User's Manual for the Quick Domenico Groundwater Fate-and-Transport Model

Environmental Cleanup and Brownfields

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Preface

This Quick Domenico user's manual documents the application of QD to groundwater fate-and-transport problems and is intended to encourage more consistent use of the model. It should help users appreciate the many factors that come into play with modeling. It has been written with an emphasis on the use of sound science and a conservative approach in fate-and-transport analyses. At the same time, it is recognized that the solution of these problems is limited by the data available. Some professional judgment is always involved in deciding how to apply QD to each site.

The contents of this manual reflect the experience of the Department of Environmental Protection with performing and reviewing fate-and-transport models. This document does not constitute formal DEP guidance. The responsibility for submitting an acceptable fate-and-transport analysis rests with the licensed professional geologist who seals the report submitted to DEP.

1. Introduction

1.1. Purpose of Quick Domenico

The Quick Domenico (QD) spreadsheet was developed by the Pennsylvania Department of Environmental Protection (DEP) to solve the groundwater transport equation for dissolved contaminant plumes. It incorporates a constant planar source, one-dimensional advection, three-dimensional dispersion, adsorption, and first-order decay. Solutions are presented at a point, on the centerline, and in a two-dimensional plan-view grid at any simulation time. QD is intended as a simple tool made available to the regulated community for fate-and-transport analyses.

Fate-and-transport modeling, including QD, has many important applications in site cleanups.

- Modeling is used to estimate the length of contaminant plumes to assess potential offsite impacts.

- QD predicts the plume area to determine what downgradient properties should be included in an environmental covenant.

- Fate-and-transport analyses are used to assess plume stability; that is, whether contamination will migrate in the future.

- Domenico-type models may be applied to sites for evaluating natural attenuation as a remediation strategy.

- The DEP spreadsheet SWLOAD5 implements the QD solution to indicate if a groundwater plume diffusing into surface water may cause an exceedence of water quality standards.

Fate-and-transport modeling is commonly performed for Act 2 (voluntary cleanup) and corrective action (storage tank) sites, and models are submitted for DEP review and approval. Fate and transport analyses are referred to and/or required throughout the Act 2 and Act 32 regulations (e.g., Title 25 Pa. Code Sections 250.204(f)(5) & (g), 250.303(b)(1)(ii), 250.309(c), 250.406(c), 250.408(a), 250.604(b), 250.702(b)(3)(i), 250.704(d)(2), and 250.707(a)(2)(x)(B) ; Section 245.313(b)(4)). A general discussion of groundwater fate-and-transport analyses is presented in the *Land Recycling Program Technical Guidance Manual*, Section IV.A.2. The TGM outlines the approach to modeling and DEP's reporting expectations.

Documentation is available for other Domenico-type models including EPA's BIOSCREEN, FootPrint, and BIOCHLOR. Some states have also developed documentation for their Domenico models (e.g., California). DEP has presented training on fate-and-transport modeling [*URS*, 2008]. This manual replaces DEP's QD "Introduction" document (last revised in August 2011).

Fate-and-transport analyses involve interpretations of hydrogeological conditions and they require the oversight of a licensed professional geologist. The environmental professional who submits a model to DEP is entirely responsible for using it correctly, selecting appropriate input parameter values, properly justifying his or her methods, and adequately documenting the work. Following the recommendations in this manual does not guarantee that the model will be successful or that it will be approved by DEP.

1.2. Overview of Manual

The objective of this *User's Manual for Quick Domenico* is to encourage better modeling by QD users and to improve the consistency of QD model reviews by DEP.

Quick Domenico is a solution to the solute transport equation published by *Domenico* [1987]. Its mathematical derivation is described in Appendix 1 and references therein. Section 3 defines and explains the variables in this problem (i.e., the model input parameters). More detailed discussions of two important variables, hydraulic conductivity and mechanical dispersivity, are found in Appendix 2 and Appendix 3. The QD output format is outlined in Section 4.

Procedures for calibrating Domenico models are lacking in most available documentation, and this is provided in Section 5. Section 6 describes how to run a predictive model. Two example problems are given in Appendix 4. Although *Domenico* [1987] presented an analytical solution, it is important to recognize that it is not an exact solution. Section 2 and Appendix 1 offer a critical review of the assumptions and limitations of QD modeling as well as common user errors.

1.3. System Requirements

QD may be downloaded from DEP's Land Recycling Program website. QD is written as a Microsoft Excel spreadsheet. It requires Excel version 5.0 or later. The Analysis ToolPak must be running. For Microsoft Excel 2010, do the following:

1. Click the **File** tab, click **Options**, and then click the **Add-Ins** category.
2. In the **Manage** box at the bottom, select **Excel Add-ins** and then click **Go**.
3. In the **Add-ins** box, select **Analysis ToolPak**, and then click **OK**.

2. QD Applicability

The solution of the differential equation for solute transport requires several key assumptions, and it is important to be aware of these when using QD. In addition, QD is not applicable to all groundwater contaminant transport problems, and there are some geological restrictions to its use.

Perhaps the most important limitation to any fate-and-transport analysis is the adequacy of the site data to run and calibrate the model. When data are sparse, extremely conservative input values must be used and the results may give very weak constraints. On the other hand, a properly applied and calibrated QD model can successfully simulate conditions at the site and predict contaminant distributions.

QD model assumptions and mathematical approximations are described in Appendix 1. Four critical assumptions are that aquifer properties are homogeneous and isotropic, the groundwater flow field is homogeneous and unidirectional, groundwater flow is in steady state, and the contaminant source remains constant in time. The following two sections discuss limitations to applying the model and common user errors.

2.1. Site Limitations

The user must consider conditions such as the local hydrogeology, contaminants of concern, and remedial activities to determine the applicability of QD to the site.

- QD was developed for aquifers in porous media. The conceptual site model should support the decision that this condition has been met. QD is *absolutely not* applicable to karst formations. QD modeling of contaminant transport in fractured bedrock should be performed with care and it must include calibration.

