INTRODUCTION - Revised 3/08*

SWLOAD.xls (SWL) is a Microsoft Excel spreadsheet application designed to estimate the "Qgw x Cgw" term in the equation Csw = (Qgw x Cgw)/Qsw found on page IV-14 of the December 1997 Final Draft of the Technical Guidance Manual. The application is based on An Analytical Model For Multidimensional Transport of a Decaying Contaminant Species", by P.A. Domenico, Journal of Hydrology, 91 (1987), pp 49-58. SWL solves the following equation with two modifications to be discussed below:

$$C(x,y,z,t) = \left(\frac{C_o}{8}\right)\exp\left\{\frac{x}{2\alpha_x}\left[1-\left(1+\frac{4\lambda\alpha_x}{v}\right)^{\frac{1}{2}}\right]\right\} erfc\left\{\left[x - vt\left(\sqrt{1+4\lambda\alpha_x / v}\right)\right] / 2\sqrt{\alpha_x vt}\right\}$$

$$\left\{erf\left[(y+Y/2)/2\sqrt{\alpha_y x}\right] - erf\left[(y-Y/2)/2\sqrt{\alpha_y x}\right]\right\}\left\{erf\left[(z+Z/2)2\sqrt{\alpha_z x}\right] - erf\left[(z-Z/2)/2\sqrt{\alpha_z x}\right]\right\}$$

where:

x = distance from planar source to the location of concern (i.e. property line) along the center line of the plume.

C(x,y,z,t) = the concentration of the contaminant at location x, y, z from the source at time t.

C_o = source concentration - the highest concentration of the contaminant in the groundwater at the source.

α_x = dispersivity in the x direction.

α_y = dispersivity in the y direction .

α_z = dispersivity in the z direction.

k= hydraulic conductivity.

i = hydraulic gradient

n_e = effective porosity (entered as a decimal fraction - (i.e. .25)

v = specific discharge. (ki/n_e)

λ = 1st order decay constant.

S_w = width of source area.

S_z = depth of source area.

x,y,z - these are the spatial coordinates in the horizontal, transverse and vertical directions that define the point or points where concentration information is desired.

t - this is time since the plume source started moving

In SWL this equation has been modified in two ways.

First, “v” has been modified to include a retardation factor
defined as 1+ (KOC*foc*p_b/ n_e).
where:
KOC = the organic carbon partition coefficient
foc = fraction of organic carbon expressed as a decimal percent
p_b= the dry bulk density of the aquifer matrix
and n_e = effective porosity.

Secondly, the term “Z/2” in the last two error function terms of the equation have been replaced by “Z” as described by Domenico (1987), page 53, to account for dispersion in the vertical axis in only the downward direction, as would occur with contaminants at the water table in a thick uniform aquifer and the source geometry for which this application is designed.

SYSTEM REQUIREMENTS

IBM Compatible PC
Windows 3.1 or later
Microsoft Excel 5.0 or later - with Analysis Tool Pack running. (On menu bar, click Tools, AddIns, Analysis ToolPak)
Intel 486 or better processor recommended.

GENERAL APPLICATION INFORMATION

Overview

The Domenico equation allows the calculation of the concentration of a chemical anywhere in a contaminant plume. SWL uses the Domenico equation to calculate the concentrations of a decaying retarded plume in a vertical cross-section of a plume at a distance that can be set equal to the distance to a stream or other discharge boundary which are displayed as a 11 x 11 grid. The concentrations are then added and multiplied by the flow in each cell to yield a mass loading estimate in mg/day through the cross-section. This is the "Qgw x Cgw" in the equation on page IV-14 of the TGM. SWL assumes that all of the calculated loading is discharged to the subject stream.

SWL is intended to provide only an estimate of the mass loading and is intended as screening tool. Therefore, if the mass loading is within the neighborhood of 30-50% of the level that would violate a stream standard, more rigorous in-stream sampling, monitoring and modeling efforts should be considered.

The kinds of contaminants for which SWL is intended are dissolved organic contaminants whose fate and transport are can be described or influenced by first order decay and reaction with organic carbon in the soil. The model allows for first order decay, retardation and three dimensional dispersion, which will be discussed below.

Upon selection and input of the final input parameters, the output can be printed on any Windows compatible printer using a pre-set print area.

