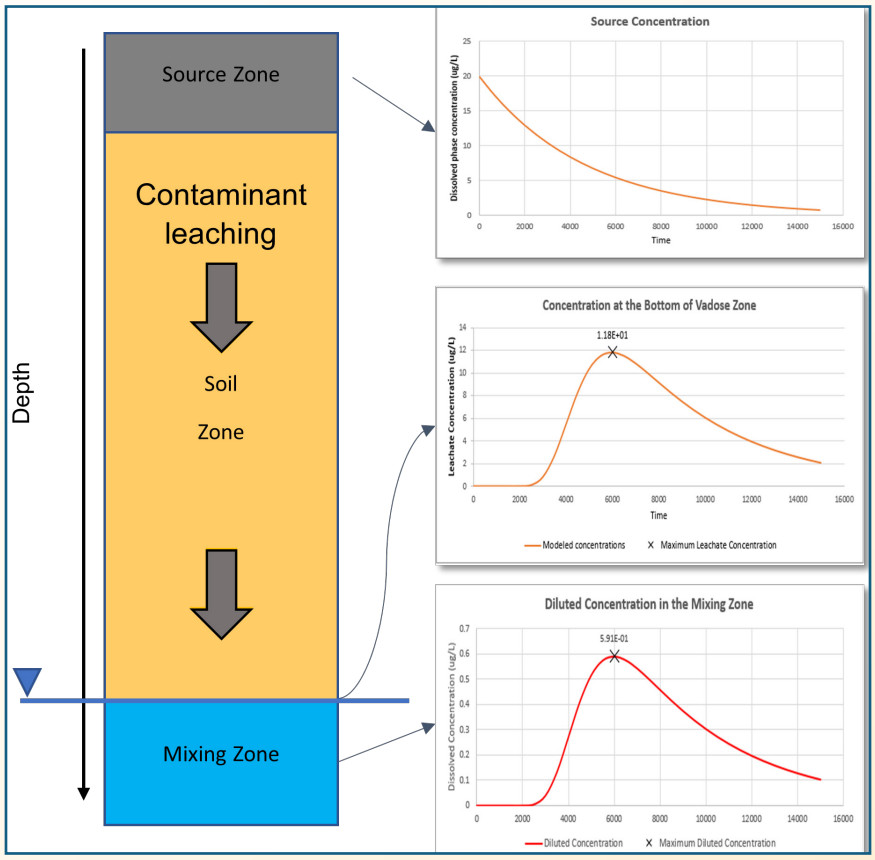
SOIL INFILTRATION AND LEACHING TOOL (SILT)



USER GUIDE

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INTRODUCTION

- The Soil Infiltration and Leaching Tool (SILT) is a Microsoft Excel-based spreadsheet tool that allows users to simulate one-dimensional contaminant fate and transport processes in a simple, user-friendly, and efficient manner
- The mathematical theory and conceptual methodology utilized in SILT follows the approach applied in the *SSM* package developed by V. Bedekar *et al*. (2012)

SOFTWARE USE

- The user can specify fate and transport parameters for the contaminant of concern in the soil source zone before it leaches to the vadose zone (See **Step 1 – Source Zone**) and as it is transported through the vadose zone (See **Step 2 – Vadose Zone**)
- The model utilizes both analytical and semi-analytical methods to solve the Convection-Dispersion Equation (CDE) with reactions to model leachate concentrations out of the vadose zone
- Dilute leachate concentrations in the mixing zone directly beneath the vadose zone can be calculated by selecting or calculating one of four built-in Dilution Attenuation Factors (See **Step 3 – Mixing Zone**)
- Model output from SILT is multi-faceted. Leachate concentrations can be used to evaluate loss processes in the vadose zone, as a screening level comparison against published groundwater standards, or as the *source term* for a groundwater contaminant plume model, such as *TS-CHEM* (See **Step 4 – Plume Model Source Steps**)
- The spreadsheet is distributed with empty, unpopulated model input parameter cells. There are no default values assigned to the cells, however:
  - The user may click the ***Sanders 1995 Example Model*** button on the *1 SourceZone* Tab to automatically populate the necessary model input parameter cells for an example model from the literature that simulates leachate breakthrough for Trichloroethylene (TCE). This allows the user to quickly see how the spreadsheet tool is set up, and how it functions
  - Any SILT workbook may be saved with a different name after a model run has been completed to preserve the model input parameters and model outputs (i.e. Save As -> "SILT TCE.xlsm")
  - SILT implements a *unit conversion* feature. The user may enter a variety of commonly used units for most input parameters, which are converted to the units needed by the model *before running model calculations*. This feature prevents unnecessary confusion related to units and ensures model output is consistent and accurate, while also allowing greater flexibility for the user
- In-depth explanations of the procedures and parameters utilized in SILT are provided in the step-by-step guide included later in this User Guide

SYSTEM REQUIREMENTS

- **Microsoft Office Excel**

  SILT is a Macro-Enabled Microsoft Excel Workbook (".xlsm") and was developed in Microsoft Excel 365. It is compatible with previous versions of Microsoft Excel (2016, 2013, 2010, 2007).

- Operating System
  - **Windows**
    - **Windows 10**
    - **Windows 8.1**
    - **Windows 7**
  - **Mac OS**
    - **macOS 13**
    - **macOS 12**
    - **macOS 11**
    - **macOS 10**

ACTIVATING THE SPREADSHEET

Many of the processes in the SILT spreadsheet tool are controlled by macros written in the Visual Basic for Applications (VBA) coding language. The following two steps ***must be taken*** to make SILT into a Microsoft trusted document before attempting to use it.

[**NOTE:** The macros contained within SILT do not affect your computer's system files in any away.]

1. UNBLOCK THE MACRO-ENABLED WORKBOOK

By default, macro-enabled excel workbooks (".xlsm") that are downloaded from the internet have their macros blocked and they will not activate until the following instructions are followed:

1. Navigate to the location on the computer where the SILT.xlsm workbook is located
2. Right-click on the SILT.xlsm file
3. Select *Properties* from the pop-up menu
4. Navigate to the bottom of the General Tab in the pop-up window
5. Check the "Unblock" box next to the Security section
6. Click Apply then OK to close the pop-up window

[**NOTE:** This will only need to be done once per *SILT download*. After the user unblocks the SILT workbook they downloaded from the SILT webpage, they will not need to unblock that SILT workbook again *unless they re-download SILT from the SILT webpage*)

The user may refer to https://learn.microsoft.com/en-us/deployoffice/security/internet-macros-blocked for further information.

2. ENABLE THE MACROS IN THE WORKBOOK

Upon opening SILT, the user will be prompted with a yellow message at the top of the screen that will tell the user that macros have been disabled as a security measure. Click the *Enable Content* button that appears beside this warning. This will activate the macros needed for SILT to function.

The user may refer to https://support.microsoft.com/en-us/office/enable-or-disable-macros-in-microsoft-365-files-12b036fd-d140-4e74-b45e-16fed1a7e5c6 for further information.

MODEL LIMITATIONS AND ASSUMPTIONS

- The analytical solutions used in the SILT spreadsheet are strictly one-dimensional. It does not simulate two- or three-dimensional flow and transport processes
- Air partitioning is limited to *only* the source zone to calculate the dissolved contaminant concentration before transportation through the vadose zone. The model does not consider the soil air phase in the vadose zone
- SILT allows for a maximum of 20,000 time steps between 0 and Tmax (See Step 1 – Source Zone). Any number higher than this will result in an error window appearing
- Air and water content parameters (θ_a and θ_w) are assumed to be decimal percentages ranging from 0 to 1. If the user inputs a value greater than 1, an error message will appear
- Water content is assumed to be constant throughout the entire vadose zone and is independent of depth; it is also independent of time and represents the average value over the period of the simulation
- SILT assumes instantaneous and reversible partitioning for the solid and air phases (in the Source Zone) and for the solid phase (in the Vadose Zone)
- SILT assumes first-order source decay rates. Certain conditions apply when providing or calculating source decay rates (See Step 1 – Source Zone)
- First-order reaction rates for the soil and water phases are assumed to be independent (See Step 2 – Vadose Zone)
- All dissolved contaminant concentrations utilized in SILT are in micrograms per liter (µg/L) since those units are commonly utilized in environmental applications
- Source step concentrations are linearly interpolated between the user-selected times
- Microsoft Excel cannot solve the transport equation for conditions in which the argument passed to the EXP() function is greater than 709. In cases where the dispersivity of the vadose zone is very low and/or the vadose zone is very thick, internal calculations may encounter a number too large for Microsoft Excel to use. If those conditions occur, an error message will appear to notify the user when they attempt to calculate the soil leachate concentration
- Molecular diffusion is not considered in the Convection-Dispersion Equation model used in SILT
- Vadose and saturated zone (mixing zone) properties are assumed to be homogeneous in the individual domains
- Flow is steady in the vadose zone and mixing zone

MODEL OVERVIEW

Vadose Zone Transport Conceptual Model

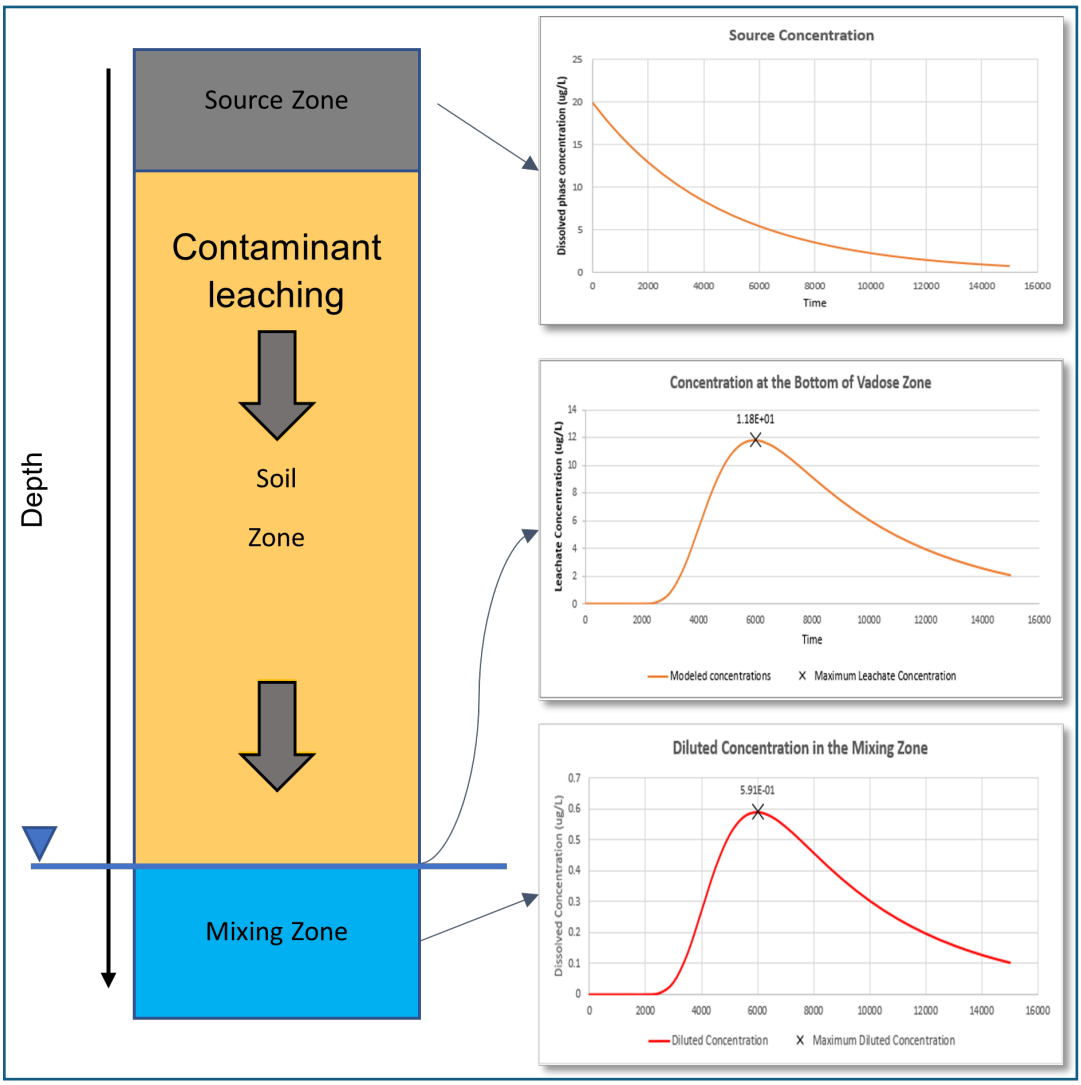


Figure 1: *Vadose Zone Transport Conceptual Model for SILT. The SILT spreadsheet tool models solute/contaminant transport from a source zone through the unsaturated soil zone down to a mixing zone contained within the saturated zone (aquifer). The concentration and travel time of the leachate will change as a function of physical and chemical processes that are occurring within all three of these zones.*

CONTAMINANT FATE AND TRANSPORT THROUGH THE VADOSE ZONE

SILT simulates contaminant transport through the vadose zone in 2 general steps:

1. The initial source zone water concentration, located in the Source Zone (of user-specified vertical thickness), is calculated after partitioning of the user-specified Source Zone Total Soil Concentration among the solid-, air- and dissolved phases
2. The dissolved phase contaminant source is transported vertically downward through the Vadose Zone, being acted upon by dispersion and degradation processes, until it reaches the groundwater table, producing a leachate breakthrough curve

Groundwater Source Term Conceptual Model

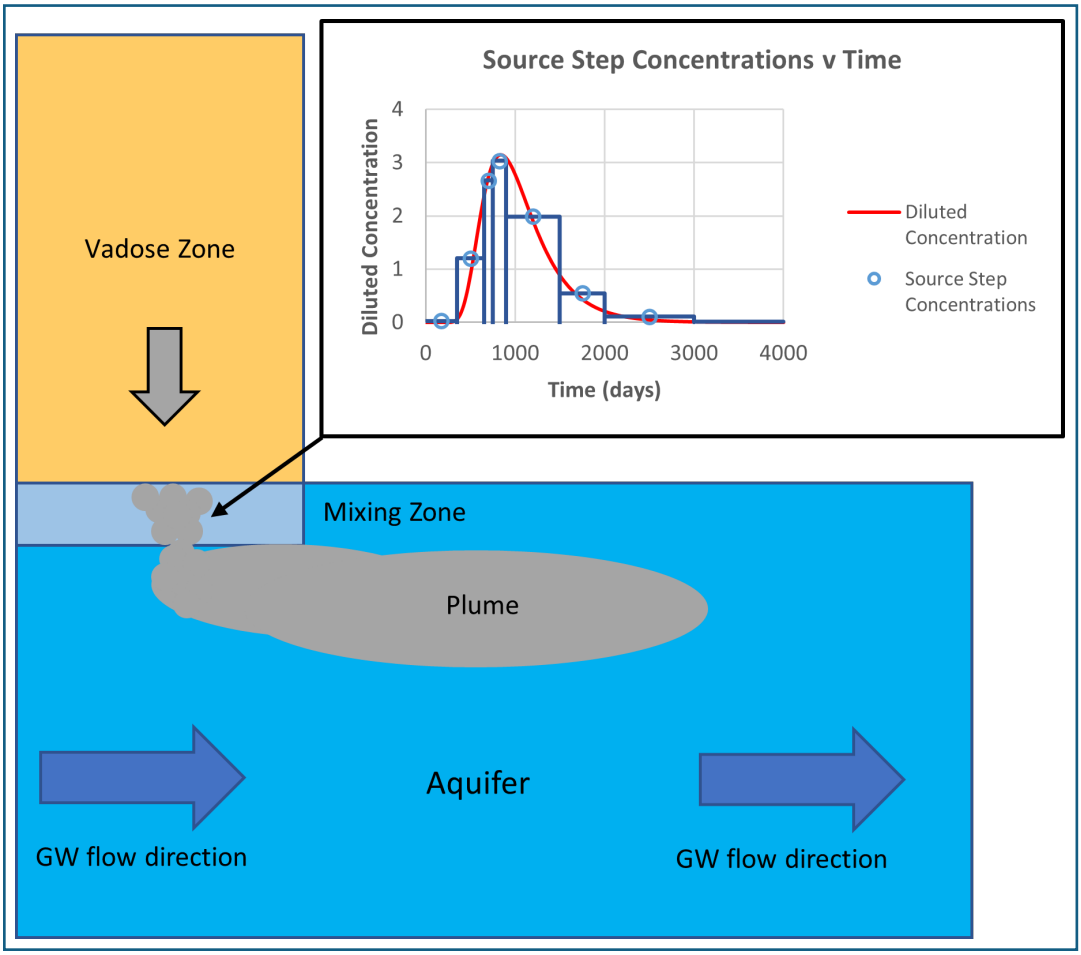


Figure 2: *Groundwater Source Term Conceptual Model for SILT. The SILT spreadsheet tool allows the user to calculate discrete source term concentrations to pair with analytical groundwater plume transport models. The user will take the diluted concentration time series calculated by one of the four Dilution Attenuation Factor options and then discretize it into a user-specified number of source step concentrations.*

CONTAMINANT CONCENTRATION IN THE GROUNDWATER MIXING ZONE

At the bottom of the vadose zone, leachate (at the calculated flux rate and concentration) is delivered to a mixing zone at the top of the water table. When the infiltrating soil water reaches the water table, it is mixed with groundwater and the contaminant is diluted, resulting in a lower concentration. A dilution-attenuation factor (DAF) is used to account for this process (NJDEP 2008).