- QD simulates only the first-order decay of dissolved contaminants during transport. For instance, it is appropriate for petroleum hydrocarbons and polycyclic aromatic hydrocarbons (PAHs), and it can also represent radioactive decay. It does not account for the formation of daughter products from parent compounds (e.g., trichloroethylene → cis-1,2-dichloroethylene → vinyl chloride). Biochlor is a preferable model for chlorinated VOCs.

- QD is intended for modeling organic contaminants. Nonreactive inorganic solutes do not experience natural degradation, and the first-order decay constant (λ) should be set to zero. The sorption of inorganics on soil particles is a complex process which is not adequately represented by the linear isotherm of QD. Therefore, the user should also input the adsorption parameters (K_{oc} and f_{oc}) as zero when modeling inorganics.

- QD is applicable to problems of natural attenuation of contaminants. Extreme caution should be exercised with its use at sites where there has been active remediation. A calibration to conditions before or during remediation may not be appropriate for the post-remediation period. Likewise, a calibration to onsite wells in the vicinity of the remedial work may not extrapolate to offsite conditions.

- Similarly, QD does not simulate decaying sources. If there is evidence for source decay (as opposed to transport decay) the user should consider using Bioscreen-AT (see Example A4.2).

- Ethanol is now a standard component of gasoline, and it has a significant influence on the fate and transport of petroleum contaminants. Because ethanol degrades faster than other constituents, electron acceptors in the aquifer are depleted, preventing the biodegradation of BTEX and other hydrocarbons. With time and distance, ethanol concentrations in the plume decline, and this makes biodegradation of other contaminants favorable. QD cannot simulate longitudinally variable values of the decay constant (λ). An alternative model is EPA's FootPrint.

- QD cannot be used to model the fate and transport of non-aqueous phase liquids (NAPL), also known as separate phase liquids or free product. However, with adequate supporting information QD can represent the dissolved plume originating from a NAPL source by inputting effective solubilities of the contaminants for the source concentrations.

2.2. Common Errors

DEP has repeatedly seen the following mistakes by QD users. DEP may reject the submitted model and report for any of these reasons.

- **Modeling a plume without any downgradient calibration points within the zone of impact** (see Section 5).
Under some circumstances extremely conservative models may be accepted without calibrations, but they require careful selection of parameter values. The first-order decay rate should be zero or very low. Calibration is usually essential to a defensible model.

- **Using inconsistent data for calibration, such as well data collected at different times**.
Contaminant concentrations should be measured at the same time (or period) for the source and calibration wells.

- **Selecting and/or varying input parameters without justification** (see Section 3).
Values should be based on site-specific data, calibrations, and appropriate literature references. Uncertain parameters must be adequately conservative, and all values must fall within physically plausible ranges.

- **Using an inappropriate degradation rate (λ)** (see Section 3.3).
A site-specific natural (bulk) attenuation rate may be estimated from onsite contaminant measurements. When using values from Ch. 250, Table 5A (labeled as "degradation coefficient (K)"), which are only representative empirical rates, one must convert from inverse years (yr^{-1}) to inverse days (day^{-1}) for input in QD. The degradation rate should generally be a calibration variable. Conservative models may assume $\lambda = 0$.

- **Choosing an unsupported hydraulic conductivity (K)** (see Section 3.7 and Appendix 2).
Hydraulic conductivity is ideally based on multiple well tests at the site. Data and solutions for

the conductivity must be fully documented. When using a literature value of K, the choice must be explained and properly referenced. It should be a conservative choice taken from representative values for the hydrostratigraphic unit. When treating K as a calibration variable, its value should be within a reasonable range. We recommend uncertainty analyses to understand the influence of K.

- **Using excessively large dispersivities (α)** (see [Section 3.2](#) and [Appendix 3](#)).
  Insofar as dispersivity scales with plume length, users often presume that longer plumes and correspondingly higher dispersivities are always more conservative. However, larger dispersivities can spread the plume out, reducing centerline concentrations. Large values of α may introduce errors in the QD solution ([Section A1.3](#)). Dispersivity should be scaled with respect to the distance to the nearest calibration point and/or receptor within the plume.

- **Modeling with QD when groundwater flow is complicated**.
  Groundwater flow should be unidirectional and relatively constant in time.

- **Appling QD to contaminants that degrade to regulated breakdown products**.
  QD is not recommended for chlorinated VOCs. EPA's [Biochlor](#) is an alternative for plumes undergoing reductive dechlorination.

- **Using QD for inorganic contaminants**.
  Inorganics may be modeled under certain circumstances. Parameter values must be chosen carefully, and the approach must be justified.

- **Using old data to develop a QD model**.
  The QD solution should be based on recent monitoring data.

- **Demonstrating attainment with QD.**
  A remediator cannot use a fate-and-transport model to demonstrate attainment of a groundwater standard at the point of compliance. Act 2 requires that this be accomplished with the statistical analysis of monitoring well data (Title 25 Pa. Code Section 250.704(b)).

- **Failing to map the observed area of impact**.
  Concentration maps using contemporaneous monitoring well data should be submitted for all contaminants of concern. (Refer, for example, to Title 25 Pa. Code Section 245.313(b)(4)(i).)

- **Failing to plot the modeled plume area on a map, with the centerline shown**.
  The maximum plume extent in plan view should be depicted.

- **Failing to map impacted downgradient properties**.
  All potentially affected properties (both down- and side-gradient), as predicted by the QD solution, should be depicted on the map. This is essential if there is to be an environmental covenant.

- **Submitting a report without the seal of a licensed professional geologist**.
  Fate-and-transport modeling constitutes a subsurface interpretation. A professional seal is required for such analyses under DEP's regulations (e.g., Title 25 Pa. Code Sections 245.314 and 250.408(a)).

