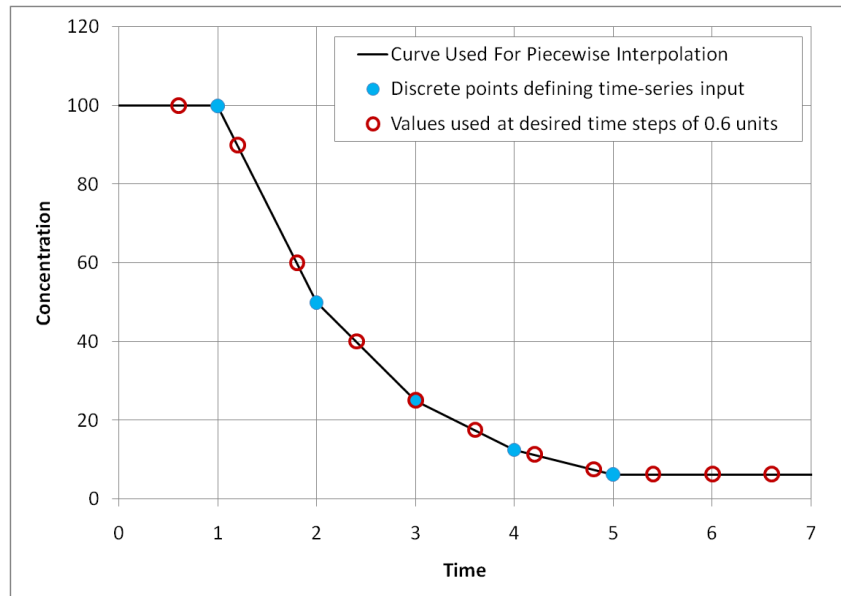


Figure B7. Implementation of time-varying concentration boundary

A Fortran code is also available that implements the analytical solution for transport across the vadose zone. The program is called OneD. However, it should be noted that the solution represents a special, degenerate, case of one of the solutions implemented in the ATRANS that is discussed in the next section (Neville, 2005).

As a check on the implementation of the solution we can also examine the results for large values of time (i.e., steady-state conditions). The solution for steady-state conditions should yield the following asymptotic results:

- For a decaying source, the steady-state concentration is 0.0 across the full thickness of the vadose zone;
- For a constant source, with no decay in the vadose zone, the steady-state concentration is C_0 across the full thickness of the vadose zone; and
- For a constant source with decay in the vadose zone, substituting for $t \rightarrow \infty$ yields:

$$C_2(z,t) = \frac{C_0}{2} \left[\exp \left\{ \frac{v'_2 z}{2D'_2} + \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\} (0) + \exp \left\{ \frac{v'_2 z}{2D'_2} - \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\} (2) \right]$$

Simplifying:

$$C_2(z,t) = C_0 \exp \left\{ \frac{v'_2 z}{2D'_2} - \frac{z}{\sqrt{D'_2}} \left(\frac{(v'_2)^2}{4D'} + \lambda_E \right)^{1/2} \right\}$$

Appendix C

Calculation of dissolved concentration in the aquifer

Approach

The conceptual model for transport in the aquifer is shown schematically in Figure C1. The analysis considers one-dimensional flow in the aquifer, with three-dimensional dispersion, equilibrium sorption, and first-order transformation reactions. In the analysis the source is represented as a “patch” along the inflow boundary. Although the patch shown in Figure C1 has general vertical coordinates Z_1 and Z_2 , in the analyses the patch will extend from the water table ($z = Z_2 = B$) to some penetration depth D ($z = Z_1 = B - D$). The patch may have a concentration history $C_0(t)$ that varies in a general way through time.