SILT provides the user with 4 options for specifying or computing the DAF: **(1)** user-specified, **(2)** default (USEPA default of 20); **(3)** calculated DAF using a user-specified mixing depth; or **(4)** calculated mixing depth and DAF using the method of Charbeneau (2000). For more information see Section 3.1 below.

USES OF THE MIXING ZONE CONTAMINANT CONCENTRATION

- **1. For Comparison with Published Groundwater Standards**

  As a first step, the user may compare the SILT-calculated groundwater mixing zone contaminant concentration against some relevant published groundwater standard or screening level (e.g. USEPA MCL or State promulgated groundwater quality standard). For SILT analyses in which the leachate concentration, and thus the mixing zone concentration, change with time, the maximum calculated concentration should be used for the comparison. (To facilitate this comparison, SILT displays on its charts the time and value of the maximum calculated leachate and mixing zone concentrations).

  For a higher-level analysis of potential soil source leaching impacts at a groundwater downgradient location of interest (site property boundary, point of compliance, or receptor point of exposure), the SILT mixing zone contaminant concentration history can be applied as the source of a contaminant plume transport model, as described in the following section.

- **2. Using Leachate Concentrations as a Source Term for Groundwater Plume Models**

  After the leachate concentration has been reduced in the groundwater mixing zone by applying a user specified DAF (See Step 3 – Mixing Zone), the user may apply the mixing zone concentration through time as the source term concentration for a groundwater plume transport (advection-dispersion) computer model. For simple analyses, analytical plume models like BIOSCREEN, ATRANS or TS-CHEM may be used, although the SILT-generated source term could also be applied in numerical groundwater fate and transport models like MODFLOW-MT3D, MODFLOW-SURFACT, FEFLOW and others. The resulting groundwater plume model can then be used to address a variety of environmental applications including Classification Exception Areas (CEAs), Natural Resource Damages (NRD) cases, commingled plume analyses, remedial system design and evaluation, among others.

  The concentration versus time source term may be generated and exported from SILT in two ways. For the entire groundwater source zone (mixing zone) concentration history, the mixing zone concentration at each SILT calculation time (up to 20,000 output times) may be copied from the Chart Data tab. A simpler representation of the source concentration as 5 or 10 concentration steps can be easily calculated and displayed using SILT's built-in capability. Once the proper user-specified step start and end times have been input to create a good match to the mixing zone concentration history, those step data (start time, end time, and concentration) can be exported for use in an analytical model like ATRANS4 or TS-CHEM that can easily represent time-varying sources by analytical superposition.

Parameter Input Cells

SILT was developed to allow for user-friendly model construction. As such, SILT utilizes a simple and intuitive method for ensuring that the user knows where to enter model input parameters. All worksheets in SILT follow the same rule for inputting data into cells: ***the user interacts with blue cells and ignores white cells***. An example of one of the parameter input sections in SILT is shown below:

			Input Values
Source Concentration			
Water content	[-]	θ_{w_src}	0.20
Air content	[-]	θ_a	0.20
Density of water	kg/m^3	ρ_{w_src}	1000.00
Soil bulk density	kg/m^3	ρ_{b_src}	1300.00
Soil-water partitioning coeff	m^3/kg	K_{d_src}	1.00E-04
Henry's law partitioning coeff	[-]	k_H	0.37
Soil Concentration	kg/kg	C_{soil}	2.50E-07
Infiltration rate	m/d	I	0.0015
Initial Concentration in Source Zone Water	ug/L	C_0	806.45
Parameter Name	Units	Symbol	Input Value

Note the white cell for the parameter *Initial Concentration in Source Zone Water*. This cell contains an Excel formula that utilizes the parameters provided by the user in the blue cells above. There are multiple cells within SILT that are populated with Excel formulas. These cells will always be white, like the above example, and are protected to prevent unintentional modifications of the formulas within the cells.

Unit Conversion Feature

The parameters used in the fate and transport models incorporated into SILT are locked to specific units to ensure internal consistency and accuracy. Those units are shown in the second column, located to the right of the column containing parameter names. While these units work well mathematically, some of them are not often used in common practice and may be difficult to relate to real-world applications. SILT's built-in unit conversion feature grants the user flexibility in how they enter model parameters, while also preventing unnecessary confusion related to units. An example of the unit conversion feature is shown below:

			Input Values	Common Units		Common Units		Common Units	
Source Concentration				Value	Units	Value	Units		
Water content	[-]	θ_{w_src}	0.20						
Air content	[-]	θ_a	0.20						
Density of water	kg/m^3	ρ_{w_src}		1.00	g/cm^3		lb/ft^3		
Soil bulk density	kg/m^3	ρ_{b_src}		1.30	g/cm^3		lb/ft^3		
Soil-water partitioning coeff	m^3/kg	K_{d_src}	1.00E-04		ml/g		L/kg		
Henry's law partitioning coeff	[-]	k_H	0.37						
Soil Concentration	kg/kg	C_{soil}	2.50E-07		mg/kg		ug/kg		
Infiltration rate	m/d	I		21.00	in/yr		cm/yr		mm/yr

The SILT unit conversion feature allows the user to input values for parameters in up to three commonly used units. See below for a zoomed in version:

		Input Values	Common Units		Common Units		Common Units	
entration			Value	Units	Value	Units		
[-]	θ_{w_src}	0.20						
[-]	θ_a	0.20						
kg/m^3	ρ_{w_src}		1.00	g/cm^3		lb/ft^3		
kg/m^3	ρ_{b_src}		1.30	g/cm^3		lb/ft^3		
m^3/kg	K_{d_src}	1.00E-04		ml/g		L/kg		
[-]	k_H	0.37						
kg/kg	C_{soil}	2.50E-07		mg/kg		ug/kg		
m/d	I		21.00	in/yr		cm/yr		mm/yr

In this example, the user has entered values into SILT in the units shown to the left of the parameter symbol for all parameters except density of water, soil bulk density, and infiltration rate. The user has decided to use the unit conversion feature for those parameters and has entered data in common units. After the user clicked the "Calculate" button located on the worksheet, the unit conversion took place and a "Converted" flag appeared in blue next to the parameters that were converted:

		Input Values	Common Units		Common Units		Common Units		
entration			Value	Units	Value	Units			
[-]	θ_{w_src}	0.20							
[-]	θ_a	0.20							
kg/m^3	ρ_{w_src}	1000.00	1.00	g/cm^3		lb/ft^3			Converted
kg/m^3	ρ_{b_src}	1300.00	1.30	g/cm^3		lb/ft^3			Converted
m^3/kg	K_{d_src}	1.00E-04		ml/g		L/kg			
[-]	k_H	0.37							
kg/kg	C_{soil}	2.50E-07		mg/kg		ug/kg			
m/d	I	0.0015	21.00	in/yr		cm/yr		mm/yr	Converted

Note how the *Input Values* column is no longer empty in the three rows representing the converted parameters. They have now been populated with values that are in the correct units needed for the model.

STEP 1 – SOURCE ZONE

Worksheet Layout

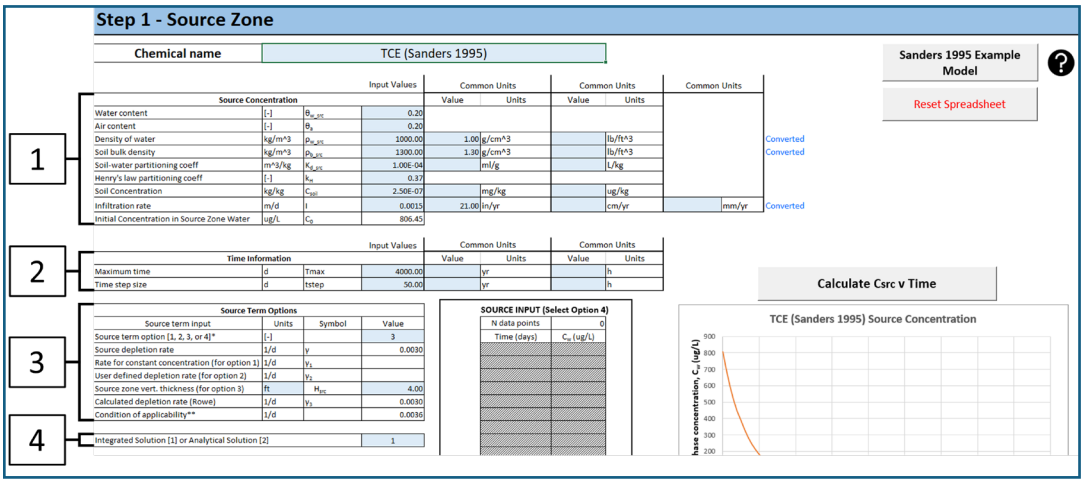


Figure 3: *Worksheet layout for the* 1 SourceZone *Tab. The components on this tab will be utilized by the user to perform all necessary functions for Step 1 of the SILT spreadsheet: the source zone.*

[**NOTE:** For the purposes of this User Guide, the Sanders (1995) Example Model – available in SILT by clicking on the "Sanders 1995 Example" button on the 1 Source Zone tab – will be utilized to show an example of the Tab layouts populated with model input parameters and model outputs]

The *1 SourceZone* Tab contains the model inputs and outputs related to the contaminant source zone. This section will cover the components of this worksheet. The worksheet is organized into four main components:

1. Source Concentration
2. Time Information
3. Source Term Options
4. Solution Options

The following section will briefly discuss the model input parameters required for each of these sections. A more detailed discussion of the mathematical theory and concepts related to the Source Zone calculations can be found in Appendix A.

1.1 SOURCE ZONE INPUT

1.1.1 Source Concentration

			Input Values
Source Concentration			
Water content	[-]	θ_{w_src}	0.20
Air content	[-]	θ_a	0.20
Density of water	kg/m^3	ρ_{w_src}	1000.00
Soil bulk density	kg/m^3	ρ_{b_src}	1300.00
Soil-water partitioning coeff	m^3/kg	K_{d_src}	1.00E-04
Henry's law partitioning coeff	[-]	k_H	0.37
Soil Concentration	kg/kg	C_{soil}	2.50E-07
Infiltration rate	m/d	I	0.0015
Initial Concentration in Source Zone Water	ug/L	C_0	806.45

Water content: The average volume (throughout the source zone and averaged over time) of water per total volume of soil or porous media in the source zone. Values are entered as decimal values between 0 and 1. A value of 1 indicates that the soil is completely saturated.

Air content: The volume of air per total volume of soil or porous media in the source zone. Values are entered as decimal values between 0 and 1. A value of 1 indicates that the soil is completely unsaturated.

Density of water: Mass of water per unit volume of water. This value is typically set to 1000 kg/m^3.

Soil bulk density: The mass of solids per total volume of soil or porous media in the source zone.

Soil-water partitioning coefficient (or soil adsorption coefficient): Coefficient that quantifies contaminant adsorption to the solid phase.

Henry's Law partitioning coefficient: Coefficient used to quantify contaminant partitioning to the air phase.

Soil Concentration: The total mass of contaminant per mass of solids.

Infiltration rate: Velocity of vertical flow through the source zone and vadose zone.

Initial Concentration in Source Zone Water: The initial dissolved contaminant concentration after air- and solid-phase partitioning (*See* Appendix A).

1.1.2. Time Information

			Input Values
Time Information			
Maximum time	d	Tmax	4000.00
Time step size	d	tstep	50.00

Maximum time: The last time step where the model will calculate source and leachate concentrations.

Time step size: The value used to discretize the source and leachate concentration time series from t = 0 to t = Tmax. The total number of time steps is defined as Tmax/tstep, and modeled concentrations will be output at each time step.

1.1.3. Source Term Options

Source Term Options			
Source term input	Units	Symbol	Value
Source term option [1, 2, 3, or 4]*	[-]		3
Source depletion rate	1/d	γ	0.0030
Rate for constant concentration (for option 1)	1/d	γ_1	
User defined depletion rate (for option 2)	1/d	γ_2	
Source zone vert. thickness (for option 3)	ft	H_{src}	4.00
Calculated depletion rate (Rowe)	1/d	γ_3	0.0030
Condition of applicability**	1/d		0.0036

Source term option: The user selects a number from 1 – 4 in the drop-down menu to identify which of the four source options they would like to use to represent the source in the Source Zone. Each of the methods below are explained in more detail in Appendix A:

1. Constant Source
2. First-order decaying source (User-defined depletion rate)
3. First-order decaying source (Depletion rate calculated by Rowe method)
4. Time-variable source concentration

Source depletion rate: The depletion rate for the currently selected source term option.

Rate for constant concentration (for option 1): The source depletion rate used for Option 1 – Constant Source. For a constant source the source depletion rate is always equal to zero.

User defined depletion rate (for option 2): The depletion rate entered by the user for Option 2 – First-order Decaying Source (User-defined).

Source zone vertical thickness (for option 3): The thickness of the source zone above the vadose zone. Used to calculate a depletion rate with the method introduced in Rowe (1991).

Calculated depletion rate (Rowe): The source depletion rate calculated by applying the method published by Rowe (1991) using the source zone vertical thickness and other source zone parameters (See *Appendix A*).

Condition of applicability: Calculated parameter which determines whether the user should select solution option 1 (analytical solutions) or 2 (integrated solution) when using first-order decaying sources (Source Term Options 2 and 3). The user should refer to *Appendix A* for more information on the conceptual and mathematical basis behind the condition of applicability.

1.1.4. Solution Option

Integrated Solution [1] or Analytical Solution [2]	1

The user enters either 1 or 2 into the blue cell to choose the solution method for the model. There are two options:

1. Integrated Solution
2. Analytical Solution

SILT can solve the vadose zone fate and transport model by using a semi-analytical solution (Solution Option 1), or analytical solutions (Solution Option 2). The two solution options are explained in detail in *Appendix A*.

After all parameters have been entered and a source term and solution option have been chosen, the user will need to click:

Calculate Csrc v Time

After clicking the button, SILT will run the model for the source term option selected and generate an output plot. Additionally, the output data from the plot are present on the Chart Data Tab so that the user can view the model output in a non-graphical format.

[**NOTE:** The Source Concentration v Time Chart has an Export Chart button if the user would like to save the chart locally to their computer as a .png or .jpg image file.]

1.2 SOURCE ZONE OUTPUT

1.2.1 Option 1: Constant Source Concentration

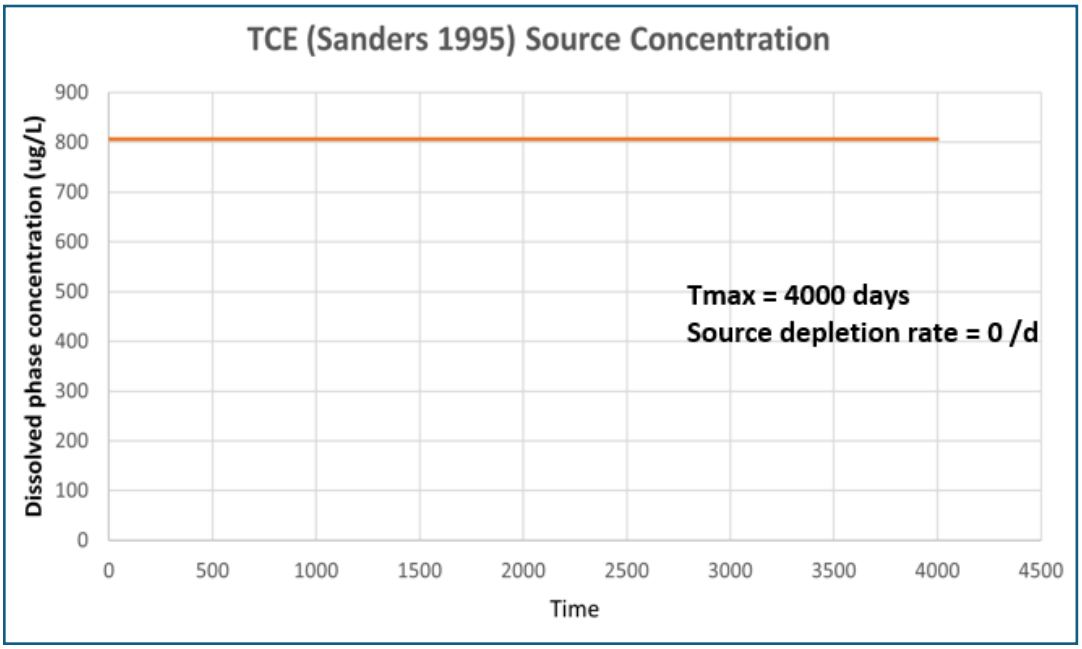


Figure 4: *Constant source term time series. This option assumes that there is no depletion in the source. The initial dissolved phase concentration (C_0) is applied for the entire duration defined by the user (t = 0 to t = Tmax).*

1.2.2 Option 2: First-order decaying source (User-defined depletion rate)

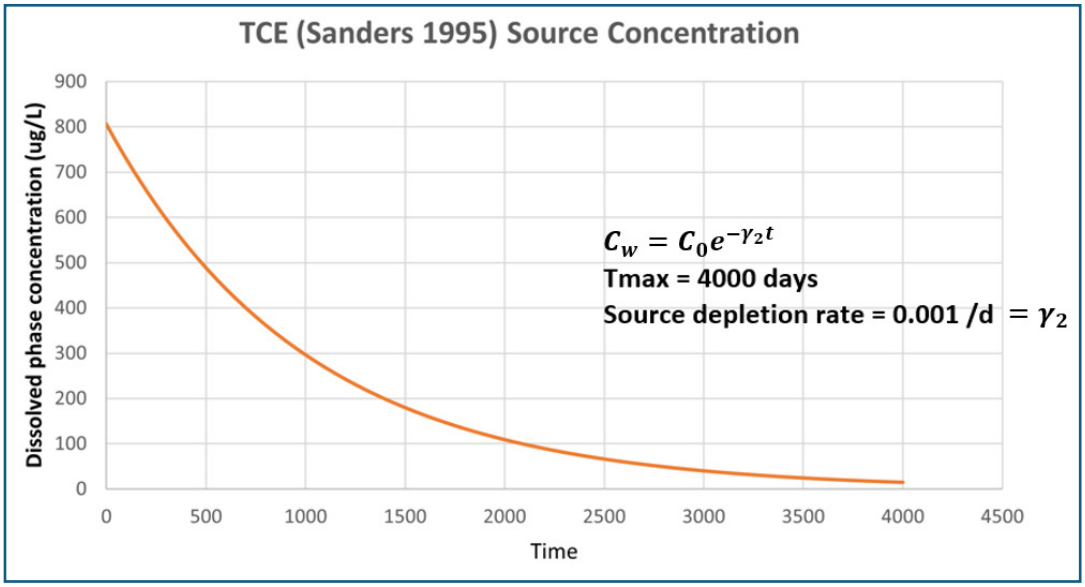


Figure 5: *First-order decay source time series with user-defined rate. The depletion rate entered by the user is represented by the term* γ_2.