Limitations

SWL is based on the Domenico analytical model referenced above. Only a single value of any one of the 20 or so flow and transport parameters required by the model are allowed at any one time. Therefore the model should not be used where any of these parameters vary significantly in direction or magnitude over the model domain. Further, SWL uses physical properties of the soil such as dry bulk density and fraction organic carbon which are difficult to relate to or determine for fractured bedrock aquifers. Therefore SWL should be used with caution in these environments. SWL is primarily intended for use in unconsolidated (soil) aquifers with reasonably uniform physical and hydrogeologic properties.

SWL is primarily intended for use with dissolved organic compounds and radioactive compounds that may react with organic carbon in the soil and/or may be subject to biodegradation or reaction that can be described by 1st order decay. The first order decay constant (lambda) should be set to zero where the biodegradability of the compound or its decay rate is questionable. (e.g. MTBE). SWL does not consider the transformation of a parent compound into daughter compounds (e.g. TCE to DCE). SWL considers compounds individually and assumes no reaction between compounds.

SWL is inherently conservative in that it assumes a finite source that is continuous.

Despite these many limitations, the Domenico model has been successfully applied to actual data from contaminated sites. In addition, SWL has application as a “conceptual” model where hypothetical or “worst case” conditions are investigated. By using conservative input assumptions, SWL may be useful in Pennsylvania’s Land Recycling Program in lending quantitative support to qualitative fate and transport analyses based solely on professional experience or opinion at sites which do appear to justify the time, expense and data requirements associated with more rigorous numerical modeling efforts.

NOTE: Because fate and transport models are usually calibrated to horizontal plume dimensions and concentrations, it may be useful to use the Quick Domenico model first to establish the input parameters for SWL.

Color Scheme

The cells in the spreadsheet have been color coded to assist in use and understanding.
Light Green - these cells allow the user to enter data.
Light Yellow - these cells are locked and calculated by the spreadsheet.
Other Colors - these cells are used for labels and other information not critical to use of the application.

Units

Where input requires a certain unit of measurement, it has been indicated. Because the spreadsheet contains internal formulas that depend on the units of the input data, use of improper units may result in spurious results.

Cell By Cell Description - Input Data

The following section discusses the information that is input cell by cell. The discussion will emphasize conservative selection of parameters where appropriate.

B2:D2 Enter project name

B3 Enter the date that application was prepared.

B4 Enter the name of the contaminant being evaluated.

G4 Enter the name of the person and company preparing the application.

A9 Source Concentration in mg/l - SWL allows one source concentration which is applied to the entire width and thickness dimensions of the source. The source is presumed to be continuous, which makes SWL inherently conservative for use at sites where sources have been removed or remediated. For conservative use, enter the highest concentration in the groundwater determined from the site characterization.

B9 Longitudinal Dispersivity - (Ax) - dispersion parallel to the direction of groundwater flow and water table.

C9 Transverse Dispersivity - (Ay) - dispersion perpendicular to the direction of groundwater flow and parallel to the water table.

D9 Vertical Dispersivity - (Az) - dispersion perpendicular to the direction of groundwater flow and water table. In SWL, only vertical dispersion downward below the water table is considered.

These parameters are dispersion terms which describe the extent to which contaminants spread out from the source into areas that cannot be accounted for by advective transport alone. Initially these parameters are often estimated and

then adjusted in order to calibrate a model to better fit actual field conditions. Several relationships have been proposed for initial estimates of Ax, Ay, and Az.

These are:
Ax = X/10 where X is the distance a contaminant has traveled by advective transport (i.e. velocity x time)

Ay = Ax/10

Az = Ax/20 to Ax/1000. In general, it is recommended for conservative use of SWL to use a very small vertical dispersion of, say, .001, unless vertical monitoring can reliably justify a larger number. Because of the way SWL is set up, a vertical dispersion of zero cannot be used.

E9 Lambda ($days^{-1}$) - this is the first order decay constant. It is determined by dividing .693 by the half-life of the compound (in days). The value is determined from literature or by calibration to existing data. Dispersivity values and lambda are the two most important calibration terms available in this application. SWL is very sensitive to the lambda term. For conservative use of SWL, use the lowest lambda from the range of values listed in literature references. For compounds that are not biodegradable or at sites where biodegradation is not occurring use a lambda of zero.

For initial estimates of lambda, see Appendix A, Table 5 of the Act 2 regulations. Values in Appendix A are in $years^{-1}$. Divide these values by 365 to get lambda in $days^{-1}$ for use in SWL.

F9 Source Width (ft) - enter the maximum width of the area of contaminated soils that have been impacted, or the maximum width of free product or smear zone of contamination measured perpendicular to the direction of groundwater flow. Data should be based on and justified by site characterization data.