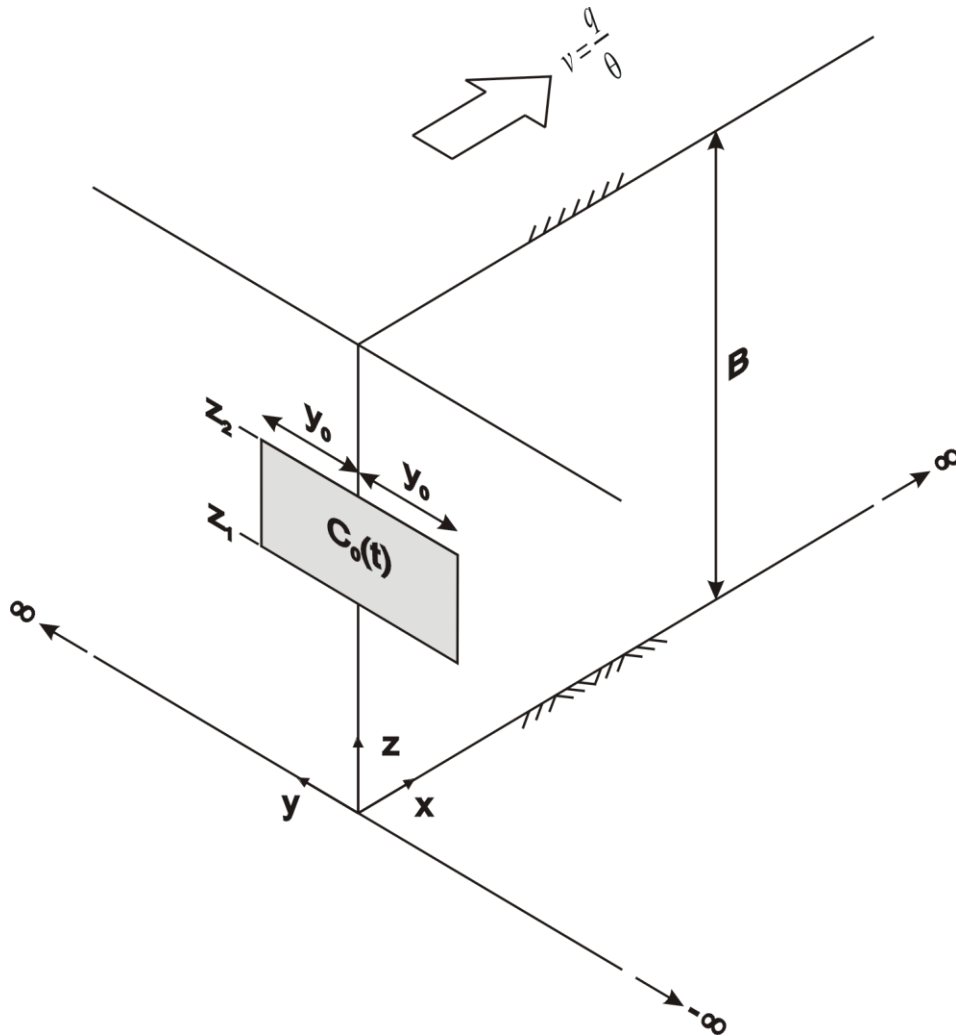


Figure C1. Conceptual model for transport in the aquifer

Dilution Factor

We have introduced a dilution factor, DF , to account for a reduction in concentration as solute exiting from the vadose zone mixes with the ambient lateral groundwater flow in the saturated zone. As used here, DF is assigned values greater than or equal to 1.

Dilution factor DF can be calculated using a simple mixing formula (WAC 173-340-747).

$$DF = (Q_p + Q_a)/Q_p$$

where,

Q_p = Volume of water infiltrating [L^3/T]

Q_a = Ground water flow [L^3/T]

For dilution factor input option 3, flow rates Q_a and Q_p are calculated using user-defined cross-sectional areas A_a and A_p , respectively. The calculations are as follows:

$$Q_a = A_a \times q_3$$

$$Q_p = A_p \times q_2$$

For dilution factor input option 4, flow rate Q_a is calculated using penetration depth H and Q_p is calculated using a user-defined source length, L , defined as the length of source along the direction of flow. Both Q_a and Q_p , assume a unit width for the source area. The calculations are as follows:

$$Q_a = 1 \times H \times q_3$$

$$Q_p = 1 \times L \times q_2$$

where, H is the penetration depth calculated as follows (Charbeneau, 2000):

$$H = H_a + H_d = B \left(1 - \exp \left\{ -\frac{q_2 L}{q_3 B} \right\} \right) + \sqrt{2\alpha_{TV} L}$$

Here:

H_a is the penetration depth due to advection [L]; and

H_d is the penetration depth due to dispersion [L].