1.2.3 Option 3: First-order decaying source (Depletion rate by Rowe Method)

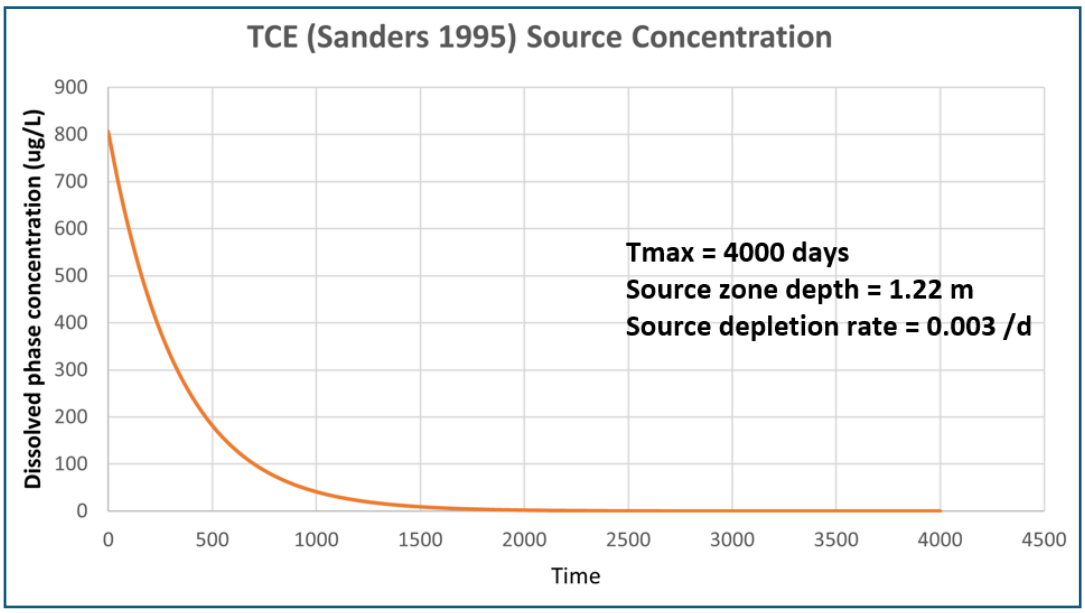


Figure 6: *First-order decay source time series with depletion rate calculated with the method of Rowe (1991). The calculated depletion rate is represented by the term* γ_3.

The source depletion rate from Rowe (1991) is calculated as follows:

$$\gamma_3 = \frac{I}{H_m}$$

Where:

γ_3 = the calculated source decay rate (1/d)

I = the infiltration rate (m/d)

H_m = the mass of the source per unit area of the source zone

Thus, H_m is defined as:

$$H_m = \frac{M_0}{C_0 H_{src}}$$

Where:

M_0 = the initial total mass of source in the source zone

C_0 = the initial dissolved concentration of the source in the source zone

H_{src} = the source zone vertical thickness

1.2.4 Option 4: Time-variable source concentration

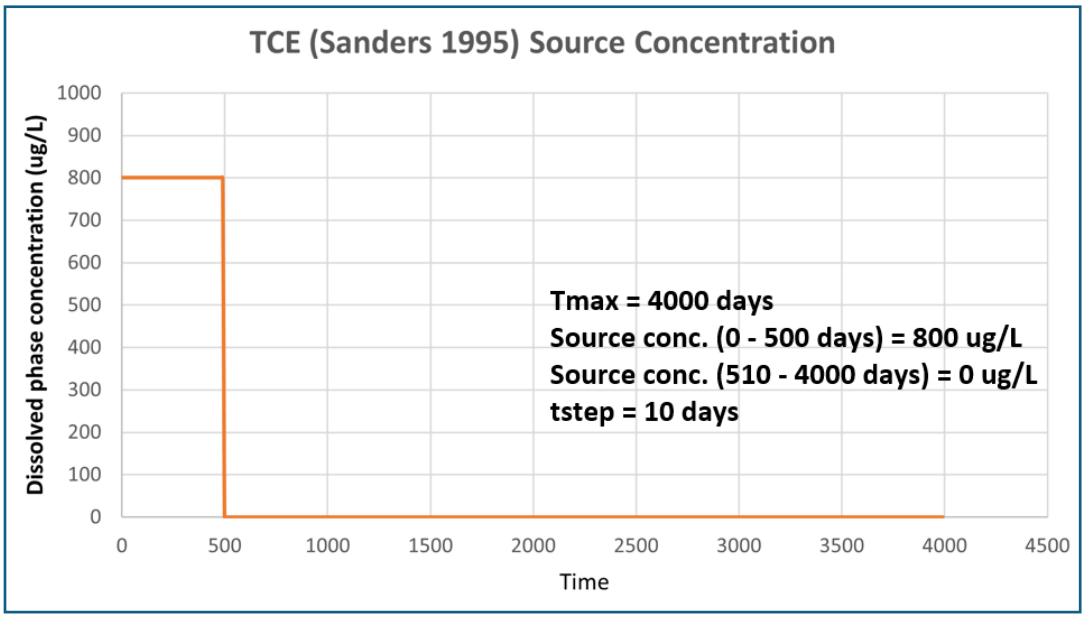
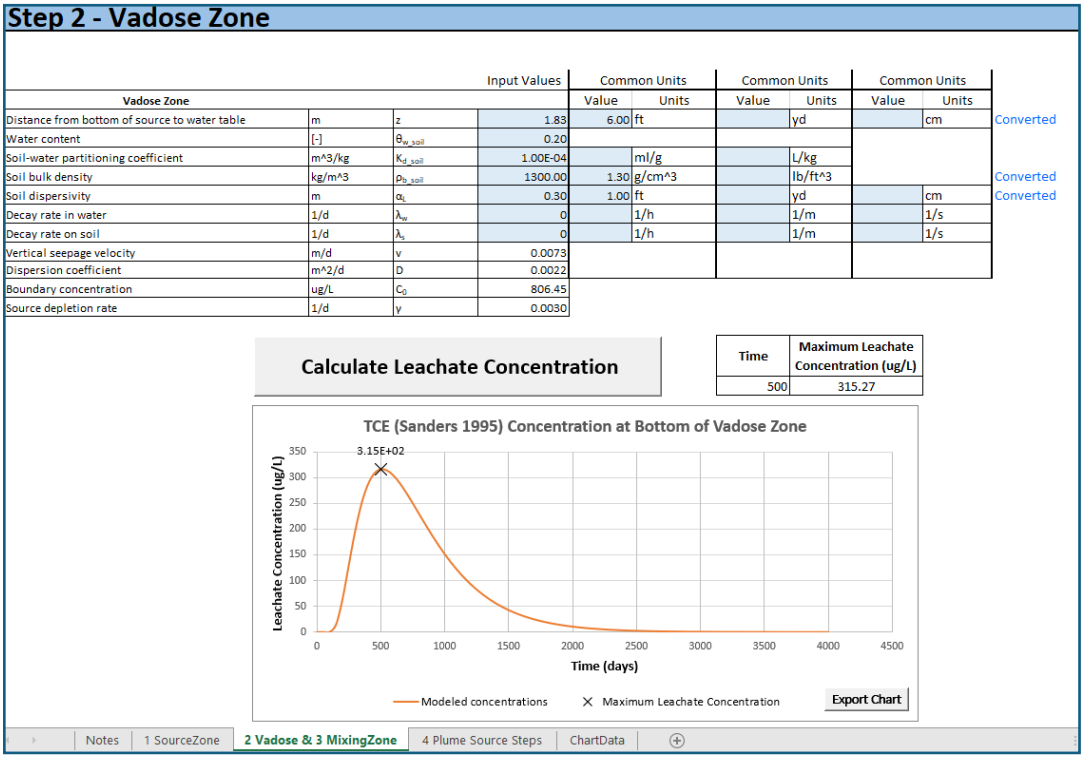


Figure 7: *Time-variable source time series with user-specified, linearly interpolated depletion rates.*

The time-variable source option allows the user to define more complex scenarios for the source. The user enters time-concentration pairs into the *Source Input (Select Option 4)* table based on concentrations measured over time or known changes in concentration, such as excavation of the source. Concentration is *linearly interpolated* between time-concentration pairs provided in the table, therefore the user should make sure that the provided time-concentration pairs have a temporal resolution high enough to account for changes in concentration (above example includes source removal after 500 days. The time parameter *tstep* was reduced from 50 days to 10 days to account for rapid reduction in source concentration).

STEP 2 – VADOSE ZONE

Worksheet Layout



Step 2 - Vadose Zone

Vadose Zone			Input Values	Common Units Value	Common Units Units	Common Units Value	Common Units Units	Common Units Value	Common Units Units	
Distance from bottom of source to water table	m	z	1.83	6.00	ft		yd		cm	Converted
Water content	[-]	θ_{w_soil}	0.20							
Soil-water partitioning coefficient	m^3/kg	K_{d_soil}	1.00E-04		ml/g		L/kg			
Soil bulk density	kg/m^3	ρ_{b_soil}	1300.00	1.30	g/cm^3		lb/ft^3			Converted
Soil dispersivity	m	α_L	0.30	1.00	ft		yd		cm	Converted
Decay rate in water	1/d	λ_w	0		1/h		1/m		1/s	
Decay rate on soil	1/d	λ_s	0		1/h		1/m		1/s	
Vertical seepage velocity	m/d	v	0.0073							
Dispersion coefficient	m^2/d	D	0.0022							
Boundary concentration	ug/L	C_0	806.45							
Source depletion rate	1/d	y	0.0030							

Calculate Leachate Concentration

Time	Maximum Leachate Concentration (ug/L)
500	315.27

Figure 8: *Worksheet layout for the* 2 Vadose & 3 MixingZone *Tab. The components on this section of the tab will be utilized by the user to perform all necessary functions for Step 2 of the SILT spreadsheet: the vadose zone.*

[**NOTE:** For the purposes of this User Guide, the Sanders (1995) Example Model will be utilized to show an example of the Tab layouts populated with model input parameters and model outputs]

The *2 Vadose & 3 MixingZone* Tab contains the model inputs and outputs related to the Vadose Zone and the Mixing Zone. This section will cover the components of the Vadose Zone portion.

The following section will briefly discuss the model input parameters required for the vadose zone model calculations. A more detailed discussion of the mathematical theory and concepts related to the Vadose Zone calculations can be found in ***Appendix A***.

2.1 VADOSE ZONE INPUT

			Input Values
Vadose Zone			
Distance from bottom of source to water table	m	z	1.83
Water content	[-]	θ_{w_soil}	0.20
Soil-water partitioning coefficient	m^3/kg	K_{d_soil}	1.00E-04
Soil bulk density	kg/m^3	ρ_{b_soil}	1300.00
Soil dispersivity	m	α_L	0.30
Decay rate in water	1/d	λ_w	0
Decay rate on soil	1/d	λ_s	0
Vertical seepage velocity	m/d	v	0.0073
Dispersion coefficient	m^2/d	D	0.0022
Boundary concentration	ug/L	C_0	806.45
Source depletion rate	1/d	γ	0.0030

Distance from bottom of source to water table: represents the total length of the vadose zone that is not part of the source zone. The source zone boundary is at the top of the vadose zone.

Water Content: The volume of water per total volume of soil or porous media in the vadose zone. Values are entered as decimal values between 0 and 1. A value of 1 indicates that the soil is completely saturated.

Soil-water partitioning coefficient (or soil adsorption coefficient): Coefficient that quantifies contaminant adsorption to the solid phase in the vadose zone.

Soil bulk density: The mass of solids per total volume of soil or porous media in the vadose zone.

Soil dispersivity: Term used to represent local variations in pore-water velocity in the direction of fluid flow in the vadose zone.

Decay rate in water: First-order transformation rate for solute in the pore water.

Decay rate on soil: First-order transformation rate for solute adsorbed to the soil.

Vertical seepage velocity: The velocity at which water seeps through the available pore-space in the vadose zone. It is calculated by dividing the infiltration rate by the average water content θ_w.

Dispersion coefficient: A coefficient that represents the hydrodynamic dispersion of the solute as it is transported through the vadose zone. It is defined as the vertical seepage velocity multiplied by the soil dispersivity.

Boundary concentration: The initial concentration of the source applied to the vadose zone upper boundary (taken from Step 1 – Source Zone).

Source depletion rate: The source depletion rate taken from Step 1 – Source Zone based on which source term option was selected by the user.

After the user has supplied all of the necessary model input parameters, click:

Calculate Leachate Concentration

After clicking the button, SILT will run the model for the vadose zone and generate an output plot showing leachate concentrations over time at the *bottom* of the vadose zone (*leachate breakthrough*). Additionally, the output data from the plot are present on the Chart Data Tab so that the user can view the model output in a non-graphical format.

2.2 VADOSE ZONE OUTPUT

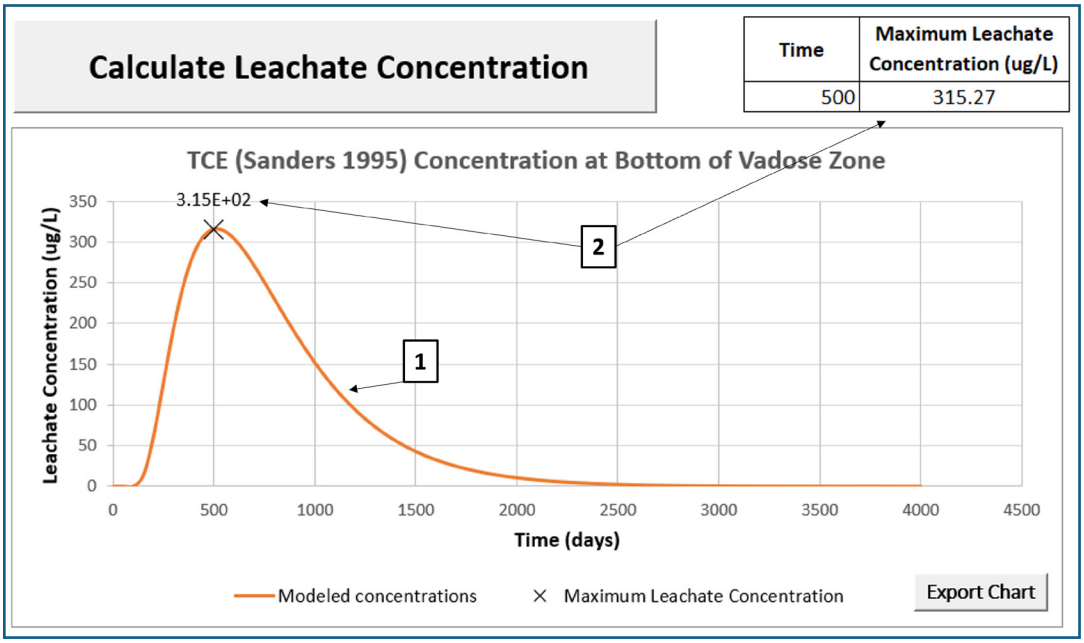
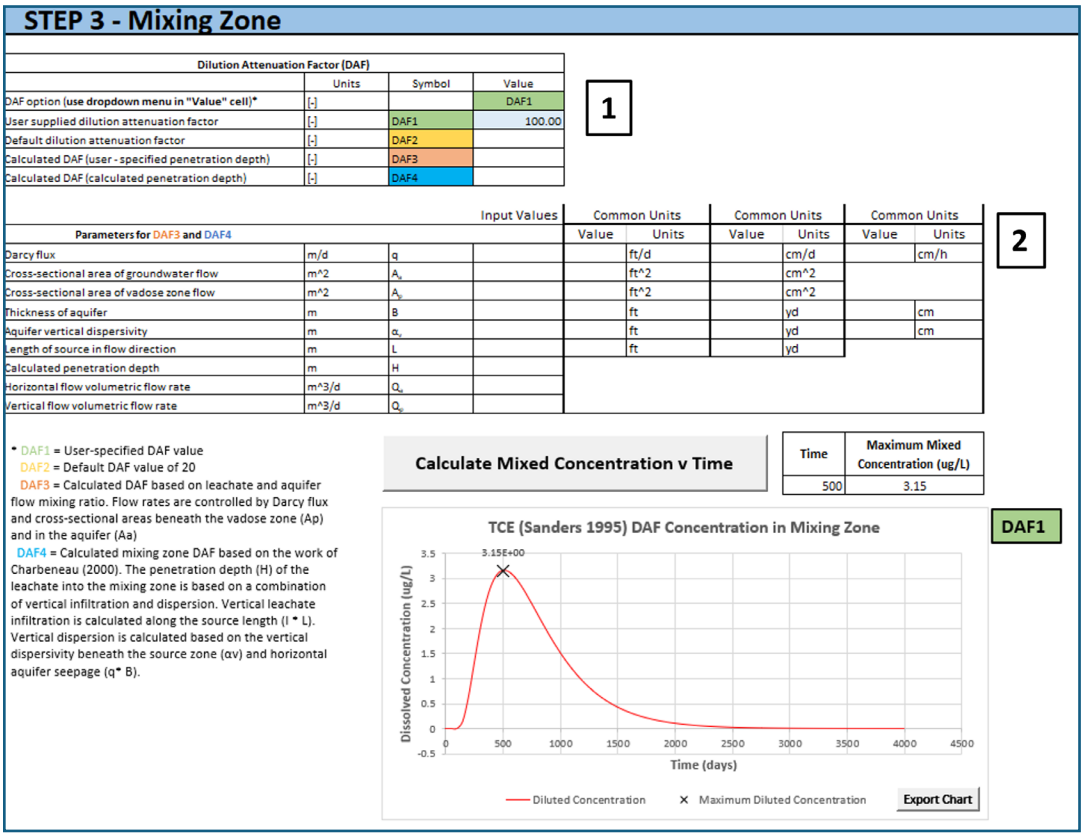