3. QD Model Input Parameters

This section describes each of the input parameters in the QD model. The user must ensure that appropriate site-specific values are input for each parameter, as the default selections are not generally applicable, and that the units are correct. We emphasize the selection of conservative values.

The sensitivity of the model to changes in the values is indicated below in a qualitative manner. More attention should be paid to high-sensitivity parameters in the calibration. The sensitivity of the solution should be evaluated by the user for every site model (Section 5.2). Keep in mind that different aspects of the solution (e.g., centerline concentrations, plume length, plume width, mass loading) are not all sensitive to the same parameters. Here sensitivity is indicated with respect to centerline concentrations.

The QD coordinate system is defined as:
    x—flow direction (longitudinal)
    y—perpendicular to flow (transverse)
    z—vertical.

The QD spreadsheet cells have been color-coded to assist in data entry.
    Light green—these cells are for the input parameters
    Light yellow—these cells are locked and they are calculated by the spreadsheet
    Other colors—these cells are used for labels and other information not critical to using QD.

3.1. Source Concentration

Symbol: C_0	**Units:** mg/L	**Sensitivity:** High

The model assumes a uniform, constant aqueous phase source concentration. That is, the contaminant source does not vary spatially, and it does not decay with time. The source takes the form of a vertical plane oriented perpendicular to the groundwater flow direction. It should be located at the downgradient limit of the identified source area. This might be the zone of impacted soils, the extent of LNAPL, the area of maximum groundwater concentrations, the tank field, or the spill area.

The source concentration should be selected from well data that is concurrent with the calibration point data. Therefore, one should not use historic source concentrations and current calibration well concentrations. If C_0 is uncertain (e.g., there are no wells at the source), then it should be a variable, in which case measured values would serve as a lower bound.

If the source concentration has decayed significantly over time, then QD is *not an appropriate model*. Source decay occurs via mass loss from dissolution and other processes. EPA's Bioscreen or the Bioscreen-AT model may be used to simulate an exponentially decaying source; see Example A4.2. Historical data may be used to estimate the decay rate or source half-life. Applying QD to problems where there has been source loss may *not* be conservative.

3.2. Dispersivities

Symbol: α	Units: ft	Sensitivity: High

Dispersion is the process of mechanical mixing of a solute in groundwater. Dispersion is a property of the aquifer, not the contaminant. It causes some spreading of the contamination forward of the advective front as well as laterally. The user inputs three dispersivities: longitudinal (α_x), transverse (α_y), and vertical (α_z).

Dispersivities cannot be measured in the field, and values must be estimated (Appendix 3). It is important to recognize that dispersion is a function of the transport scale; the larger the scale, the larger the dispersion. Therefore, dispersion likely increases with x rather than having a fixed value as in QD.

Several relationships for dispersivity have been published. DEP recommends an initial value of $\alpha_x = 0.1x$ where x is the distance to a calibration point, the nearest receptor, or the plume length, depending on the scale of concern.

The transverse dispersivity is commonly defined as $\alpha_y = 0.1\alpha_x$. Calibrating α_y could be accomplished if there is sufficient site data to delineate the plume width. The vertical dispersivity should be small for conservative modeling ($\alpha_z = 0.001$ ft) as this approximates two-dimensional transport. Larger values of α_z might be used if vertical contaminant profiles support estimation and calibration of downward dispersion of the plume.

Fate and transport modeling has a significant sensitivity to the dispersivities. If dispersivities are zero or are too small, then the modeled plume length and width will be underestimated. If the dispersivities are too large, then the plume will be spread out in an unrealistic manner, reducing the centerline concentrations. A common error is to assume a long plume and consequently a large value of α_x. This is not necessarily a conservative approach, and modeled concentrations at the nearest receptor may be underestimated.

Further information on dispersivities is found in Appendix 3. The mathematical errors associated with excessively large dispersivities are described in Section A1.3.

3.3. Decay Constant

Symbol: λ	Units: day^{-1}	Sensitivity: High

The first-order decay rate represents the degradation of the contaminant as it moves through the aquifer with time. We call this the *transport decay*, and it is distinct from the *source decay*. The decay constant is related to the half-life by $\lambda = 0.693/t_{1/2}$. The degradation rate is a critical parameter because it influences the downgradient change in contaminant concentrations more than any other.

There is a large uncertainty in degradation rates, and actual rates depend on site-specific conditions. Therefore, λ should be a calibration parameter in most QD models. Starting values may be found in the literature [e.g., *Howard et al.*, 1991] or Ch. 250, Appendix A, Table 5A.

However, these are estimated values or ranges based on limited field studies or experiments; the user cannot assume that they reflect conditions at every site. For instance, anaerobic conditions in an aquifer might cause decay rates to be much slower than measured in an aerobic environment. Initial site-specific values may also be estimated from the bulk attenuation rate constant derived from field data [*Newell et al.*, 2002].

When calibrating the model, it is important for the user to be able to recognize source decay and distinguish it from transport decay. Note that the constant-source assumption in QD (zero source decay) means that concentrations throughout the plume will only increase and reach a constant value at steady state. Decay of a source will result in the eventual decline of downgradient concentrations with time, and a calibrated value of λ in QD can be exaggerated. Applying QD to problems with source decay is not conservative. Refer to Example A4.2 for a comparison of models with and without source decay.

If site data do not exhibit transport decay, then the decay constant should be input as zero. When modeling inorganic contaminant transport, $\lambda = 0$.

3.4. Source Width

Symbol: Y	Units: ft	Sensitivity: Medium

The source width should equal the maximum width of known or inferred groundwater contamination at the site. This could be indicated by impacted soils from sampling or visual observations, the presence of NAPL, or elevated dissolved concentrations in monitoring wells. The source is oriented perpendicular to the direction of groundwater flow in the model.

Centerline concentrations tend to increase with increasing source widths (though this relationship depends on the value of α_y). The source width will control the plume width, so it can be significant for identifying impacted properties cross-gradient to the plume centerline. The source width is critical to the plume mass loading. Therefore, when modeling stream impacts this parameter must be accurate.