Analysis

Transport in the aquifer is simulated with an analytical solution. The analytical solution is described briefly in Zheng and Bennett (2002; p. 114), and in more detail in Neville (2005). The solution is derived using integral transform methods, following the approaches adopted in Cleary and Ungs (1978) and Wexler (1992). The solution is a generalization of the solutions implemented in the U.S. EPA codes EPACMTP (Sudicky and others, 1988) and MULTIMED (Salhotra and others, 1995).

The governing equation for transport in the aquifer is:

$$\theta \frac{\partial C_3}{\partial t} + \rho_b \frac{\partial \bar{C}_3}{\partial t} = -q_3 \frac{\partial C_3}{\partial x} + \theta D_x \frac{\partial^2 C_3}{\partial x^2} + \theta D_y \frac{\partial^2 C_3}{\partial y^2} + \theta D_z \frac{\partial^2 C_3}{\partial z^2} - \theta \lambda_{w3} C_3 - \rho_b \lambda_{s3} \bar{C}_3$$

; over: $0 \leq x < \infty$, $-\infty < y < \infty$, $0 \leq z \leq B$

Here:

C_3 = dissolved concentration [M solute/ L³ water];

\bar{C}_3 = sorbed concentration [M solute/ M solids];

x, y, z = spatial coordinates [L];

t = time [T].

θ = saturated water content [L³ water/ L³ porous medium];

ρ_b = bulk density [M solids/ L³ porous medium];

q_3 = Darcy flux [L/ T];

D_x, D_y, D_z = dispersion coefficients [L²/ T];

λ_{w3} = first-order decay coefficient in the dissolved phase (water) [T⁻¹]; and

λ_{s3} = first-order decay coefficient in the sorbed phase (solids) [T⁻¹]; and

The dispersion coefficients are defined as the sum of mechanical dispersion and diffusion coefficients:

$$D_x = \alpha_L \frac{|q|}{\theta} + D^* = \alpha_L v + D^*$$

$$D_y = \alpha_{TH} \frac{|q|}{\theta} + D^* = \alpha_{TH} v + D^*$$

$$D_z = \alpha_{TV} \frac{|q|}{\theta} + D^* = \alpha_{TV} v + D^*$$

Here:

α_L = longitudinal dispersivity [L];

α_{TH} = horizontal transverse dispersivity [L];
 α_{TV} = vertical transverse dispersivity [L]; and
 D^* = effective diffusion coefficient [L²/T].

The sorbed phase concentration is related to the dissolved phase concentration according to:

$$\bar{C}_3 = K_d C_3$$

Here K_d is the linear sorption partitioning coefficient [L³/M].

The initial and boundary conditions are:

$$C_3(x, y, z, 0) = 0$$

$$C_3(0, y, z, t) = C_{0-3}(t) [H(y + Y_0) - H(y - Y_0)] [H(z - Z_1) - H(z - Z_2)]$$

$$C_3(\infty, y, z, t) = 0$$

$$C_3(x, -\infty, z, t) = 0$$

$$C_3(x, \infty, z, t) = 0$$

$$\frac{\partial C_3}{\partial z}(x, y, 0, t) = 0$$

$$\frac{\partial C_3}{\partial z}(x, y, B, t) = 0$$

Here:

$C_{0-3}(t)$ = arbitrary time-varying function;

Y_0 = half-width of source;

Z_1 = bottom of source; and

Z_2 = top of source.

The term $H(\cdot)$ denotes the Heaviside step function, defined as:

$$\begin{aligned} H(\xi - \xi_0) &= 0 \text{ if } \xi < \xi_0 \\ &= 1 \text{ if } \xi > \xi_0 \end{aligned}$$

The source function for the aquifer, $C_0(t)$, is calculated as the concentration at the bottom of the vadose zone, scaled by the dilution factor:

$$C_{0-3}(t) = \frac{C_2(L_2, t)}{DF}$$

The general solution for a concentration history at the patch that varies as a general function of time is:

$$C_3(x, y, z, t) = \frac{x}{4B\sqrt{\pi D'_x}} \int_0^t C_{0-3}(\tau) \frac{1}{(t-\tau)^{3/2}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} \right\} \\ \cdot \left[\left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y(t-\tau)}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y(t-\tau)}} \right\} \right] \right. \\ \cdot \left. \left[(z_2 - z_1) + \frac{2B}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} (t-\tau) \right\} \right] \right] d\tau$$