Figure 9: *Modeled contaminant concentration time series at the bottom of the vadose zone (leachate breakthrough) after completion of* Step 2 – Vadose Zone. *The leachate breakthrough time series plot will have a concentration curve that is dependent on which source source type was chosen in* Step 1 – Source Zone (1). *In addition, SILT will find the time step where the maximum leachate concentration is calculated. It will display this value at the appropriate time step in scientific notation on the plot, and also in a small table above the plot (2).*

[**NOTE:** The Concentration at the Bottom of the Vadose Zone v Time Chart has an Export Chart button if the user would like to save the chart locally to their computer as a .png or .jpg image file]

STEP 3 – MIXING ZONE

Worksheet Layout



STEP 3 - Mixing Zone

Dilution Attenuation Factor (DAF)	Units	Symbol	Value
DAF option (use dropdown menu in "Value" cell)*	[-]		DAF1
User supplied dilution attenuation factor	[-]	DAF1	100.00
Default dilution attenuation factor	[-]	DAF2	
Calculated DAF (user - specified penetration depth)	[-]	DAF3	
Calculated DAF (calculated penetration depth)	[-]	DAF4	

1

Parameters for DAF3 and DAF4	Units	Symbol	Input Values	Common Units Value	Common Units Units	Common Units Value	Common Units Units	Common Units Value	Common Units Units
Darcy flux	m/d	q			ft/d		cm/d		cm/h
Cross-sectional area of groundwater flow	m^2	A_a			ft^2		cm^2		
Cross-sectional area of vadose zone flow	m^2	A_p			ft^2		cm^2		
Thickness of aquifer	m	B			ft		yd		cm
Aquifer vertical dispersivity	m	α_v			ft		yd		cm
Length of source in flow direction	m	L			ft		yd		
Calculated penetration depth	m	H							
Horizontal flow volumetric flow rate	m^3/d	Q_a							
Vertical flow volumetric flow rate	m^3/d	Q_p							

2

* DAF1 = User-specified DAF value
DAF2 = Default DAF value of 20
DAF3 = Calculated DAF based on leachate and aquifer flow mixing ratio. Flow rates are controlled by Darcy flux and cross-sectional areas beneath the vadose zone (Ap) and in the aquifer (Aa)
DAF4 = Calculated mixing zone DAF based on the work of Charbeneau (2000). The penetration depth (H) of the leachate into the mixing zone is based on a combination of vertical infiltration and dispersion. Vertical leachate infiltration is calculated along the source length (l * L). Vertical dispersion is calculated based on the vertical dispersivity beneath the source zone (αv) and horizontal aquifer seepage (q* B).

Calculate Mixed Concentration v Time

Time	Maximum Mixed Concentration (ug/L)
500	3.15

DAF1

Figure 10: *Worksheet layout for the* 2 Vadose & 3 MixingZone *Tab. The components on this section of the tab will be utilized by the user to perform all necessary functions for Step 3 of the SILT spreadsheet: the mixing zone.*

The Step 3 – Mixing Zone portion of the *2 Vadose & 3 MixingZone* Tab contains inputs and outputs related to the diluted leachate concentration which is found in the mixing zone. This section will cover the two input components of this worksheet:

1. Selection of a Dilution Attenuation Factor (DAF)
2. Parameters needed to calculate DAF3 and DAF4

The following section will briefly discuss the parameters required for each of these sections. A more detailed discussion of the mathematical theory and concepts related to DAF option 3 and 4 calculations can be found in *Appendix A*.

3.1. SELECTION OF A DILUTION ATTENUATION FACTOR (DAF)

Dilution Attenuation Factor (DAF)			
	Units	Symbol	Value
DAF option (**use dropdown menu in "Value" cell**)*	[-]		DAF1
User supplied dilution attenuation factor	[-]	DAF1	100.00
Default dilution attenuation factor	[-]	DAF2	
Calculated DAF (user - specified penetration depth)	[-]	DAF3	
Calculated DAF (calculated penetration depth)	[-]	DAF4	

In this section, the user is able to select from four available methods for defining or calculating a Dilution Attenuation Factor (DAF) that will be applied to the leachate concentration modeled in Step 2 – Vadose Zone. A DAF is first selected from a dropdown menu in the *Value* column of the first row. The DAF options are numbered and color-coded so the user can easily identify which option they have currently selected. The options are defined as follows:

DAF1 – User supplied dilution attenuation factor

DAF2 – Default dilution attenuation factor

DAF3 – Calculated dilution attenuation factor (user – specified penetration depth)

DAF4 – Calculated dilution attenuation factor (calculated penetration depth)

A brief description of each method is given in the following section:

DAF1: The user supplies a dilution attenuation factor in the blue cell shown to the right of *DAF1*. The blue cell acts as an input cell like all other blue cells in the SILT spreadsheet.

DAF2: A default value of 20 is shown in the white cell next to *DAF2*. This value is consistent with the DAF specified in the USEPA Soil Screening Guidance (1996). It is also consistent with the DAF value derived from representative New Jersey aquifer conditions (average aquifer hydraulic gradient and aquifer hydraulic conductivity) and is discussed in more detail in the "Soil and Soil Leachate Remediation Standards for the Migration to Groundwater Exposure Pathway, Basis and Background" document located at https://www.nj.gov/dep/srp/guidance/rs. The user ***does not*** provide input for this option.

DAF3: The user provides parameter information in the blue input cells in the table shown in Section 3.2.1 explained below. The mixing zone penetration depth is calculated internally based on a leachate and aquifer flow mixing ratio. The user supplies the dimensions of the mixing zone by defining a cross-sectional area beneath the vadose zone (for the volumetric flow rate in the vertical direction) and the cross-sectional area of the aquifer (for the volumetric flow rate in the horizontal direction).

DAF4: The user provides parameter information in the blue input cells in the table shown in Section 3.2.2 explained below. The mixing zone penetration depth is calculated internally based on the method derived in Charbeneau (2000) (See *Appendix A*). The user provides information about the length of the source in the direction of aquifer flow and the aquifer's hydraulic properties, namely the vertical dispersivity. The penetration depth of the source into the mixing zone is then calculated based on vertical leachate infiltration and vertical dispersion.

3.2. PARAMETERS NEEDED TO CALCULATE DAF3 AND DAF4

3.2.1. DAF3 Selected

39	**Dilution Attenuation Factor (DAF)**			
40		Units	Symbol	Value
41	DAF option (**use dropdown menu in "Value" cell**)*	[-]		DAF3
42	User supplied dilution attenuation factor	[-]	DAF1	
43	Default dilution attenuation factor	[-]	DAF2	
44	Calculated DAF (user - specified penetration depth)	[-]	DAF3	35.21
45	Calculated DAF (calculated penetration depth)	[-]	DAF4	
46				
47				Input Values
48	**Parameters for DAF3 and DAF4**			
49	Darcy flux	m/d	q	0.05
50	Cross-sectional area of groundwater flow	m^2	A_a	10.00
51	Cross-sectional area of vadose zone flow	m^2	A_p	10.00
52	Thickness of aquifer	m	B	
53	Aquifer vertical dispersivity	m	α_v	
54	Length of source in flow direction	m	L	
55	Calculated penetration depth	m	H	
56	Horizontal flow volumetric flow rate	m^3/d	Q_a	0.50
57	Vertical flow volumetric flow rate	m^3/d	Q_p	0.01

Darcy flux: the horizontal darcy flow velocity in the aquifer.

Cross-sectional area of groundwater flow: the area of a cross-section sliced vertically through the aquifer. The groundwater flow will flow *horizontally* through this cross-section.

Cross-sectional area of vadose zone flow: the area of a cross-section placed horizontally beneath the bottom of the vadose zone. Leachate flowing out of the vadose zone will flow *vertically* through this cross-section.

Horizontal flow volumetric flow rate: the volume of water per unit time which flows through the aquifer in the horizontal direction.

Vertical flow volumetric flow rate: the volume of water per unit time which flows into the aquifer from the vadose zone in the vertical direction.

3.2.2. DAF4 Selected

Dilution Attenuation Factor (DAF)			
	Units	Symbol	Value
DAF option (**use dropdown menu in "Value" cell**)*	[-]		DAF4
User supplied dilution attenuation factor	[-]	DAF1	
Default dilution attenuation factor	[-]	DAF2	
Calculated DAF (user - specified penetration depth)	[-]	DAF3	
Calculated DAF (calculated penetration depth)	[-]	DAF4	28.42
			Input Values
Parameters for DAF3 and DAF4			
Darcy flux	m/d	q	0.05
Cross-sectional area of groundwater flow	m^2	A_a	
Cross-sectional area of vadose zone flow	m^2	A_p	
Thickness of aquifer	m	B	10.00
Aquifer vertical dispersivity	m	α_v	1.82
Length of source in flow direction	m	L	6.10
Calculated penetration depth	m	H	4.89
Horizontal flow volumetric flow rate	m^3/d	Q_a	0.24
Vertical flow volumetric flow rate	m^3/d	Q_p	0.0089

Darcy flux: the horizontal darcy flow velocity in the aquifer.

Thickness of aquifer: the total aquifer thickness measured from the average groundwater table depth to the base of the aquifer or confining unit.

Aquifer vertical dispersivity: term used to represent local variations in groundwater flow velocity in the vertical direction.

Length of source in flow direction: the horizontal length of the source zone in the direction of groundwater flow.

Calculated penetration depth: the depth that the mixing zone will penetrate into the aquifer based on Charbeneau (2000) (See *Appendix A*).

Horizontal flow volumetric flow rate: the volume of water per unit time which flows through the aquifer in the horizontal direction.

Vertical flow volumetric flow rate: the volume of water per unit time which flows into the aquifer from the vadose zone in the vertical direction.

3.3. MIXING ZONE OUTPUT

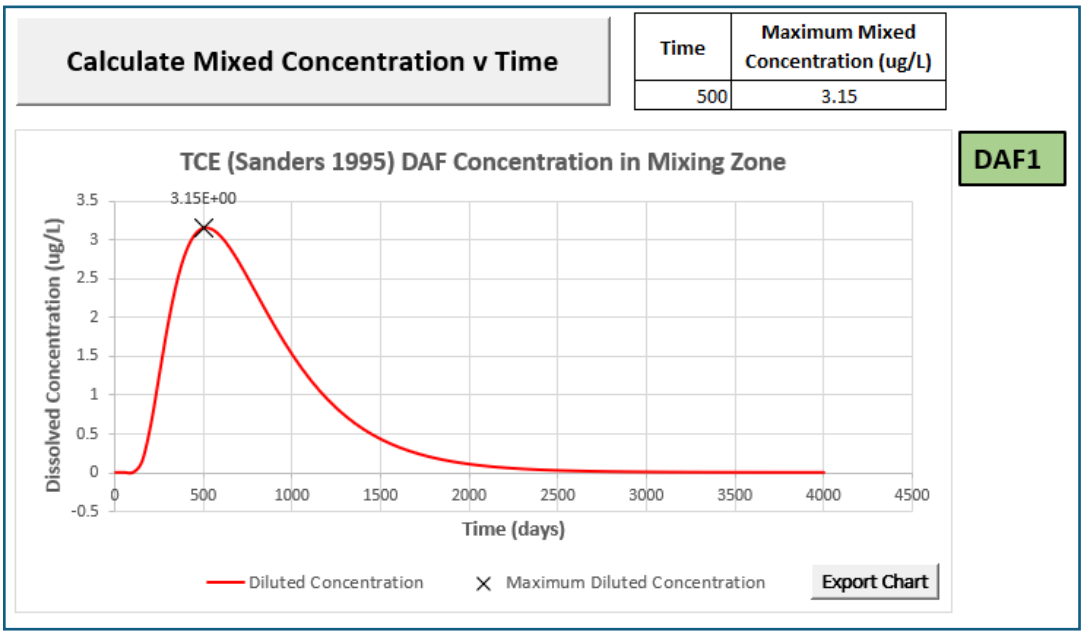


Figure 11: *Diluted leachate concentration time series for* Step 3 – Mixing Zone.

After the user clicks Calculate Mixed Concentration v Time the selected DAF value will be applied to the modeled concentrations from *Step 2 – Vadose Zone*. Each point on the leachate breakthrough curve will be divided by the DAF value, resulting in a plot of diluted concentration values (**Figure 11**). The diluted concentration plot should have the same shape as the leachate breakthrough curve since it is the same curve, but with reduced concentrations. The plot produced by SILT for Step 3 – Mixing Zone, like the plot produced in *Step 2 – Vadose Zone* (**Figure 9**), has the maximum concentration value shown on the plot and in a small table above the plot. Additionally, a small color-coded box next to the plot indicates which DAF option was used to generate the plot (DAF1, DAF2, DAF3 or DAF4). This allows for the user to always know which DAF was used to produce the *current* results, even if another DAF option is selected from the drop-down menu at a later time. If the user wants to calculate the dilute concentration curve with a different DAF option, they can select another DAF option from the drop-down menu and click *Calculate Mixed Concentration v Time* again.

[**NOTE:** The Dilute Concentration in the Mixing Zone Chart has an Export Chart button if the user would like to save the chart locally to their computer as a .png or .jpg image file]

STEP 4 – PLUME MODEL SOURCE STEPS

WORKSHEET LAYOUT

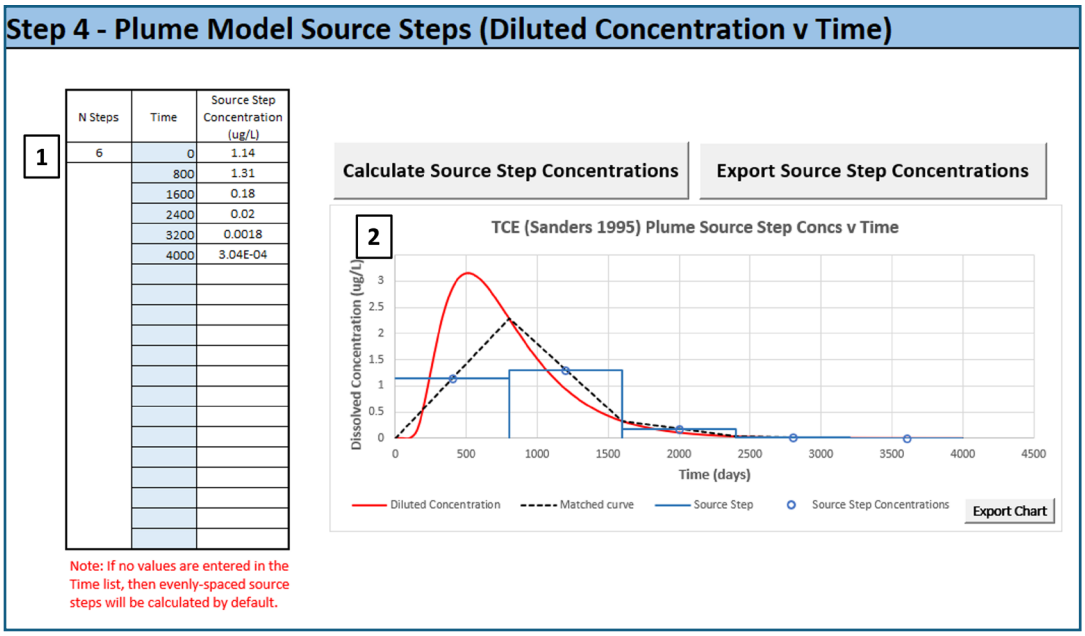


Figure 12: *Worksheet layout for the* 4 Plume Source Steps *Tab. The components on this section of the tab will be utilized by the user to perform all necessary functions for Step 4 of the SILT spreadsheet: Plume Model Source Steps.*

The *4 Plume Source Steps* Tab is utilized to define discrete steps of diluted concentration data from Step 3 – Mixing Zone to incorporate into a groundwater contaminant plume model as a source term. The user can refer to *Appendix A* for a detailed description of the discretizing procedure used to calculate the source step concentrations.