3.5. Source Thickness

Symbol: Z	Units: ft	Sensitivity: Low

The source thickness should equal the maximum depth range of contamination in the aquifer at the source (i.e., below the seasonally high water table). For petroleum contaminants this is the smear zone. The depth of contamination in the saturated zone is best determined using nested wells to vertically delineate the source.

The predicted centerline concentrations and plume length have virtually no sensitivity to the source thickness. However, the source thickness is critical to the plume mass loading. Therefore, when modeling stream impacts this parameter must be defined carefully.

3.6. Time

Symbol: t	Units: days	Sensitivity: Medium

Time is measured from the date of the release. Steady state is achieved when the farthest downgradient concentrations no longer change with increasing time. The user should determine when steady state occurs because thereafter the calibrations and predictions will not be sensitive to the age of the plume. Under typical conditions steady state is realized within a few years. When there is source decay (e.g., in Bioscreen models) time is much more important because the model never attains steady state.

3.7. Hydraulic Conductivity

Symbol: K	Units: ft/day	Sensitivity: High

Contaminant transport is dominated by advective groundwater flow. The groundwater velocity is primarily controlled by the hydraulic conductivity and hydraulic gradient. Properly selecting the hydraulic conductivity with well test data, model calibration, or appropriately conservative literature values is essential for a valid analysis. Refer to Appendix 2 for more information on hydraulic conductivity.

The recommended sources of hydraulic conductivity are the results of pump tests or multiple slug tests at the site. These results should not be considered exact values of hydraulic conductivity for the site because there can be large spatial and directional variations. Therefore, hydraulic conductivity should be a calibration parameter in the model solutions.

If there is no well test data, then other information sources may be used (Appendix 2). However, calibration is key for such models. Under some circumstances a very conservative value of K may be selected without calibrating the model. The user should not assume that only large values of K are conservative (Example A4.1).

If there is no transport decay ($\lambda = 0$), steady state QD model results will have no dependence on K.

3.8. Hydraulic Gradient

Symbol: i	Units: ft/ft	Sensitivity: Medium

Hydraulic gradient is the slope of the potentiometric surface in the direction of groundwater flow. It is calculated from static water level measurements at monitoring wells. This parameter must be based on site measurements and not be an estimate. Any longitudinal variation of the gradient should be evaluated. A useful calculator for determining the maximum gradient of a planar surface fit to hydraulic head measurements may be found at EPA's Online Tools for Site Assessment website.

The groundwater flow velocity is proportional to the hydraulic gradient. The gradient should not be a calibration variable in the QD model because the uncertainty in the flow velocity is accounted for by varying the hydraulic conductivity (Section 3.7).

3.9. Effective Porosity

Symbol: n_e	**Units:** —	**Sensitivity:** Low

Effective porosity is the nondimensional ratio of interconnected void space to the bulk volume of the aquifer material. (It is less than the total porosity which includes all void spaces.) Values for unconsolidated sediments can vary greatly, from 0.01 to ~0.40. An appropriate value for porous media is 0.3, but the user should select a porosity corresponding to the aquifer material at the site.

The groundwater flow velocity is inversely proportional to the effective porosity. It is also a factor in the retardation factor calculation (Section 3.16). The effective porosity should not be a calibration variable in the QD model because the uncertainty in the flow velocity is better accounted for by varying the hydraulic conductivity (Section 3.7).

3.10. Bulk Density

Symbol: ρ_b	**Units:** g/cm^3	**Sensitivity:** Low

The aquifer matrix bulk density is input on a dry basis. A typical value for unconsolidated materials is 1.7 g/cm^3.

The bulk density is used to calculate the solute adsorption, or retardation, factor, R (Section 3.16). The retardation, in turn, affects the contaminant velocity. Therefore, the bulk density should not be varied in the QD calibration; the uncertainty in the velocity is accounted for by varying the hydraulic conductivity (Section 3.7).

3.11. Organic Carbon Partition Coefficient

Symbol: K_{oc}	**Units:** L/kg	**Sensitivity:** Low

The partition coefficient relates the affinity of the dissolved contaminant for organic carbon in the soil. Values are chemical specific. Larger values reflect a greater tendency to adsorb onto the soil. The user should input values found in Ch. 250, Appendix A, Table 5A. Alternative values should be fully justified.

The organic carbon partition coefficient is used to calculate the solute adsorption, or retardation, factor, R (Section 3.16). The retardation, in turn, affects the contaminant velocity. K_{oc} is a relatively well determined quantity, and it should never be treated as a variable when calibrating QD. For inorganic solutes $K_{oc} = 0$.

3.12. Fraction of Organic Carbon

Symbol: f_{oc}	**Units:** —	**Sensitivity:** Low

This is the weight fraction of natural organic carbon in the uncontaminated aquifer soil matrix. It determines the organic carbon available for hydrocarbons to adsorb to the solid phase. It is desirable to measure this quantity in samples from the site, but it is more commonly estimated. Typical values are 0.0002–0.005. An appropriate default value is 0.002. A conservative value in some bedrock formations would be zero.

The fraction of organic carbon is used to calculate the solute adsorption, or retardation, factor, R (Section 3.16). The retardation, in turn, affects the contaminant velocity. Therefore, the f_{oc} should not be a variable in the QD calibration; the uncertainty in the velocity should be accounted for by adjusting the hydraulic conductivity (Section 3.7). For inorganic solutes $f_{oc} = 0$.

3.13. Point Concentration Location

Symbol:	(x_s, y_s, z_s)	**Units:**	ft	**Sensitivity:**	None

The user may calculate a contaminant concentration at a solution point in the aquifer (x_s, y_s, z_s). Maximum surface centerline concentrations are at (x_s, 0, 0). These coordinates are not model variables and they only affect the output information.