Here λ denotes the effective first-order reaction rate (decay coefficient) in the saturated zone. The effective first-order reaction rate is calculated from the specified reaction rates in the dissolved (water) and sorbed (solids) phases according to:

$$\lambda = \frac{1}{R_3} \left(\lambda_{w3} + \frac{\rho_b \lambda_{s3} K_d}{\theta} \right)$$

The term R_3 is the retardation factor in the saturated zone, defined as:

$$R_3 = 1 + \frac{\rho_b}{\theta} K_d$$

In our opinion, it is appropriate to leave the solution in its most general form, as we cannot assume *a priori* that the concentration at the bottom of the vadose zone can be represented by a simple closed-form function. If the concentration at the bottom of the vadose zone is approximated by a set of discrete steps up to the elapsed time t , the solution for the concentration in the aquifer at any location and time is given by:

$$C_3(x, y, z, t) = \frac{x}{4B\sqrt{\pi D'_x}} \sum_{i=1}^{N(t)} \Delta C_i \int_0^{t-t_i} \frac{1}{\tau^{3/2}} \exp \left\{ -\lambda\tau - \frac{(x-v'\tau)^2}{4D'_x\tau} \right\} \\ \cdot \left[\left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y\tau}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y\tau}} \right\} \right] \right. \\ \cdot \left. \left[(z_2 - z_1) + \frac{2B}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \tau \right\} \right] \right] d\tau$$

Here the concentration history at the bottom of the vadose zone is represented as a sequence of steps ΔC_i that start at times t_i . The magnitudes of the concentrations steps incorporate any reductions arising from the dilution factor.

Implementation of the analytical solution

For source screening analysis, the analytical solution is implemented in Excel 2007 and is called “SSA_Analytical.xlsm”. Standard formulae available in Excel are used. For robustness of the solution over a wide range of possible input values standard formula for calculating the complimentary error function $erfc(y)$ was evaluated using an asymptotic expansion of the complimentary error function (Abramowitz and Stegun, 1972) for all values of y greater than or equal to 3.4 and values of y less than 14, where y is a positive real number.

The asymptotic expansion is evaluated only to two terms and is given by the relation:

$$erfc(y) = \left(\frac{e^{-y^2}}{y\sqrt{\pi}} \right) \left(1 - \frac{1}{2y^2} \right)$$

Here, y is a positive number for which complimentary error function is evaluated. For negative values of y , following symmetry relation is applied.

$$erfc(-y) = 2 - erfc(y)$$

Fourier series calculation uses 20 terms in the calculations. Calculations using more than 20 terms was found to make insignificant contribution to the overall solution and therefore the Fourier series calculation was limited to 20 terms.

Integration function for the saturated zone calculations was coded using a VBA macro that runs in the background during a simulation. The macro uses trapezoidal rule to approximate integration. The number of steps in which the function is discretized depends on the time variables specified by the user. Number of steps is calculated by dividing the maximum time by the time step size.

The analytical solution is also implemented in the package ATRANS (Neville, 2005). Although the solutions are implemented in Fortran codes, the ATRANS package has a straightforward graphical user interface, ATRANSlive, [http://www.sspa.com/atranslive/\(S\(qpuloyuqnajwom45glpwape4\)\)/Default.aspx](http://www.sspa.com/atranslive/(S(qpuloyuqnajwom45glpwape4))/Default.aspx).

S.S. Papadopoulos & Associates, Inc. has also implemented within Excel a solution that is a special case of the solution presented here. The solution is for an aquifer that is infinitely thick and is implemented in the code BIOSCREEN-AT. The BIOSCREEN-AT code provides an exact solution that complements the popular screening tool BIOSCREEN (Karanovic and others, 2007). The BIOSCREEN-AT package is available at <http://www.sspa.com/Software/bioscreen.shtml>.