The worksheet contains two elements shown in **Figure 12: (1)** a table which contains time steps and source step concentrations for grouped diluted leachate concentrations in the mixing zone, and **(2)** a plot to allow the user to visualize the currently grouped source step concentrations.

4.1. DEFINING TIME-VARYING STEPS FOR DILUTE LEACHATE CONCENTRATIONS

The user can optionally provide times in the blue cells of the Time column. Any integer value can be entered ranging from t = 0 to t = *Tmax* (as it was defined in *Step 1 – Source Zone*). If the user does not provide any time values in the blue cells, then five evenly-spaced source steps ranging from t = 0 to t = *Tmax* will be calculated by default (**Figure 12**). The total number of discrete source step concentrations is equal to the number *N Steps* shown in the input table.

Once the default time values are used, or user-defined time values are provided, then the user should click Calculate Source Step Concentrations to calculate the discrete source step concentrations.

[**NOTE:** The Source Step Concentrations v Time Chart has an Export Chart button if the user would like to save the chart locally to their computer as a .png or .jpg image file]

4.2. INTERPRETING AND EXPORTING THE SOURCE STEP CONCENTRATIONS

After grouping, the source step concentration data will be represented by a number of discrete columns equal to *N Steps* – 1. **When using the default time values, there will always be six times used to generate six source steps.** (Recognize that the sixth "step" extends at constant concentration from the last specified time – 4000 days in this example – to infinity. See Appendix A, Fig A-4.) The user should define, or refine, the number of discrete columns until a reasonable representation of the dilute concentration time series is achieved. SILT provides a *matched curve* on the source step concentrations plot (black dashed line) to allow the user to visualize how closely the discretized source step concentrations match the dilute leachate concentration curve (solid red line). An example of how to group the data and interpret the source step concentration plot is provided below:

Example: In **Figure 13** below, which considers dilute TCE leachate concentrations in the mixing zone from the Sanders (1995) example, the six default source step concentrations match the red dilute concentration curve fairly well after t = 1250 days, but are poorly matched between t = 0 and t = 1250 days. This is due to a rapid increase in the rate of leachate breakthrough into the mixing zone after about 400 days. The leachate concentration in the mixing zone peaks at 850 days and then exponentially declines until the end of the modeled time defined in ***Step 1 – Source Zone*** (Tmax = 4000 days). From the plot the user can determine that uniform 800-day time intervals are too large of an increment to group the data without losing accuracy. The user can then insert additional time steps or change the default time steps to better match the curve.

N Steps	Time	Source Step Concentration (ug/L)
6	0	1.14
	800	1.31
	1600	0.18
	2400	0.02
	3200	0.0018
	4000	3.04E-04

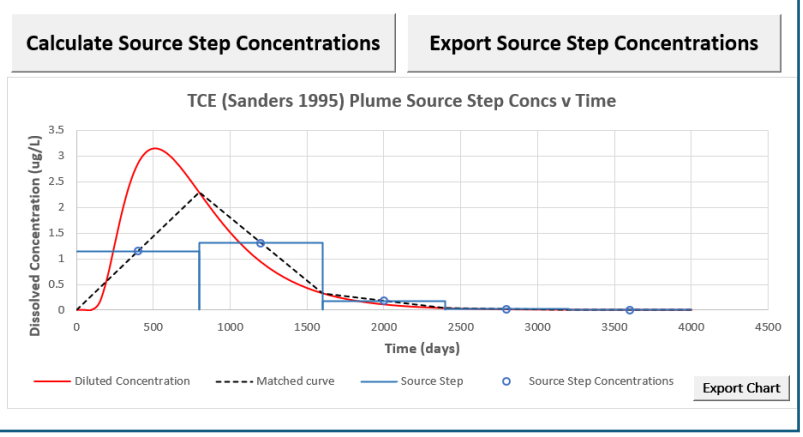
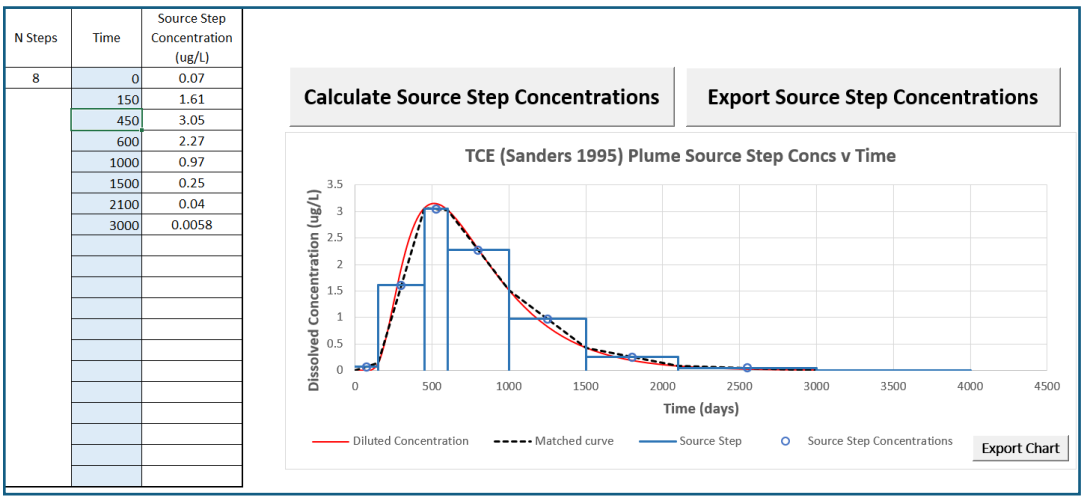


Figure 13: *Calculated source step concentrations using default discretization (five evenly-spaced source steps).*

Since the user has analyzed the default output, and has realized that the source step concentrations need to be refined, the user modifies and adds additional time step values to the *Time* column (**Figure 14**). The user ends up with time values of tt = 0, 15, 450, 600, 1000, 1500, 2100 and 3000, resulting in 8 source concentration steps. The black *matched curve* line is now matching the red diluted concentration curve very well, indicating that the defined source step concentrations will adequately represent the leachate concentration as a source term for the groundwater plume model.



N Steps	Time	Source Step Concentration (ug/L)
8	0	0.07
	150	1.61
	450	3.05
	600	2.27
	1000	0.97
	1500	0.25
	2100	0.04
	3000	0.0058

Figure 14: *Calculated source step concentrations after refining the default discretization.*

Once a reasonable set of source step concentrations has been calculated, the user may export them by clicking Export Source Step Concentrations . The time-source step concentration pairs will be exported as a comma-separated-value (.csv) file.

APPENDICES

APPENDIX A: MODEL CONCEPTS AND THEORY

A1. Vadose Zone Flow and Transport Model

The governing equation utilized in SILT for solute flow and transport in the vadose zone is the Convection-Dispersion Equation (CDE) with reactions:

$$\frac{\partial}{\partial t}(\theta_w C_w + \rho_b C_s) = -\frac{\partial}{\partial z}(I C_w) + \frac{\partial}{\partial z}\left(\theta_w D \frac{\partial C_w}{\partial z}\right) - \theta_w \lambda_w C_w - \rho_b \lambda_s C_s$$

Where:

C_w = Liquid-phase concentration in the vadose zone

C_s = Solid-phase concentration in the vadose zone

z = depth coordinate in the vadose zone, where z = 0 is the bottom of the source zone

t = Time

θ_w = water content in the vadose zone (average in vadose zone during period of simulation)

ρ_b = soil bulk density

I = Infiltration rate into the vadose zone

D = Dispersion coefficient related to transport in the vadose zone

λ_w = first-order transformation rate in the liquid-phase

λ_s = first-order transformation rate in the solid-phase

Movement of a contaminant in the vadose zone is handled through advective and dispersive transport. Infiltration at a steady rate into a soil of specified and unchanging soil moisture percentage defines the vertical flow field through the vadose zone. Advection and dispersion processes are combined to describe the movement of contamination that is dissolved from (partitioned from) the source zone into the infiltrating soil water. Advective flow is represented by the Darcy flux, *q*. Dispersive flow is related to small-scale irregularities in the flow field which result in solute spreading both parallel and perpendicular to the flow field, represented by both the average water content, θ_w, and Dispersion coefficient, *D*.

The solute concentration in the vadose zone (the zone of transport) beneath the source zone will also be subject to reductions based on physical and chemical processes. SILT incorporates adsorption to the solid phase in the vadose zone. Solid phase adsorption is assumed to be instantaneous and at equilibrium between the solid and dissolved phases, and is defined below:

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

Where:

R = Retardation factor

ρ_b = Soil bulk density

θ_w = Volumetric water content (average in vadose zone during period of simulation)

K_d = Soil-water partitioning coefficient

The retardation factor, R, is then applied to the governing equation shown above by scaling the advective and dispersive components:

$$v_{eff} = \frac{I}{\theta_w R}$$

$$D_{eff} = \frac{D}{R}$$

Where:

V_{eff} = Effective velocity, adjusted by adsorption

D_{eff} = Effective dispersion, adjusted by adsorption

θ_w = Volumetric water content (average in vadose zone during period of simulation)

D = Dispersion coefficient related to transport in the vadose zone

I = Infiltration rate into the vadose zone

R = Retardation factor

Chemical reactions are lumped together into two decay terms related to reactions in the solid-phase, λ_s, and in the dissolved phase, λ_w. A general term can be defined to accommodate adsorption effects and chemical reactions:

$$\lambda_{eff} = \frac{\left(\lambda_w + \frac{\rho_b \lambda_s K_d}{\theta_w}\right)}{R}$$

Where:

λ_{eff} = Effective chemical decay term due to reactions

ρ_b = Bulk density of the soil

K_d = Soil-water partitioning coefficient

θ_w = Volumetric water content (average in vadose zone during period of simulation)

R = Retardation factor

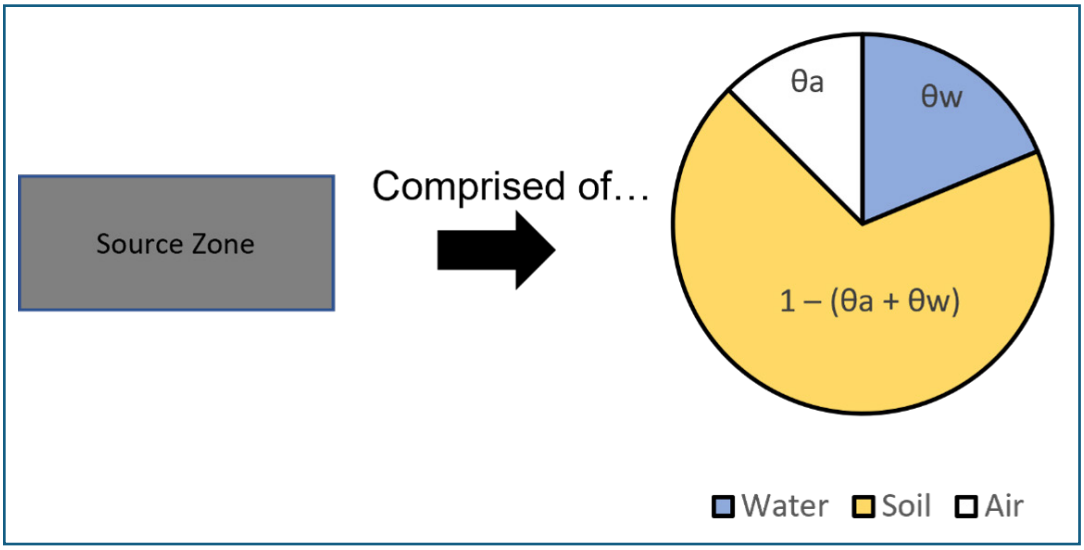
The adjusted adsorption and reaction parameters defined above can be used to reduce the governing equation to a reduced partial-differential equation that is used to model dissolved-phase leachate concentrations at the bottom of the vadose zone:

$$\frac{\partial C_w}{\partial t} = -v_{eff}\frac{\partial C_w}{\partial z} + D_{eff}\frac{\partial^2 C_w}{\partial z^2} - \lambda_{eff} C_w$$

The above governing equation is adjusted based on whether the user utilizes a semi-analytical general solution, or specific analytical solutions, depending on source type. These will be explained in further detail in Section A3.

A2. CALCULATION OF THE INITIAL DISSOLVED CONCENTRATION IN THE SOURCE ZONE

SILT considers the source zone as an accumulation of source chemical in the solid, liquid and gaseous phases, within a portion of the soil column of some specified vertical extent. The partitioning of chemical mass among the media phases within this source zone is conceptualized as shown below:



Where:

θ_a = Volumetric air content

θ_w = Volumetric water content (average in source zone during period of simulation)

The air and water content constitute the total porosity of the source zone, and the solid-phase is calculated as 1 – the total porosity. SILT allows for gas- and solid-phase partitioning in the source zone. Assuming equilibrium sorption mechanics, the initial dissolved concentration in the source zone is calculated as follows:

$$C_0 = C_{soil} \frac{\rho_b}{(\theta_w + \theta_a K_H + \rho_b K_d)}$$

Gas-phase partitioning

Solid-phase partitioning

Where:

C_0 = Initial dissolved concentration in the source zone, after partitioning

C_{soil} = Concentration of source in the solid phase

ρ_b = Soil bulk density

θ_w = Volumetric water content (average in source zone during period of simulation)

θ_a = Volumetric air content

K_H = Henry's Law constant

K_d = Soil-water partitioning coefficient

The soil concentration, C_{soil} is defined as the mass ratio between the total mass of the source species and the mass of the soil:

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

A3. SOURCE TYPE CALCULATIONS

Solute flow and transport in the vadose zone beneath the source zone are dependent on three factors: **1)** The governing equation defined in Section A1; **2)** the initial dissolved concentration from the source zone (the partitioning calculation of which is described in Section A2); **3)** The type of source that is being assumed to represent the behavior of the source species in the Source Zone.

The general initial and boundary conditions for the Convection-Dispersion Equation utilized in SILT are described below:

- C_w (z,0)=0
- C_w (0,*t*)= C_0 (*t*)
- C_w (∞,*t*)=0

SILT allows for two solution options to calculate the source concentration and leachate at the bottom of the vadose zone as a function of time:

$$C_w(z,t) = \frac{z}{2\sqrt{\pi D_{eff}}} exp\left\{\frac{v_{eff} z}{2D_{eff}}\right\} \int_0^t C_w(t_i) \frac{1}{(t-t_i)^{3/2}} exp\left\{-\left(\frac{v_{eff}^2}{4D_{eff}} + \lambda_{eff}\right)(t-t_i) - \frac{z^2}{4D_{eff}(t-t_i)}\right\} dt$$

A3.1 Integrated Solution (Bedekar et al., 2012) – Solution Option 1

Where:

C_w = Dissolved concentration of leachate at the bottom of the vadose zone

t = current time step

z = Distance from the bottom of the source to water table

V_{eff} = Effective velocity

D_{eff} = Effective dispersion

t_i = previous time step

λ_{eff} = Effective chemical decay term

The trapezoidal rule is used to approximate integration in the SILT spreadsheet. The discretization of the integration term (dt) is defined by the *tstep* parameter in ***Step 1 – Source Zone***. The parameter *tstep* should be small enough to incorporate changes in source and leachate concentration over time, especially if rapid changes occur (such as removal of a source or if a large depletion rate is used). The semi-analytical (integrated) approach is a general solution that can be applied to any of the source type options. A source concentration time-series is first calculated internally by utilizing the parameters C_0, *tstep*, *Tmax* and γ from ***Step 1 – Source Zone***. The resulting time series of C_w values are then utilized in the integrated solution shown above to calculate a time series of soil leachate values. The use of integration techniques to evaluate a time series is a more robust approach than a direct analytical solution, however it will generally take longer to calculate, depending on how small or large the parameter *tstep* is.

The semi-analytical solution is also subject to an internal limitation of Microsoft Excel, namely a memory limitation that does not allow it to return a value for the EXP() function for a value of the argument greater than 709. In instances where the model in question may have very large vadose zone thickness values (z) or very low soil dispersivity (α_L) then the first exponential term in the general solution shown above may become very large. In the event an argument greater than 709 would be passed to the EXP() function in the solution, SILT will produce an error message when the user clicks the *Calculate Leachate Concentration* button which will direct the user to reduce the thickness of the vadose zone, increase the dispersivity, or select Solution Option 2.