3.14. Model Calculation Domain

Symbol:	L, W	**Units:**	ft	**Sensitivity:**	None

The user inputs the length and width of the area where a solution is desired. The length (L) is the distance downgradient from the source. The width (W) is actually the half-width perpendicular to the flow direction (the true width is twice the input value). The solution is obtained at the same depth (z_s) as the point concentration location (Section 3.13). These distances are not model variables and they only affect the output information.

3.15. Field Data

Symbol:	x_i	**Units:**	ft	**Sensitivity:**	None
Symbol:	C_i	**Units:**	mg/L	**Sensitivity:**	None

The user enters analytical data from one or more downgradient wells to calibrate and validate the model. The centerline concentration (C_i) should be from wells on or near the plume centerline. The longitudinal distance from the source (x_i) is entered for each well. Care must be taken in selecting the data for calibration, and we recommend using average concentrations (Section 5.2).

The model-calculated solution is not affected by the calibration point data entered in the worksheet. However, the user-calibrated solution is highly sensitive to these values.

3.16. Calculated Quantities

The groundwater velocity and retardation factor are important parameters that are not input by the user because they are calculated by the model from other variables.

The interstitial **groundwater velocity** (v), or seepage velocity, is determined as follows:

$$v = \frac{Ki}{n_e}$$

K: hydraulic conductivity
i: hydraulic gradient
n_e: effective porosity

The Domenico solution is a function of the contaminant velocity. This may be less than the groundwater flow velocity owing to solute adsorption. Only one of the parameters in v (typically K) should be used as a calibration variable while best estimates of the others should be selected.

The **retardation factor** (R) is defined as:

$$R = 1 + \frac{K_{oc} f_{oc} \rho_b}{n_e}$$

K_{oc}: organic carbon partition coefficient
f_{oc}: fraction organic carbon
ρ_b: bulk density
n_e: effective porosity.

The contaminant velocity (v_c) equals the groundwater velocity reduced in proportion to the retardation factor: $v_c = v/R$. The retardation factor should equal one for inorganic substances (i.e., $K_{oc} = f_{oc} = 0$).

4. QD Model Output

Quick Domenico displays numerical and graphical outputs of the model solution.

A point concentration (mg/L) is calculated for the coordinates and time that were input. Also, contaminant concentrations (mg/L) are determined on a two-dimensional horizontal grid for the domain specified by the length and width input parameters. The grid has ten columns in the x direction (downgradient) and five rows in the y direction (cross-gradient), including the centerline.

Modeled centerline concentrations are plotted with distance from the source. Graphs with linear and logarithmic concentration scales are displayed. The centerline field data are also plotted for comparison and calibration.

5. Calibrating the QD Model

5.1. Objective

Calibration is a crucial part of fate-and-transport modeling. It allows the user to refine the parameter values by matching the simulation to field data. If successful, calibration demonstrates that the model can reproduce actual measurements, and it gives us some confidence that it can therefore be used to predict plume concentrations at other locations and times. The objective is to constrain the parameter values to improve the accuracy of the model.

Fate-and-transport model calibrations are not unique because there are several poorly determined sensitive variables (namely the first-order decay rate, the hydraulic conductivity, and the dispersivities). A successful calibration does not guarantee that the model will accurately predict conditions throughout the plume or in the future.

Although we always recommend use of calibration points, in some cases it may be acceptable to use QD without a calibration. It is not always feasible to install calibration wells at the site, and an uncertainty analysis may demonstrate that conservative parameter values result in a satisfactory outcome. In general, without a calibration the model must be run with very conservative inputs, and the parameter choices must be fully justified (e.g., see Appendix 2 and Appendix 3). The licensed professional geologist submitting the report is responsible for defending the analysis with or without a calibration.

5.2. Methodology

DEP advocates a systematic approach to model calibration. This manual describes calibration with only three significant variables: hydraulic conductivity (K), longitudinal dispersivity (α_x), and decay rate (λ). It is important to evaluate the sensitivity of the model to different combinations of these parameter values to find the most conservative result.

The user must consider whether or not a well with nondetect results is a suitable calibration point. If the plume is in steady state, and the well is truly directly downgradient of the source, we know that contamination has not and presumably will not extend that far. However, calibrating to nondetect field data will usually give only a lower bound on the transport decay rate.

We recommend the following steps to calibrate QD models.

1. **Select the calibration well(s).** Normally modeling is conducted after monitoring wells have been installed and data have been collected. The wells chosen for calibration must be downgradient of the source and close to the centerline. Off-centerline wells might be suitable if they are close enough, relative to the source width, such that the contaminant concentrations are fairly uniform across the plume. If not, then you could attempt to calculate the concentration at the off-centerline location (i.e., $y \neq 0$). If no existing wells will serve as calibration points, then one or more new wells may need to be installed. Generally, when there are more wells available for calibration the model will be better constrained, though in some instances no solution will match the field data from all of the calibration wells. In this

situation you must exercise your judgment to fit the model and decide which wells best represent the contaminant distribution.

2. **Measure the distance of the well(s) from the source.** This should be done with proper accuracy.

3. **Determine the calibration values.** Concentration data should be available for the wells in at least four consecutive quarters for the final model. Concentrations may vary significantly from quarter to quarter, and the calibration can be very sensitive to the value used. Picking a single measurement to calibrate the model may bias the results if it is not representative of the typical concentrations in that area at that time. For this reason you should average a few quarters of data at each well. Alternatively, you can calibrate the model to the highest observed value to be conservative. These steps must be taken for each contaminant of concern at each calibration well.

4. **Determine the calibration time.** This is the time since the release, whether known or estimated. It should not be the time since the source concentration (C_0) was measured in a well because QD presumes a constant source over time. The model will be sensitive to this time if it isn't in steady state.

5. **Choose the "known" parameter values.** Of the three key parameters, only hydraulic conductivity is likely to be constrained based on well testing or knowledge of the soil type or lithology of the aquifer (Appendix 2). The starting values of the other parameters, longitudinal dispersivity and decay rate, can be estimated using standard quantities (e.g., one-tenth the calibration distance for α_x and Ch. 250 Table 5A values for λ). These values will need to be varied in the calibration.