Appendix D

Implementation in Excel

Calculations and analytical solution as detailed in Appendices A through C were implemented in MS Excel 2007 using standard formulae available in Excel. For integration calculations required for transport calculations in saturated zone a VBA macro was written. The implementation has been tested with the latest available version of Excel, Excel 2016.

The source concentration is calculated in the spreadsheet “InputParameters_Vadose” and all other calculations are performed in the spreadsheet “Calculations”. Intermediate variables and coefficients are calculated in column “E” of the “Calculations” spreadsheet, vadose zone calculations are broken up in columns “H” through “O” and columns “BD” through “BL”, and saturated zone calculations are performed in the macro and intermediate calculated terms are written in columns “T” through “Y”. Calculated saturated concentrations are written to column “AE” of the “Calculations” spreadsheet. Further technical details of the implementation are provided in appropriate appendices.

Most of the Excel file is write-protected to avoid inadvertent edits. Cells that are editable in order to provide input are highlighted. Breakthrough curves provided in the worksheet “Charts” are not write-protected and may be used to customize plots. Basic error checking is performed in the cells by applying conditional formatting feature of Excel. If entered parameter values are outside of an acceptable range, for example negative water content, the cell changes to a red color indicating an error.

Integration function for the saturated zone calculations was coded using a VBA macro that runs in the background during a simulation. Given below is the relevant listing of the macro. The macro uses trapezoidal rule to approximate integration. The number of steps in which the function is discretized depends on the time variables specified by the user. Number of steps is calculated by dividing the maximum time by the time step size.

```
Sub AnalSol_01()  
    'Declare variables  
    Dim N As Integer, OrigTotim As Double, totim As Double, delT As Double  
    Dim B As Double, z_1 As Double, z_2 As Double, D_z As Double, pi As Double  
    Dim lambda As Double, x As Double, y As Double, y0 As Double, v As Double, Dx  
    As Double, Dy As Double  
    Dim t_tau1 As Double, t_ti1 As Double, zv As Double, D2 As Double, V2 As  
    Double, Lam2 As Double  
    Dim Csource(1 To 30000) As Double, Tsource(1 To 30000) As Double, expv(1 To  
    30000) As Double  
    Dim Csource2(1 To 30000) As Double  
    Dim term3 As Double, term4 As Double  
    Dim Nv As Integer, gamma As Double  
    Dim t_tau As Double, t_ti As Double  
    Dim tStart As Date, tEnd As Date, tSimSec As Double  
    Dim Temp As Double, c0 As Double  
    Dim erfcDens(1 To 20000) As Double, cVadose(1 To 20000) As Double, Exp1(1 To  
    20000) As Double, Erfc1(1 To 20000) As Double, Erfc2(1 To 20000) As Double,  
    zTerm(1 To 20000) As Double
```



```

Dim coEf As Double, C3 As Double
Dim fnctn(1 To 20000) As Double
Dim y11 As Double, y22 As Double, y1 As Double, s1 As Double, erfcc As
Double, erfce As Double

tStart = Time

'For the vadose zone calculations
Calculate

'Initialize constants
zv = Worksheets("InputParameters_Vadose").Cells(15, 5)
D2 = Worksheets("Calculations").Cells(7, 5)
V2 = Worksheets("Calculations").Cells(6, 5)
Lam2 = Worksheets("Calculations").Cells(8, 5)
term3 = Worksheets("Calculations").Cells(12, 5)
term4 = Worksheets("Calculations").Cells(13, 5)
B = Worksheets("InputParameters_Saturated").Cells(4, 5)
z_1 = Worksheets("InputParameters_Saturated").Cells(9, 5)
z_2 = Worksheets("InputParameters_Saturated").Cells(10, 5)
D_z = Worksheets("calculations").Cells(27, 5)
pi = Application.WorksheetFunction.pi
lambda = Worksheets("InputParameters_Saturated").Cells(25, 5)
y0 = Worksheets("InputParameters_Saturated").Cells(5, 5)
x = Worksheets("InputParameters_Saturated").Cells(6, 5)
y = Worksheets("InputParameters_Saturated").Cells(7, 5)
v = Worksheets("Calculations").Cells(28, 5)
Dx = Worksheets("Calculations").Cells(25, 5)
Dy = Worksheets("Calculations").Cells(26, 5)
coEf = Worksheets("Calculations").Cells(30, 5)

Worksheets("Calculations").Range("T4:AE30006").Clear
Worksheets("Calculations").Range("p4:p30006").Clear
Application.Calculation = xlCalculationManual
totim = Worksheets("InputParameters_Vadose").Cells(27, 5)
delT = Worksheets("InputParameters_Vadose").Cells(28, 5)
N = totim / delT 'Number of time-steps
Application.ScreenUpdating = False
'Worksheets("Calculations").Activate

If (Worksheets("InputParameters_Vadose").Cells(32, 5) = 4 Or _
    ((Worksheets("InputParameters_Vadose").Cells(40, 5) = 1) And _
    ((Worksheets("InputParameters_Vadose").Cells(32, 5) = 2) Or _
    (Worksheets("InputParameters_Vadose").Cells(32, 5) = 3)))) Then
    If (Worksheets("InputParameters_Vadose").Cells(32, 5) = 4) Then
        Nv = Worksheets("InputParameters_Vadose").Cells(32, 8)
        If (Nv <= 0) Then
            MsgBox "Set number of points in cell H32 >= 1"
        End If
    End If
    For i = 1 To Nv
        Tsource(i) = Worksheets("InputParameters_Vadose").Cells(33 + i, 7)
        Csource2(i) = Worksheets("InputParameters_Vadose").Cells(33 + i, 8)
    Next i
ElseIf (Worksheets("InputParameters_Vadose").Cells(40, 5) = 1) Then
    If (Worksheets("InputParameters_Vadose").Cells(32, 5) = 2) Then
        gamma = Worksheets("InputParameters_Vadose").Cells(35, 5)
    ElseIf (Worksheets("InputParameters_Vadose").Cells(32, 5) = 3) Then
        gamma = Worksheets("InputParameters_Vadose").Cells(37, 5)
    Else
        MsgBox "Logic failed. Simulation terminated."
    End If
End If