A3.2 Analytical Solutions – Solution Option 2

SILT also allows the user to select from a variety of analytical solutions to represent the four available source types, which will be individually explained in the following section.

A3.2.1 – Constant Source Concentration (Source Term Option 1)

For a **constant source**, the upper boundary condition is changed to:

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

Which indicates that enough mass is being applied over time to ensure that the dissolved concentration is constant, and equal to its initial concentration.

The analytical solution for leachate transport with a constant source is generalized from Ogata and Banks (1961):

$$C_w(z,t) = \frac{C_0}{2}\left[\exp\left\{\frac{v_{eff}}{2D_{eff}} + \frac{z}{\sqrt{D_{eff}}}\left(\frac{(v_{eff})^2}{4D_{eff}} + \lambda_{eff}\right)^{1/2}\right\}\operatorname{erfc}\left\{\frac{z}{2\sqrt{D_{eff}t}} + \left(\frac{(v_{eff})^2}{4D_{eff}} + \lambda_{eff}\right)^{1/2}\right\}\sqrt{t}\right.$$
$$\left. + \exp\left\{\frac{v_{eff}}{2D_{eff}} - \frac{z}{\sqrt{D_{eff}}}\left(\frac{(v_{eff})^2}{4D_{eff}} + \lambda_{eff}\right)^{1/2}\right\}\operatorname{erfc}\left\{\frac{z}{2\sqrt{D_{eff}t}} - \left(\frac{(v_{eff})^2}{4D_{eff}} + \lambda_{eff}\right)^{1/2}\right\}\sqrt{t}\right]$$

A3.2.2 – First-order decaying source (Source Term Options 2 and 3)

For a ***first-order decaying source***, the upper boundary condition is changed to:

$$C_w(0,t) = C_0 \exp(-\gamma t)$$

Where γ is a source depletion rate that is either defined by the user (Source Term Option 2) or calculated using the Rowe (1991) Method (Source Term Option 3) explained in Section 1.2.3 of this User Guide. When this source type is selected the model assumes that the mass of the source will be depleted at an exponential rate over time.

The analytical solution for leachate transport with a decaying source is also generalized from Ogata and Banks (1961) and presented in Bedekar et al. (2012):

$$C_w(z,t) = \frac{C_0}{2}\exp(-\gamma t)\left[\exp\left\{\frac{v_{eff}z}{2D_{eff}} + \frac{z}{\sqrt{D_{eff}}}\left(\frac{(v_{eff})^2}{4D_{eff}} + (\lambda_{eff} - \gamma)\right)^{1/2}\right\}\operatorname{erfc}\left\{\frac{z}{2\sqrt{D_{eff}t}} + \left[\left(\frac{(v_{eff})^2}{4D_{eff}} + \lambda_{eff}\right)t\right]^{1/2}\right\} + \exp\left\{\frac{v_{eff}z}{2D_{eff}} - \frac{z}{\sqrt{D_{eff}}}\left(\frac{(v_{eff})^2}{4D_{eff}} + (\lambda_{eff} - \gamma)\right)^{1/2}\right\}\operatorname{erfc}\left\{\frac{z}{2\sqrt{D_{eff}t}} - \left[\left(\frac{(v_{eff})^2}{4D_{eff}} + (\lambda_{eff} - \gamma)\right)t\right]^{1/2}\right\}\right]$$

The analytical solutions for Source Term Options 2 and 3 are uniquely subject to a *condition of applicability* since the analytical solution for a decaying source is not entirely robust. The condition of applicability is defined below:

$$\gamma < \frac{v_{eff}^2}{4D_{eff}} + \lambda_{eff}$$

This condition is a mathematical check that ensures the user-defined or calculated depletion rate, γ, is not large enough to cause the following term in the analytical solution to result in a negative square-root (i.e. mathematically unsolvable):

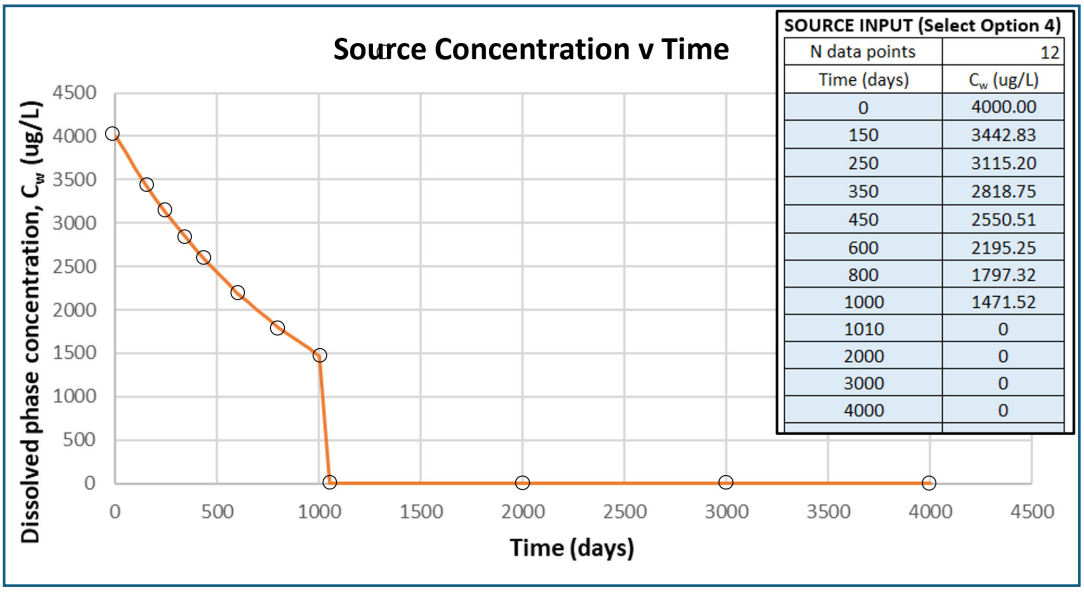
$$\left(\frac{(v_{eff})^2}{4D_{eff}} + (\lambda_{eff} - \gamma)\right)^{1/2}$$

The condition of applicability is also a physics-based constraint on the analytical solution. If the above condition is violated, then that infers that the mass flux from the source to the vadose zone is insufficient to maintain positive mass compared to the relatively high advective velocities and decay rates which remove mass from the soil zone near the source.

SILT contains a built-in error check which will inform the user of whether the condition of applicability has been violated and will direct the user to utilize Solution Option 1 (Integrated Solution) instead.

A3.2.3 – Time-variable source concentration (Source Term Option 4)

For source histories that cannot be fully represented by a constant source or first-order degradation mechanics, the user can provide discrete time-concentration pairs in the provided table for Source Term Option 4 (See Section 1.2.4 of this User Guide). The source concentration time series is first calculated internally by using piecewise linear interpolation between each provided time-concentration pair. A conceptual representation of an interpolated source concentration time series having first-order degradation followed by source excavation is shown in **Figure A-1** below:



SOURCE INPUT (Select Option 4)	
N data points	12
Time (days)	C_w (ug/L)
0	4000.00
150	3442.83
250	3115.20
350	2818.75
450	2550.51
600	2195.25
800	1797.32
1000	1471.52
1010	0
2000	0
3000	0
4000	0

Figure A-1: *Linearly interpolated time-variable source concentration. Between t = 0 and t = 1000, the source is subject to a first-order depletion rate of 0.001/d. After source removal at t = 1010 days, the source concentration is set to 0 µg/L.*

The orange line represents the linearly interpolated source concentration based on the *reference points* (black circles) provided by the user in the *Source Input* table. The user should keep two points in mind when utilizing Source Term Option 4: **1)** The user must ensure that they provide enough time-concentration pairs to adequately capture the source concentration history when linearly interpolating between data points; **2)** The user should make sure that their time step size, tstep in *Step 1 – Source Zone* is appropriate to represent changes in source concentration over time, similar to discretizing the time series for Solution Option 1 (*See* Section A3.1). In the above example, the parameter *tstep* is set to 10 days to ensure that the linear interpolation between 1000 and 1010 days adequately demonstrates the removal of the source, which resulted in an abrupt change in source concentration.

The analytical solution for vadose zone transport using a user-provided time-variable source follows the approach utilized for discrete source concentrations employed in the ATRANS analytical groundwater fate and transport model (Neville, 2005):

$$C_w(z,t) = \sum_{i=1}^{NP} \frac{\Delta C_{wi}}{2} \left[\exp\left\{ \frac{v_{eff} z}{2D_{eff}} + \frac{z}{\sqrt{D_{eff}}} \left(\frac{v_{eff}^2}{4D_{eff}} + \lambda_{eff} \right)^{1/2} \right\} \operatorname{erfc}\left\{ \frac{z}{2\sqrt{D_{eff}(t-t_{si})}} + \left(\frac{v_{eff}^2}{4D_{eff}} + \lambda_{eff} \right)^{1/2} \sqrt{(t-t_{si})} \right\} + \right.$$
$$\left. \exp\left\{ \frac{v_{eff} z}{2D_{eff}} - \frac{z}{\sqrt{D_{eff}}} \left(\frac{v_{eff}^2}{4D_{eff}} + \lambda_{eff} \right)^{1/2} \right\} \operatorname{erfc}\left\{ \frac{z}{2\sqrt{D_{eff}(t-t_{si})}} - \left(\frac{v_{eff}^2}{4D_{eff}} + \lambda_{eff} \right)^{1/2} \sqrt{(t-t_{si})} \right\} \right]$$

Where:

NP = total number of discrete points provided by the user

ΔC_{wi} = Change in dissolved concentration between the given time, *t*, and the *ith* discrete time-concentration pair

t_{si} = The start time of the *ith* discrete time-concentration pair

A4. DAF CALCULATIONS FOR DAF OPTIONS 3 AND 4

As leachate from the bottom of the vadose zone is introduced to the aquifer, it mixes with groundwater and dilutes the solute concentration. The dilution occurs within the *mixing zone*, an area beneath the vadose with a size that is dependent on a combination of soil and aquifer hydraulic properties.

SILT provides the user with four options for applying a Dilution Attenuation Factor (DAF) to the mixing zone (*See* Section 3.1 *of this User Guide*), however DAF options 1 and 2 do not explicitly take the size of the mixing zone into account; being user-provided or default values, respectively. In the sections below the DAF options which allow for calculation of the DAF based on mixing zone size (DAF options 3 and 4) will be discussed. SILT calculates a dilution factor based on site-specific estimates of infiltration and groundwater flow volume using a flow mass balance method described in Washington State regulation WAC 173-340-747 as discussed in the Washington State Department of Ecology "Model Toxics Control Act Regulation and Statute"

The mass balance dilution method utilized in SILT to calculate DAF values for both DAF options 3 and 4, is expressed as:

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

Where:

DAF = Dilution Attenuation Factor

Q_p = Volumetric flow rate in the vertical direction through the vadose zone

Q_a = Horizontal volumetric flow rate through the aquifer lateral to groundwater flow

The general mixing method requires an estimate of the depth of the mixing zone that is then used to calculate the horizontal influx of groundwater into the mixing zone based on a Darcy's Law calculation. The methods of estimating the depth of the mixing zone for DAF Method 3 and Method 4 are described in the Sections A4.1 and A4.2 below.

A4.1 DAF Option 3 - User-Specified Penetration Depth

For DAF Option 3, the user needs to provide information about the Darcy *flux*, *q*, and a cross-section area for groundwater flow, A_a, and the vadose zone, A_p. The mixing zone dimensions are conceptualized in **Figure A-2** below:

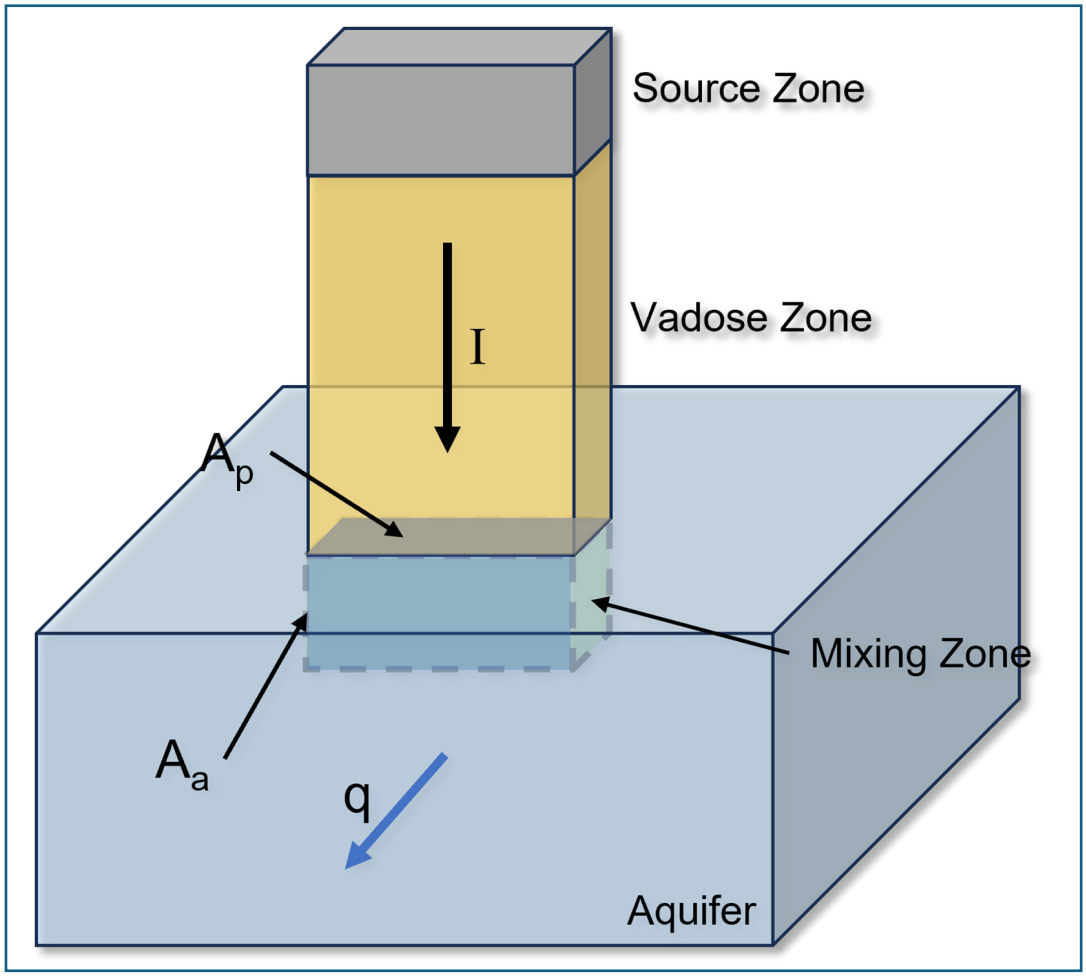


***Figure A-2**: Conceptual model of the mixing zone delineated by user-defined surface area planes in the vertical (A_p), and horizontal (A_a) directions.*

Where:

A_a = Cross-sectional area of groundwater (lateral) flow

A_p = Cross-sectional area of vadose zone (vertical) flow

q = Darcy flux in the direction of flow in the aquifer

I = Infiltration rate into the vadose zone (Defined in Step 1 – Source Zone)

After the user provides information about the above parameters, a DAF is calculated by first calculating Q_a and Q_p as defined below:

$$Q_a = A_a * q$$

$$Q_p = A_p * I$$

The DAF is then calculated by inserting the values of Q_a and Q_p into the general equation given in the introduction of Appendix Section A4 above.