6. **Assess acceptable ranges for the parameters.** No values are known with certainty, and they typically vary spatially and/or with changing subsurface conditions. Therefore, even a site measurement of hydraulic conductivity will not be a unique model input. Decide what reasonable ranges of the parameter values are. This will normally be one or two orders of magnitude (Appendix 2 and Appendix 3).

7. **Choose a parameter to vary.** Only one of the unknown parameters (K, α_x, or λ) will be varied at a time. The other parameters are initially assigned estimated or preferred values. Change this parameter's value within the acceptable range until you obtain the best fit to the calibration data. If the fit is not satisfactory, explore changes to the other parameters to improve the match. You may need to reassess the acceptable ranges or other parameters if the solution still doesn't agree with the field data.

8. **Vary each of the other calibration parameters.** With three significant parameters there will be multiple possible solutions. You will need to systematically vary each parameter within the acceptable range to obtain a suite of solutions. Obviously this method could result in numerous model runs and different results. In practice, though, you can focus on the conservative parameter values and some combinations will be rejected because they don't reproduce the calibration data. Many solutions will look alike because the steady state Domenico curves have the same shape.

9. **Compile the successful parameter combinations.** Record the combinations of parameter values that give models matching the calibration data. These will serve as the basis for the predictive models.

Example. Suppose repeated slug tests at multiple wells at the site yielded an average hydraulic conductivity of $K = 1.4$ ft/day. The distance from the source to the nearest calibration point is 100 ft, so we select one-tenth of this distance for the estimated longitudinal dispersivity, $\alpha_x = 10$ ft. The contaminant of concern is benzene, and DEP's Ch. 250 Table 5A degradation coefficient is $\lambda = 9.6 \times 10^{-4}$ day^{-1}. These are the starting values of each of these parameters. We assume an uncertainty in both K and α_x of a factor of ten, and the uncertainty in λ could be greater than that. Therefore, the calibration ranges are $K = 0.14$–14 ft/day and $\alpha_x = 1$–100 ft, and λ is an entirely free parameter (that is, it can have any value greater than or equal to zero).

We run a sequence of models, systematically changing K and α_x within their ranges and varying λ as necessary in each run until the solution fits the calibration data. The model inputs would be as follows:

Model	K (ft/day)	α_x (ft)
1	1.4	10
2	1.4	1
3	1.4	100
4	0.14	10
5	0.14	1
6	0.14	100
7	14	10
8	14	1
9	14	100

Also see Examples A4.1 and A4.2.

5.3. Model Validation

The calibration will result in multiple possible models that explore the range of likely parameter values and that match the field data at one point in time. Whenever possible, these models should be validated by obtaining solutions at other times and comparing the resulting concentrations to the field data at those times. (This is also known as "history matching" or verifying the model.) If a solution cannot reproduce the data at other times, then it can be rejected. This process allows the user to refine the number of acceptable models. If the data indicate that the plume is in steady state, then the user might not be able to validate the model in this way. If calibration well concentrations are decreasing, then that implies source decay, and QD is not an appropriate model; the user should consider Bioscreen or Bioscreen-AT.

6. Running a Predictive Model

6.1. Methodology

Having defined a range of parameter combinations that can reproduce the field measurements, the user can next run predictive models. These models will estimate the contaminant concentrations at other locations and times to estimate plume lengths and widths, potential impacts at downgradient potable wells and streams, etc.

Because the calibration procedure likely yielded multiple plausible models (Section 5.2), each of these will be run as a predictive model. For the example at the end of Section 5.2, up to nine calibrated models would be run to simulate the plume. The user will select the most conservative result for each contaminant (e.g., the longest benzene plume).

Keep in mind that for QD the concentration at a given distance from the source only increases with time until the model reaches steady state. DEP recommends evaluating the results at 30 yr, but the user should verify that the model is in steady state by then. Steady state may be much earlier (e.g., if K is relatively high), and the calibrated solution may already be at steady state. In this case the results at 30 yr would be unchanged from the calibration time. SWLOAD calculates a solution at infinite time (10^{99} days).

It's important to recognize that if the source is decaying, then the concentration at a given distance will initially increase and then decrease with time. There is no steady state. The model time is critical to a non–steady state solution, and the worst case (maximum concentrations or longest plume) may be at the present, not in the future. (See Example A4.2.)

6.2. Results

6.2.1. Point of Compliance

Concentrations are calculated at the centerline distance to the point of compliance. The model with the highest concentration is selected for evaluating potential exceedences.

6.2.2. Plume Morphology

QD is a valuable model for mapping the planform shape of the plume to determine where it exceeds Statewide health standard (SHS) medium-specific concentrations (MSCs) and/or practical quantitation limits (PQLs). This must be known for preparing post-remediation care plans and environmental covenants. The predictive models are run iteratively by varying the point concentration solution location (x_s) to determine the centerline distance to each MSC or PQL. The models with the longest distances are selected as the most conservative. The plume morphology will depend on the downgradient transport distance relative to the source width. Typically the plume width will be approximately equal to the source width because transverse dispersivity is relatively low.

6.2.3. Downgradient Impacts

If the concentration at a specific point (x_s, y_s) needs to be estimated, for instance at a drinking water or public supply well, then the user runs models for that location. The model with the highest concentration is selected.

6.2.4. Stream Loading

To evaluate loading of the plume to a surface water body, the user transfers the calibration model parameters to SWLOAD. SWLOAD is run for each parameter combination to determine the average concentration and groundwater influx rate to the stream. (See the Act 2 *Technical Guidance Manual*, Section IV.A.3.) The model with the highest average concentration is selected.