```

```

        c0 = Worksheets("InputParameters_Vadose").Cells(11, 5)
    Else
        MsgBox "Logic failed. Simulation terminated."
    End
End If
iL = 1
For i = 1 To N
    t_tau = i * delT
    'interpolate source conc from time series provided
    If (Worksheets("InputParameters_Vadose").Cells(32, 5) = 4) Then
        If (t_tau <= Tsource(1)) Then
            Csource(i) = Csource2(1)
        ElseIf (t_tau >= Tsource(Nv)) Then
            Csource(i) = Csource2(Nv)
        Else
            For isrc = iL To (Nv - 1)
                If (t_tau > Tsource(isrc) And t_tau <= Tsource(isrc + 1)) Then
                    Csource(i) = ((Csource2(isrc + 1) - Csource2(isrc)) * (t_tau - Tsource(isrc)) / (Tsource(isrc + 1) - Tsource(isrc))) + Csource2(isrc)
                    iL = isrc
                    Exit For
                End If
            Next isrc
        End If
    Else
        Csource(i) = c0 * Exp(-t_tau * gamma)
    End If
    expv(i) = Exp(-(V2 * V2 / (4 * D2)) + Lam2 * (t_tau)) - ((zv * zv) / (4 * D2 * t_tau)))
Next i

For k = 1 To N 'Loop through time-steps 1 to N
    For i = 1 To k ' k*delT is the current time
        fnctn(i) = 0 'Initialize integral term
        t_tau = i * delT
        t_ti = k - i
        If t_ti = 0 Then
            c0 = 0
        Else
            c0 = Csource(t_ti)
        End If
        fnctn(i) = (c0 / (t_tau ^ 1.5)) * expv(i)
    Next i
    integral = 0
    ' fnctn(1) = 0
    For i = 2 To k
        integral = integral + 0.5 * (fnctn(i) + fnctn(i - 1)) * delT
    Next i
    c2 = integral * Exp(term3) * term4 / Application.WorksheetFunction.SqrtPi(1)
    Worksheets("Calculations").Cells((k + 3), 16) = c2
Next k
Calculate
End If
For i = 1 To N
    cVadose(i) = Worksheets("calculations").Cells(i + 3, 15)
    't_tau = Worksheets("calculations").Cells(i + 3, 18)
    't_tau_pk = i * delT
    'diff_pk = diff_pk + Abs(t_tau - t_tau_pk)
    t_tau = i * delT
    'EXP1 term
    Exp1(i) = Exp((-lambda * t_tau) - ((x - v * t_tau) ^ 2 / (4 * Dx * t_tau)))