- **A4.2 DAF Option 4** - Calculated Penetration Depth based on Charbeneau (2000)

DAF Option 4 utilizes the work of Charbeneau (2000) to calculate the penetration depth of the mixing zone based on both advective flow and vertical dispersion into the aquifer:

$$H = B\left(1 - \exp\left\{-\frac{IL}{qB}\right\}\right) + \sqrt{2\alpha_v L}$$

Where:

B = Thickness of the aquifer

I = Infiltration rate into the vadose zone

L = Length of source in the direction of flow

q = Darcy flux in the direction of groundwater flow in the aquifer

α_v = Aquifer vertical dispersivity

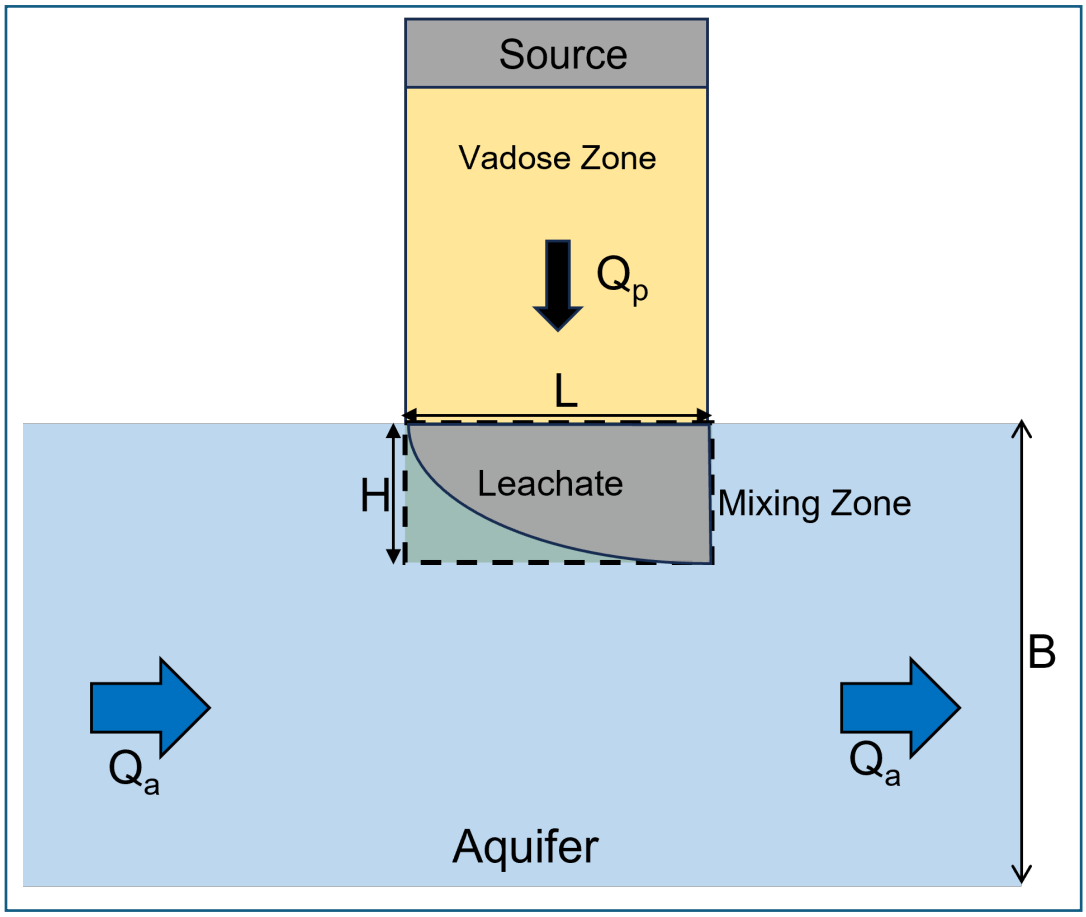


Figure A-3: *Conceptual model of the mixing zone penetration depth and length as calculated by the method of Charbeneau (2000).*

The volumetric flow rates in the horizontal and vertical direction are then calculated as follows:

$$Q_a = H * q$$

$$Q_p = I * L$$

The DAF is then calculated by inserting the values of Q_a and Q_p into the general equation given in the introduction of Appendix Section A4 above.

A5. USING MIXING ZONE CONCENTRATION HISTORY AS THE SOURCE TERM FOR PLUME TRANSPORT MODELS

As described in Section A4, SILT calculates contaminant concentration through time in the groundwater mixing zone beneath a soil source area. This produces the output curve displayed in **Figure 11**.

Groundwater flowing through and away from this mixing zone will result in the formation of a downgradient plume of groundwater contamination. Thus, the SILT mixing zone concentrations through time can be used to create a time-varying source term for a contaminant plume fate and transport model.

Mixing zone concentration versus time data calculated by SILT may be used in two ways: **(1)** the entire history of time step and concentration data pairs can be extracted and processed in any way the analyst desires for a high-temporal-resolution depiction of the source term, or **(2)** SILT can represent the concentration versus time curve as a set of several concentration steps of user-specified durations to create a much simpler representation of the mixing zone concentration history. These two methods are described further below.

A5.1 High-Resolution Concentration Time Series

After Step 3 – Mixing Zone has been completed the user may click on the ChartData tab to access the Mixing Zone concentration versus time data that SILT calculated at each time step from t = 0 to t = *Tmax*:

Mixing Zone		DAF1
Time (days)	C_dilute (ug/L)	
0	0	
50	0	
100	2.06029E-26	
150	4.38794E-11	
200	2.67714E-06	
250	0.000483668	
300	0.009054357	
350	0.057397952	
400	0.199039697	
450	0.474552292	
500	0.881235491	
550	1.373331002	
600	1.883899561	
650	2.348919023	
700	2.722331146	
750	2.980565584	
800	3.119897478	
850	3.150646764	
900	3.091065481	
950	2.962360132	
1000	2.785280091	
1050	2.578146816	
1100	2.355980339	

These time concentration data pairs may then be copied from the Chart Data tab in SILT and inserted into any post-processing program that can use comma-separated or excel values to create a high-temporal-resolution depiction of the contamination source term for a computer model of plume transport (similar to **Figure 11**).

A5.2 SILT-Generated Mixing Zone Source Step Concentrations

Certain plume transport models (e.g. analytical plume models) benefit from a more simple representation of the source in which the source concentration time series is applied as a series of discrete steps. Each step in the sequence specifies the source concentration for a particular time duration.

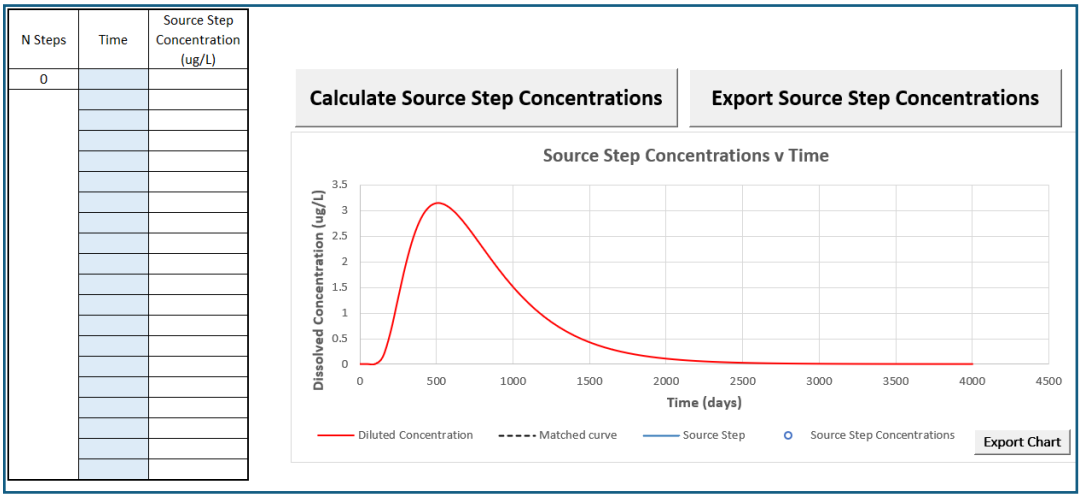
SILT has a built-in feature for generating this simplified step representation of the mixing zone concentration. The user examines the Mixing Zone concentration plot and enters a set of times that form the start and end of the desired concentration steps. SILT displays the stepped representation of the concentration history, and the user can adjust the times until an acceptable representation is achieved. SILT then allows export of discrete time-concentration pairs that can be used as the source term input data for a contaminant plume transport model.

When adequately stepped this process allows the user to **1)** capture concentration trends in the time series and reduce the amount of data points required for the groundwater model to a manageable level – while retaining a sufficiently accurate representation of the source, and **2)** track the fate and transport of a soil source through the vadose zone in groundwater, and downgradient in the saturated zone to potential receptor locations. A combination of the two transport processes allows the user to analyze questions related to soil impacts to groundwater, and environmental applications related to groundwater contamination such as Classification Exception Areas (CEAs), Natural Resource Damages (NRD) cases, Commingled Plume analyses, Remedial System Design and Evaluation, among others.

The methodology upon which this SILT Mixing Zone stepped concentration feature is based is presented below:

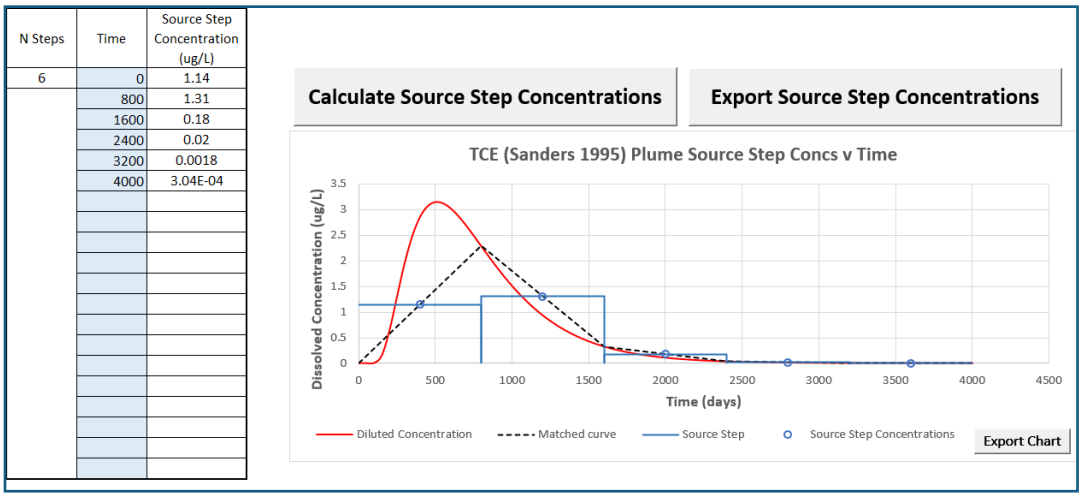
- **A5.2.1:** Calculation of Default Source Step Concentrations

Upon completion of Step 3 – Mixing Zone the user will find the worksheet *4 Plume Source Steps* as it appears below, with an empty time-concentration pairs table, and a plot showing only the dilute concentration time-series calculated in the previous step:



If the user does not enter any times into the "Time" column next to the plot, and clicks *Calculate Source step concentrations*, then SILT will automatically calculate five evenly spaced source steps (SS) from t = 0 to t = Tmax, and display them to the user:

In the example from **Figure 13** Tmax = 4000 days, so SILT discretized the time series into 6 source steps with each source step duration (Δt_{SS}) defined by the conditions given below:



[**NOTE:** The default source steps shown above (from **Figure 13**) would not be considered a good fit but they can be used as a baseline for refining the source steps, as explained later in this section]

$$\Delta t_{DEFAULT} = \frac{Tmax}{5} = \frac{4000\ days}{5} = 800\ days; t \leq Tmax$$

$$\Delta t_{DEFAULT} = \infty\ ; t > Tmax$$

The delineation of the default source steps is conceptualized in **Figure A-4**:

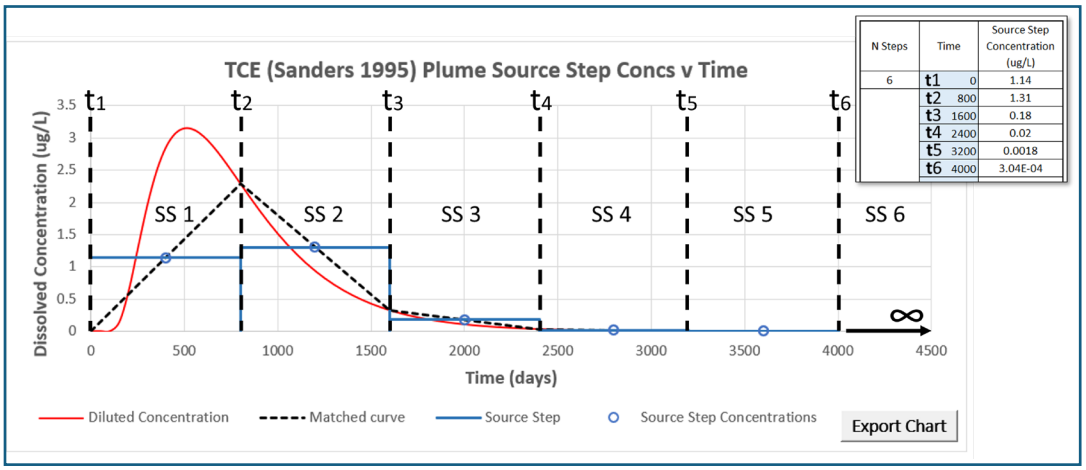


Figure A-4: *Conceptual figure for source step (SS) delineation using SILT default source step durations ($\Delta t_{DEFAULT}$).*

The source step concentrations (SSC) are calculated by taking the dilute concentrations at each time step and averaging them, then applying that average concentration across the SS (**Figure A-5**):

$$SSC_i = C_{ti \rightarrow ti+1} = (C_{ti+1} - C_{ti})/2$$

Where:

SSC_i = Source Step Concentration for the *ith* source step

C_{ti} = Modeled dilute leachate concentration at time *t*

- **A5.2.2:** Calculation of User-Defined Source step concentrations

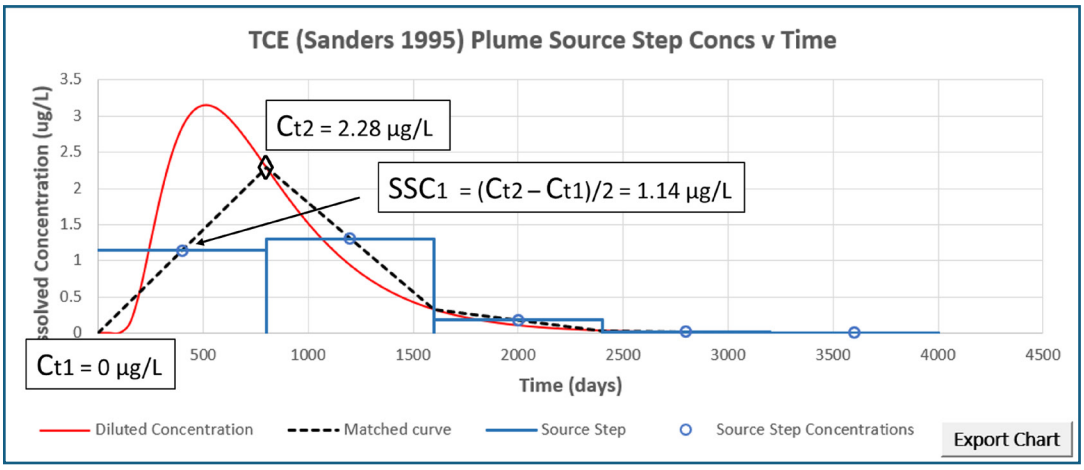
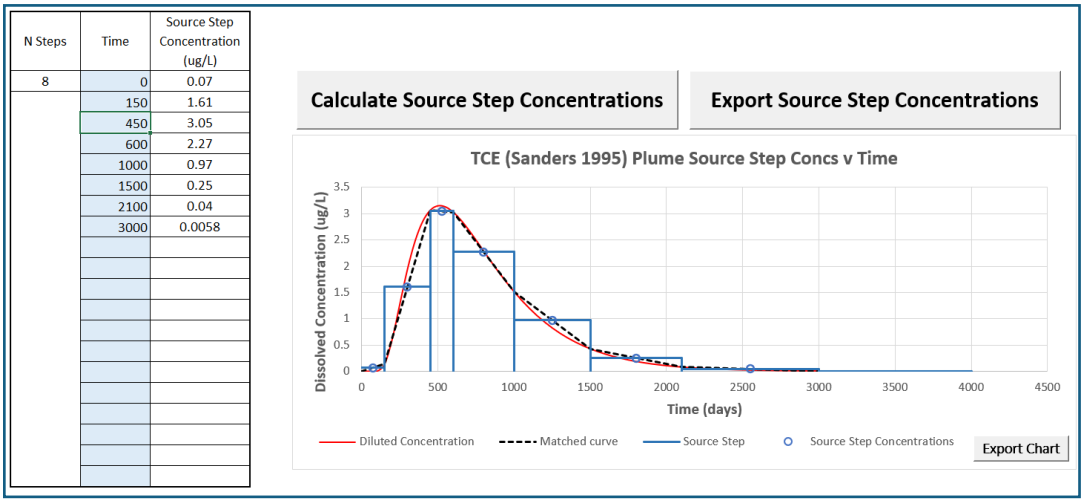


Figure A-5: *Calculation of a source step concentration (SSC).*

Due to the complex nature of environmental problems, the default source step concentrations will likely be an inadequate representation of the leachate breakthrough as a source term for a groundwater plume model. However, the default groupings can still provide the user with an initial look at how well the discretized data fits the results from the vadose zone model. The user can then add or refine the time steps to the *"Time"* column on the *4 Plume Source Steps* Tab to improve the discretization (**Figure A-6**):



N Steps	Time	Source Step Concentration (ug/L)
8	0	0.07
	150	1.61
	450	3.05
	600	2.27
	1000	0.97
	1500	0.25
	2100	0.04
	3000	0.0058

Figure A-6: *User-defined source step concentrations. The user has defined 9 time steps to delineate source steps for the diluted concentration data ranging from t = 0 to t =* Tmax.

In this case, the duration (Δt_{SS}) of each source step is calculated considering the change in time between each user-defined time:

$$\Delta t_{SS} = t_{i+1} - t_i \; ; t \leq Tmax$$

$$\Delta t_{SS} = \infty \; ; t > Tmax$$

The concentration for each SSC is calculated using the same averaging equation as the default method given in Section A5.1.

