INTRODUCTION – Revised 3/08*

Quick Domenico.xls (QD) is a Microsoft Excel spreadsheet application of "An Analytical Model For Multidimensional Transport of a Decaying Contaminant Species", by P.A. Domenico, Journal of Hydrology, 91 (1987), pp 49-58. QD solves the following equation with two modifications to be discussed below:

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

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.

erf = error function

erfc = complementary error function

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 QD 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Secondly, the term “Z/2” in the last two error function terms of the equation have been replaced by “Z” as described by Domenico (1987), page 53, to account for dispersion in the vertical axis in only the downward direction, as would occur with contaminants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 comaptible) or later processor recommended.

General Application Information

Overview

Quick Domenico(QD) calculates the concentration of contaminant species at any point and time downgradient of a source area of known width, thickness and strength. The kinds of contaminants for which QD 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. In addition, QD calculates the concentrations in a two dimensional 5x10 grid whose length and width are set by the user. The output of the grid is plotted on an Excel chart each time the any element of the input data is changed. This allows users to see almost immediately the effects of changes in input data.

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

QD 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, QD 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 QD should be used with caution in these environments. QD is primarily intended for use in unconsolidated (soil) aquifers with reasonably uniform physical and hydrogeologic properties.

QD 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). QD is not appropriate for use with organic compounds that are undergoing transformation to daughter compounds (e.g. TCE to DCE). QD considers compounds individually and assumes no reaction between compounds.

Despite these many limitations, the Domenico model has been successfully applied to actual data from contaminated sites. In addition, QD has application as a “conceptual” model where hypothetical or “worst case” conditions are investigated. By using conservative input assumptions, QD may be useful in Pennsylvania’s Land Recycling Program in providing 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.

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 will 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.

A9 Source Concentration in mg/l - QD 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 QD 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 Distance to Location of Concern (x) (in feet) - this is the distance measured from the source, perpendicular to the water table contours, to the point where a concentration is desired.

C9 Longitudinal Dispersivity - (Ax) - dispersion parallel to the direction of groundwater flow and water table.

D9 Transverse Dispersivity - (Ay) - dispersion perpendicular to the direction of groundwater flow and parallel to the water table.

E9 Vertical Dispersivity - (Az) - dispersion perpendicular to the direction of groundwater flow and water table. In QD, 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 QD to use a very small vertical dispersion of .001, unless vertical monitoring and calibration can reliably justify a larger number. Because of the way QD is set up, a vertical dispersion of zero cannot be used. A value of about .001 is suggested for initial uncalibrated or conceptual applications.

F9 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. QD is very sensitive to the lambda term. For conservative use of QD, 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.

G9 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.

H9 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.

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. QD 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. QD assumes horizontal flow and a uniform hydraulic gradient (planar water table). 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 determine 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 QD use a reasonably low effective porosity value 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. QD 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 QD, 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.

A18 This cell is automatically filled by transfer of the 'X' coordinate in B7. The value is repeated here simply to facilitate the view of the x, y and z coordinates for which the spreadsheet calculates a solution.

B18 'y' (ft) This is the 'y' coordinate for which a solution is desired. For a solution on the centerline of the plume downgradient from the source, y would be set equal to zero. Otherwise 'y' is equal to distance that the location of concern is offset from the centerline along a line perpendicular to the centerline. Both positive or negative values may be entered; however, because QD provides a symmetrical solution, there is no difference in the values obtained.

C18 'z' (ft)This is the 'z' coordinate in the vertical axis at x,y of the location of concern. For most applications this should be left at zero since this value will yield the highest concentration which is at the water table.

D18 't' - (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, graphic chart and time 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.

C26:C27 These cells are where the user sets the grid dimensions for the 5 by 10 grid that appears in cells C29::K33. By setting length at 500 ft and width at 50 feet, for example, the grid would cover a length of 500 feet and a width of 50 feet on either side of the source origin. Concentrations in the plume are calculated increments of length/10 or 50 feet in this example, and for width/ 2 or 25 feet. By changing grid sizes, the user will very quickly see how grid dimensions are affected.

Output Data

A22:B22 These cells contain the source concentration calculated for the specific location and time defined in A18 through D18.

B29:K33 These cells contain the output for the grid defined by the grid dimension input in A26 and A27. For the grid output, z is fixed at zero by the spreadsheet.

The output from the grid is automatically displayed in a Microsoft Excel chart located above the grid.

The following data is the minimum that should be derived from the site characterization for use in many models although specific models may require more:

Source Geometry and Concentration
Groundwater Flow Direction
Hydraulic Conductivity
Hydraulic Gradient
Fraction Organic Carbon unless assumed to be .001

The following data may be derived from literature values or estimated based on other site characteristics :

Organic Partition Coefficient (Koc)
First-Order Decay Coefficient (Lambda)
Soil Bulk Density
Effective Porosity

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