```

```

Worksheets("Calculations").Cells(i + 3, 20) = Expl(i)
'erfc denominator term
erfcDens(i) = 2 * ((Dy * t_tau) ^ 0.5)
Worksheets("Calculations").Cells(i + 3, 21) = erfcDens(i)
'erf term in column V
y11 = (y - y0) / erfcDens(i)
y1 = Abs(y11)
s1 = Application.WorksheetFunction.Min(1, (1 - 1 / (2 * y1 * y1)))
erfcc = (Exp(-(y1 * y1)) * s1) / (y1 *
Application.WorksheetFunction.SqrtPi(1))
erfce = Application.WorksheetFunction.ErfC(y1)
If (y11 < 0) Then
    erfcc = 2 - erfcc
    erfce = 2 - erfce
End If
If (y1 > 3.4) Then
    Erfc1(i) = erfcc
Else
    Erfc1(i) = erfce
End If
Worksheets("Calculations").Cells(i + 3, 22) = Erfc1(i)
'erfc term in column W
y22 = (y + y0) / erfcDens(i)
y1 = Abs(y22)
s1 = Application.WorksheetFunction.Min(1, (1 - 1 / (2 * y1 * y1)))
erfcc = (Exp(-(y1 * y1)) * s1) / (y1 *
Application.WorksheetFunction.SqrtPi(1))
erfce = Application.WorksheetFunction.ErfC(y1)
If (y22 < 0) Then
    erfcc = 2 - erfcc
    erfce = 2 - erfce
End If
If (y1 > 3.4) Then
    Erfc2(i) = erfcc
Else
    Erfc2(i) = erfce
End If
Worksheets("Calculations").Cells(i + 3, 23) = Erfc2(i)
'Summation term
Temp = 0
For j = 1 To 20 '20 parts
    Temp = Temp +
        (Sin(j * pi * z_2 / B) - Sin(j * pi * z_1 / B)) * Cos(j * pi * Z / B)
* Exp(-D_z * j * j * pi * pi * t_tau / (B * B)) / j
Next j
'Zterm
zTerm(i) = (z_2 - z_1) + 2 * B * Temp / pi
Worksheets("Calculations").Cells(i + 3, 25) = zTerm(i)
Next i
integral = 0
fnctn(1) = 0
For i = 2 To k
    integral = integral + 0.5 * (fnctn(i) + fnctn(i - 1)) * delT
Next i
'-----LOOP THROUGH ALL THE TIME-STEPS TO DO SATURATED ZONE TRANSPORT
CALCULATIONS-----
For k = 1 To N 'Loop through time-steps 1 to N
    For i = 1 To k ' k*delT is the current time
        fnctn(i) = 0 'Initialize integral term
        't_tau = Worksheets("calculations").Cells(i + 3, 18)
        t_tau = i * delT
        t_ti = k - i 'Worksheets("Calculations").Cells(i + 3, 19)
    
```

```

        'Lookup vadose zone conc c0
        'c0 = Application.WorksheetFunction.VLookup(t_ti, Range("H3:O10006"), 8,
False)
        If t_ti = 0 Then
            c0 = 0
        Else
            c0 = cVadose(t_ti)
        End If
        fnctn(i) = (c0 / (t_tau ^ 1.5)) * Exp1(i) * (Erfc1(i) - Erfc2(i)) *
zTerm(i)
        Next i

        integral = 0
        fnctn(1) = 0
        For i = 2 To k
            integral = integral + 0.5 * (fnctn(i) + fnctn(i - 1)) * delT
        Next i
        C3 = integral * coEf
        'Sat zone conc at well
        Worksheets("Calculations").Cells((k + 3), 31) = C3
    Next k
End Sub

```

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