6.3. Report Contents

The Quick Domenico model analysis should be fully documented in the submitted report. The fate-and-transport content of the report should generally include the following elements, depending on the complexity of the modeling. (Refer also to the *Technical Guidance Manual*, Section IV.A.2.h.)

- A discussion of why application of QD is appropriate in the context of the conceptual site model (Section 2).

- A table of all initial and final parameter values, including parameter ranges (Section 3).

- A complete explanation of the input values used.

- Specification of the calibration wells and field data values.

- A description of the uncertainty or sensitivity analysis and calibration (Section 5).

- Predictive model conditions and results (Section 6).

- Figures showing the source location, source and calibration wells, plume centerline, and the planform shape of each contaminant of concern at the site.

- Appendices with QD worksheet printouts for calibration and predictive model runs for each contaminant of concern.

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Xu, M., and Y. Eckstein, Use of weighted least squares method in evaluation of the relationship between dispersivity and field scale, *Ground Water*, *33*, 905–908, 1995.

Note: Web links were valid as of February 24, 2014.

Web Links

California Regional Water Quality Control Board—Los Angeles Region, *Manual for Domenico Non–Steady State Spreadsheet Analytical Model.*

Commonwealth of Pennsylvania, Title 25 Pa. Code, Ch. 245, Administration of the Storage Tank and Spill Prevention Program.

Commonwealth of Pennsylvania, Title 25 Pa. Code, Ch. 250, Administration of the Land Recycling Program (Act 2).

PA DEP, Land Recycling Program Technical Guidance Manual.

PA DEP, Quick Domenico.

S. S. Papadopulos and Associates, Inc., BIOSCREEN-AT.

US EPA, BIOCHLOR.

US EPA, BIOSCREEN.

US EPA, Center for Subsurface Modeling Support.

US EPA, FootPrint.

US EPA, On-Site calculators.

USGS Pennsylvania Water Science Center

Note: Web links were valid as of February 24, 2014.

Appendix 1.   QD Model Background

A1.1. Model Derivation

Domenico [1987] published a solution to the three-dimensional differential equation for solute transport in a saturated porous medium with uniform steady-state flow, one-dimensional advection, three-dimensional dispersion, adsorption, and first-order decay [*van Genuchten*, 1985]:

$$\frac{\partial}{\partial t}(n_e C + \rho S) = \frac{\partial}{\partial x}\left(n_e D_x \frac{\partial C}{\partial x} - qC\right) + n_e D_y \frac{\partial^2 C}{\partial y^2} + n_e D_z \frac{\partial^2 C}{\partial z^2} - \lambda_w n_e C - \lambda_s \rho S \qquad \text{(A1-1)}$$

where:

Table A1.1.

Symbol	Definition	Units
C	solute concentration	$M\,L^{-3}$
S	adsorbed concentration	$M\,M^{-1}$
n_e	effective porosity	$L^3\,L^{-3}$
ρ	bulk density	$M\,L^{-3}$
D_i	coefficients of dispersion	$L^2\,T^{-1}$
q	groundwater flux (Darcy velocity)	$L\,T^{-1}$
λ_w	water decay coefficient	T^{-1}
λ_s	soil decay coefficient	T^{-1}
x	longitudinal horizontal distance	L
y	transverse horizontal distance	L
z	downward vertical distance	L
t	time	T

M: mass, L: length, T: time

See Section 3 for a discussion of these parameters.

The following assumptions apply:

- The dissolved and adsorbed contaminant decay coefficients are equal
  $\lambda = \lambda_w = \lambda_s$.

- Properties (n_e and q) are constant in space and time, so there is steady-state flow.

- Adsorption is described by a linear, reversible isotherm
  $S = K_d C$
  where K_d is an empirical distribution coefficient ($M^{-1}\,L^3$), and for organics
  $K_d = K_{oc} f_{oc}$
  where K_{oc} is the organic carbon partition coefficient and f_{oc} is the fraction of organic carbon.

See Section A.1.2 below for a further discussion of model assumptions.

The transport equation is then expressed as:

$$\frac{\partial C}{\partial t} = \frac{\alpha_x v}{R}\frac{\partial^2 C}{\partial x^2} + \frac{\alpha_y v}{R}\frac{\partial^2 C}{\partial y^2} + \frac{\alpha_z v}{R}\frac{\partial^2 C}{\partial z^2} - \frac{v}{R}\frac{\partial C}{\partial x} - \lambda C = 0 \tag{A1-2}$$

where:

Table A1.2.

Symbol	Definition	Expression	Units
R	retardation	$1 + \dfrac{\rho K_d}{n_e}$	—
α_i	dispersivity	D_i/v	L
v	interstitial groundwater velocity	q/n_e	L T^{-1}

The following initial and boundary conditions are applied:

- $C(x, y, z, 0) = 0$ (A1-3)

- $C(0, y, z, t) = C_0$ for $-\tfrac{1}{2}Y \le y \le +\tfrac{1}{2}Y$ and $0 \le z \le Z$ (A1-4)

- $\lim\limits_{x\to\infty} \dfrac{\partial C(x, y, z, t)}{\partial x} = 0$ (A1-5)

- $\lim\limits_{y\to\pm\infty} \dfrac{\partial C(x, y, z, t)}{\partial y} = 0$ (A1-6)

- $\lim\limits_{z\to\infty} \dfrac{\partial C(x, y, z, t)}{\partial z} = 0$ (A1-7)

The *Domenico* [1987] solution of Equation (A1-2) subject to these boundary conditions, and with the inclusion of adsorption, is as follows:

$$C(x, y, z, t) = \frac{C_0}{8}\exp\left[\frac{x}{2\alpha_x}\left(1 - \sqrt{1 + \frac{4\lambda R\alpha_x}{v}}\right)\right] \times \mathrm{erfc}\left(\frac{x - vt\sqrt{1 + \dfrac{4\lambda R\alpha_x}{v}}}{2\sqrt{\dfrac{\alpha_x vt}{R}}}\right) \tag{A1-8}$$

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

Note that this is a truncated, and not an exact, solution to the problem. Here it is assumed that contamination resides at the top of the aquifer and the only vertical dispersion is downwards.