G9 Source Thickness - typically this is the thickness of contaminated soils that contribute contamination to the water table plus the water table fluctuation that creates a smear zone.

H9 Time - (days) - this is the time (in days), after a contaminant began moving in the groundwater, for which a solution is desired. By adjusting the spreadsheet with the scroll bars so that both the grid, and time in cell H9 can be seen at the same time on the screen, adjusting the time progressively upward provides a graphical way to determine at what time steady state is reached for the particular set of input conditions represented by the input data.

A14 Hydraulic Conductivity (k)(ft/day) - the hydraulic conductivity of a geologic material is a measure of it's ability to transmit water. The hydraulic conductivity is determined from pumping or slug tests or, sometimes, laboratory tests using

standard ASTM or other methods described in numerous hydrogeology text books. SWL allows only one hydraulic conductivity measurement to be input. For conservative use, use the highest conductivity value measured at the site.

B14 Hydraulic Gradient (ft/ft)- this is the slope of the water table in the direction of ground water flow. SWL assumes horizontal flow and a uniform hydraulic gradient. Hydraulic gradient of the water table should be measured at each site. A minimum of three wells drilled to the same depth into the geologic formation is required to measure the hydraulic gradient.

C14 Effective Porosity - (decimal fraction- e.g. .25) – effective porosity is the dimensionless ratio of volume of interconnected void spaces in a geologic material to the total volume of material. Effective Porosity can be determined by sending soil samples to a laboratory or, if the texture of the material is well described, by estimating the value from text books or literature references. For conservative use of SWL use a reasonably low value for effective porosity from the range of measured or estimated values.

D14 Soil Bulk Density -(p_b) (g/cm^3) - this is the dry weight of a sample divided by its total volume in an undisturbed state. SWL is not particularly sensitive to this parameter. Samples can be sent to a lab for measurement or a value of 1.8 is often estimated.

E14 KOC - this is the organic carbon partition coefficient and is chemical specific. During formulation of the Act 2 regulations, the Department went to considerable time and expense, using outside expertise, to develop the most up-to-date KOC values. These are provided in Appendix A, Table 5, of the Act 2 regulations. Use these KOC values unless the KOC value is determined for the specific site.

F14 Fraction Organic Carbon (foc) - (decimal fraction) - this is the organic carbon content of the soil. This value can be determined by a soil laboratory using ASTM methods. Samples for organic carbon should be taken from the same soil horizon in which the contaminant occurs, but from an area that has not been impacted. For conservative use of SWL, use the lowest of the range of values determined or estimated. One/half of one per cent (.005) is a commonly estimated value.

G14 Retardation - the spreadsheet calculates this value automatically. It is defined as $1+ (KOC*foc*p_b/n)$.

H14 Velocity (V) - (ft/day) – is the rate of groundwater flow. The spreadsheet calculates this value automatically from the previous inputs.

C18 **Distance to Stream** - this is the distance to the stream measured perpendicular to the groundwater contour line or parallel to the direction of the hydraulic gradient.

C19 **Plume View Width** - In this cell, the user sets the total width of the cross-sectional window for which concentrations will be evaluated and displayed in the adjacent grid. This number will be divided by 10 to form the horizontal dimension of the grid on both sides of the centerline of the plume. **The grid width should be set such that it closely approximates the actual width of the dispersed plume at the distance from the source that is being evaluated.** This width is easily established by a trial and error approach whereby the value is adjusted so that the outer boundaries of the grid show very low but positive concentrations. Accuracy is not usually compromised severely if the outer cells alone (E17:E27 and O17:O27) contain a zero concentration with the next inner cells containing a low positive number.

C20 **Plume View Depth -** In this cell, the user sets the vertical thickness of the plume that he wishes to view. The "depth" entered here is divided by 10 to form the vertical dimension of the plume below the surface of the water table. This value is set by the user using the same trial and error procedure as in cell C19. The plume view depth should be set such that the lower most row contains zero or low positive numbers. Accuracy is not usually compromised severely if the lowest row contains a zero concentration with the next row up containing a low positive number. The user should adjust the grid such that the highest loading rate is estimated.

Output Data

E17:O17 - These cells contain the grid. The grid columns present the calculations for the concentrations at the centerline of the plume and at + or - distances from the centerline of the plume based on the value used in C19. The top row of the grid presents the concentrations for the water table surface. The rows below the top display the calculated concentrations at progressively lower depths depending on the value that was set in cell C20.

H29 This cell displays the mass loading estimate through the cross section of the plume in mg/day.

* Revised 3-08 to correct the porosity term (n) to effective porosity (n_e)