A5.3: Special Considerations

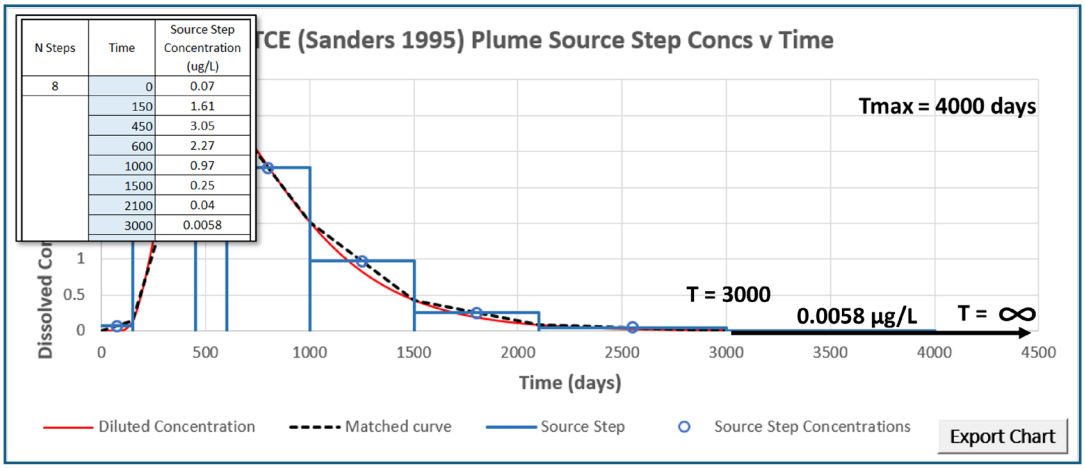
The stepping calculations for plume source step concentrations in SILT allow for some flexibility in how the user enters times into the *Time* column, namely 1) The user does not need to provide times that are evenly divisible by the time step (*tstep*); 2) The user does not need to have *Tmax* be the final time in the *Time* column.

1. *When the user does not provide times that are evenly divisible by tstep*

   The solute fate and transport models utilized in SILT define the simulated time information using the max time (*Tmax*) and time step (*tstep*) provided by the user in ***Step 1 – Source Zone***. As such, solute, leachate and dilute leachate concentrations are output by SILT for N = *Tmax/tstep* time steps at an interval equal to *tstep*. However, the user does not need to provide times that are evenly divisible by *tstep* for the SSC calculations. In such cases, the concentration is estimated through linear interpolation between the modeled dilute leachate concentration values immediately before and after the user-provided time.

2. *When the user does not have Tmax as the final time in the Time column*

   Although SILT will model source and leachate concentrations from t = 0 to t = *Tmax*, the SSC grouping calculations do not need to be temporally bounded. In the case where a user does not have *Tmax* as their final value in the *Time* column, the stepping calculations will be performed normally, however the final source step concentration will be equal to the modeled dilute leachate concentration at the last time step provided and is then assumed to be that concentration *indefinitely* (**Figure A-7**).



N Steps	Time	Source Step Concentration (ug/L)
8	0	0.07
	150	1.61
	450	3.05
	600	2.27
	1000	0.97
	1500	0.25
	2100	0.04
	3000	0.0058

Figure A-7: *Source step concentrations without using* Tmax *as the final user-defined time. The last calculated source step concentration is assumed to be constant from t = 3000 to t = ∞.*

APPENDIX B: SANDERS (1995) EXAMPLE MODEL

SILT comes packaged with a built-in example model that is based on vadose zone fate and transport parameters presented in Sanders (1995). In that work the author utilized four different vadose zone models to compare how they modeled leachate breakthrough with volatile organic compounds. The vadose zone model parameters used in Sanders (1995) are presented below, and vary depending on the model that was used:

TABLE 2
Model Input Parameters

		SLM1	PRZM	SESOIL	IMPACT
Contamination depth range (ft)	0–4	x	x	x	x
Groundwater depth (ft)	10	x	x	x	x
Bulk density of dry soil, (g/cm³)	1.3	x	x	x	x
Saturation volume of soil (v/v)	0.41	x	x		x
Field capacity of soil (v/v)	0.20	x	x		x
Wilt point of soil, (%, v/v)	9.5		x		x
Air dry moisture content (v/v)	0.05				x
Initial moisture content of soil (v/v)	0.20	x	x		x
Organic carbon content of soil (%, w/w)	0.1	*	*	x	x
Air diffusion coefficient of contaminant (m²/d)	0.43			x	x
Water diffusion coefficient of contaminant (m²/d)	4.3×10^{-5}				x
Soil layer depth		2′	5 cm	2′ and 4′	1′
SCS Runoff Curve number (AMC II)	82		x		x
Snow melt coefficient (cm/°C-d)	0.457		x		
Minimum depth to which evaporation is extracted (cm)	17.5		x		
Crop interception potential (cm)	0		x		
Maximum crop root depth (cm)	10		x		
Maximum areal crop coverage (%)	1		x		
Condition after harvest	Fallow		x		
Hydrodynamic dispersion (cm²/d)	0		x		
Effective soil porosity (v/v)	0.20			x	
Intrinsic permeability (cm²)	2e-9			x	
Disconnectedness index	6.33			x	
Freundlich exponent	1			x	
Saturated hydraulic conductivity (ft/d)	9.83				x
"m" Coefficient (Campbell's hydraulic conductivity equation)	12.8				x
"b" Coefficient (Clapp and Hornberger's soil diffusivity and soil moisture retention equations)	4.9				x
Saturation suction head (ft; Clapp and Hornberger equations)	0.72				x
Time increment (d)		7	1	1	1
Convergence criteria	0.001				x
Root zone depth (ft)	3				x
Soil dispersivity (ft)	1				x

* Model requires Kd (K_{oc} × fractional organic carbon).

ance formulation in order to calculate soil moisture behavior. Application of Eagleson's approach in SESOIL is discussed in Bonazountas and Wagner (1984) and Hetrich *et al.* (1993).

6

The relevant model parameters from Sanders (1995) as they relate to SILT are given in the following table:

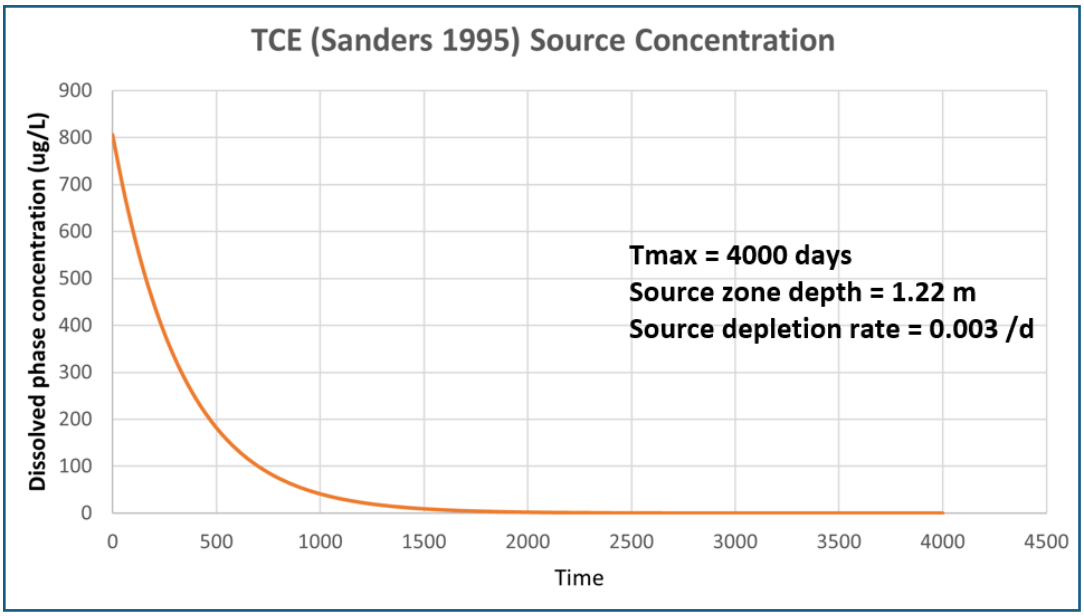
Sanders (1995) Parameter	Sanders (1995) value [units]	**SILT Parameter**	SILT value [units]
Contamination depth range	4 [ft]	**Source Zone Vertical Thickness**	1.22 [m]
Groundwater depth	10 [ft]	**Distance from bottom of source to water table**	1.829 [m
Bulk density of dry soil	1.3 [g/cm^3]	**Soil Bulk Density**	1300 [kg/m^3]
Initial volumetric water content	0.20 [-]	**Water Content**	0.20 [-]
Saturation volume of soil - initial volumetric water content	0.20 [-]	**Air Content**	0.20 [-]
Annual recharge to groundwater	21 [in/yr]	**Infiltlration Rate**	0.0015 [m/d]
Degradation rate	0 [d^{-1}]	**Decay rate in water / Decay rate in soil**	0 [d^{-1}]
Partitioning Coefficient (Koc * foc)	0.1 [ml/g]	**Soil-water partitioning coefficient**	1.00E-04 [m^3/kg]
Dilution Attenuation Factor	100	**DAF 1**	100

The parameters for the Sanders (1995) example can be populated in the spreadsheet at any time by clicking the *Sanders 1995 Example Model* button on the upper right corner of the *1 SourceZone* tab:

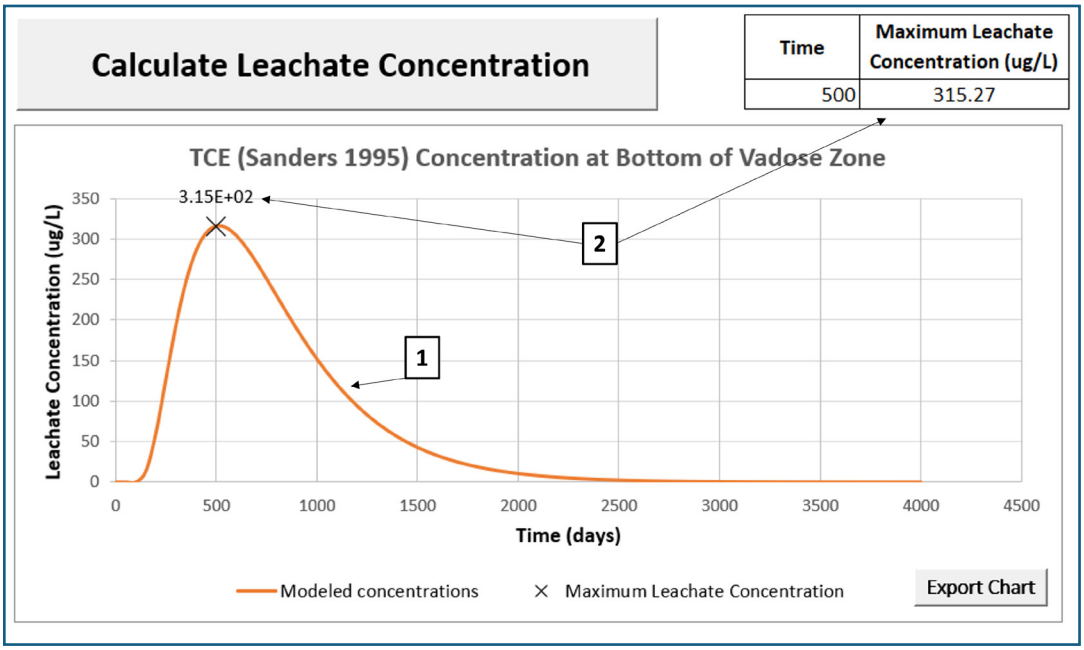
Sanders 1995 Example Model

[**NOTE:** Clicking the *Sanders 1995 Example Model* button will automatically overwrite any values included in parameter cells with the values needed for the example model. Be sure to run the example model from a blank SILT spreadsheet or save pre-parameterized models as a separate file first.]

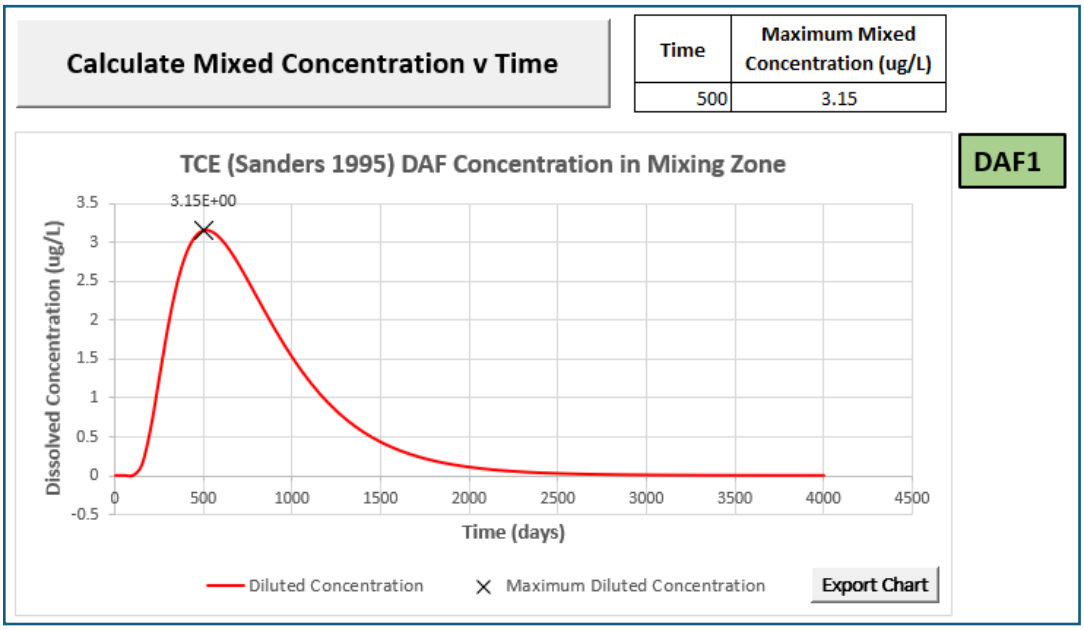
For the Sanders Example model, Source Term Option 3 was selected, and a source depletion rate of 0.003 /d was calculated. After partitioning calculations, the initial concentration in Source Zone water was 806.45 ug/L. The time series for dissolved phase concentrations in the source zone is shown below (same as **Figure 6** in *Section 1.2.3*):



The leachate breakthrough is calculated in *Step 2 – Vadose Zone*, and results in a leachate concentration curve that increases rapidly before declining at a slower pace due to the source concentration flushing out of the vadose zone and into the mixing zone (same as **Figure 9** in Section 2.2).



The peak leachate concentration occurs at approximately 850 days. After applying a Dilution Attenuation Factor of 100 (as specified in the Sanders study), the diluted leachate concentration curve in the mixing zone is shown below (same as **Figure 11** in *Section 3.3*):



The leachate breakthrough curve for TCE in SILT compares well to the leachate breakthrough curves modeled by the SLM1 and SESOIL models in Figure 2a from Sanders (1995):

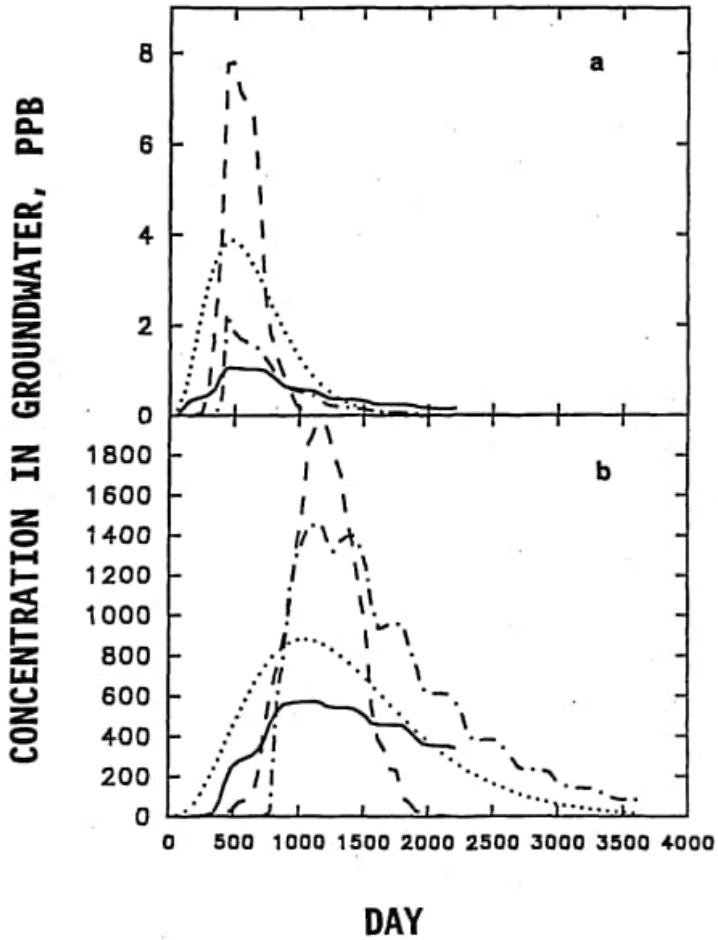


FIGURE 2. *Simulated concentrations of contaminants in groundwater vs. time using four vadose zone leaching models. Degradation was set to zero. (a) Trichloroethene (0.25 µg/g initial concentration); (b) 1,2-Dichlorobenzene (125 µg/g initial concentration).* — —, PRZM; ·····, SLM1; — · —, SESOIL; ——, IMPACT.

despite some differences in their calculated annual recharge to groundwater. This may be due to the relatively short transport times to groundwater for the chemicals studied (low K_{oc} values) and the relatively shallow water table used in the environmental scenario. This observation suggests that simplified treatment of water

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