Quick Domenico and EPA's Bioscreen apply the above solution, Equation (A1-8). Papadopulos and Associates' Bioscreen-AT application performs an exact analytic solution to Equation (A1-2) using a program called ATRANS.

EPA's Biochlor spreadsheet employs a slightly different approach. First, the longitudinal solution is not truncated, so there is a second (smaller) term with a product of an exponent and complementary error function. This will be slightly more accurate, but will not make a significant difference in practice.

Above it was assumed that the dissolved and adsorbed contaminant decay coefficients are equal. A second difference with the Biochlor solution is that the sorbed phase coefficient is zero:

$$\lambda_s = 0$$
$$\lambda = \lambda_w.$$

The resultant transport equation is then:

$$\frac{\partial C}{\partial t} = \frac{\alpha_x v}{R}\frac{\partial^2 C}{\partial x^2} + \frac{\alpha_y v}{R}\frac{\partial^2 C}{\partial y^2} + \frac{\alpha_z v}{R}\frac{\partial^2 C}{\partial z^2} - \frac{v}{R}\frac{\partial C}{\partial x} - \frac{\lambda}{R}C = 0 \tag{A1-9}$$

This is identical to Equation (A1-2) except for the last term, where λ is divided by R. Therefore, if one wishes to run Biochlor *without* assuming zero sorbed-phase decay, values of $R\lambda$ may be entered in place of λ.

A1.2. Model Assumptions

Domenico's solution to the advective–dispersive equation incorporates the following assumptions.

- Aquifer properties are homogeneous and isotropic. For instance, porosity and hydraulic conductivity are spatially uniform, and there is no directional dependence.

- The flow field is homogeneous and unidirectional. The hydraulic gradient and groundwater velocity are constant in magnitude and direction throughout the model space. There are no pumping or recharge conditions altering the natural flow. The flow field is not radial, convergent, or divergent. There are no vertical flow gradients.

- Groundwater flow is in steady state. The hydraulic gradient and groundwater velocity are constant in time.

- The source shape is defined as a vertical rectangle perpendicular to groundwater flow.

- The source dimensions and concentration are constant with time.

- The aquifer is initially free of the contaminant, other than at the source.

- Both the aqueous and sorbed contaminant phases may undergo first-order decay, and the decay rate is the same for both.

- There is no transverse or vertical contaminant decay.

- Contaminants undergo linear, reversible, isothermal adsorption.

- Flow velocities are sufficiently high that mechanical dispersion dominates diffusion.

A1.3. Mathematical Approximations

The approximations inherent to the Domenico solution have been examined by *West* et al. [2007] and *Srinivasan* et al. [2007]. They pointed out three significant mathematical inaccuracies.

- The three-dimensional solution is taken to be the product of three one-dimensional solutions. This approach does not conserve mass.

- The longitudinal solution $C(x,t)$ omits a secondary term in QD and Bioscreen. The error is large when the dispersivity (α_x) is large such that x/α_x is relatively small.

- Domenico made the time substitution $t = x/v$, where v is the groundwater velocity. This is only correct when $\alpha_x = 0$. For nonzero longitudinal dispersivity, there are sizable errors especially forward of the advective front. This time reinterpretation also exaggerates the plume width.

West et al. [2007] and *Srinivasan* et al. [2007] concluded that contaminant concentrations may be significantly underestimated on the plume centerline. Errors can be minimized when:
- longitudinal dispersivities are low (α_x)
- advection velocities are high ($v = Ki$)
- simulation times are long (t).

Users must practice caution when making site predictions using fate-and-transport models as discussed by *Konikow* [2010].

Appendix 2. Hydraulic Conductivity

A2.1. Site-Specific Measurements

The preferred source of hydraulic conductivity values for input to Quick Domenico are measurements from on-site well tests. The most common methods used are slug tests and pump tests. The user must keep in mind that site-specific values are not exact measurements of conductivity, which can vary spatially and with depth. Therefore, a conservative approach should be used when applying the results to fate-and-transport models.

If well testing results are the basis for the QD hydraulic conductivity, then all data and calculations must be submitted to support values used in the model. This should include printouts from software (e.g., AQTESOLV) and graphs showing drawdown data and the best fits of the solution method. A narrative should explain the approach to aquifer testing, the applicability of the method, and how a representative hydraulic conductivity range was obtained from the results.

A2.1.1. Slug Tests

Slug tests are performed by inserting and removing a "slug" (such as an enclosed pipe) into and out of a well (rising head test). The change in the water level with time is measured. A solution, such as the Bouwer and Rice method for unconfined aquifers, is fit to the data to derive a hydraulic conductivity [e.g., *Kruseman and de Ridder*, 1990, Ch. 16; *Bouwer*, 1989].

Slug tests give a very limited picture of the aquifer permeability. They represent the permeability in a small volume immediately around the well. This material may have been disturbed by drilling the well. Also, the recovery may be influenced by flow through the filter pack. For these reasons, results of testing just one or two wells are not sufficient for determining a hydraulic conductivity value for use in the QD model. Each well should be tested at least three times, and at least three wells should be slug tested. Wells ought to be selected in the source area and downgradient from it.

The slug test results at a site should *not* be used to determine an absolute, average value of *K* for input to QD. Instead, the test results should be evaluated to define a range of reasonable conductivities for the aquifer. This approach accounts for local heterogeneity and anisotropy, and it should be conservative. The range might be defined as the minimum and maximum values, the average plus or minus the standard deviation, or the 95% lower and upper confidence limits of the mean. These low and high conductivity values are then input to QD as part of the sensitivity analysis and calibration.

A2.1.2. Pump Tests

Pumping tests are more representative of the aquifer permeability than slug tests. They reflect a larger volume of the subsurface (encompassing the wells that respond to the pumping) and are performed for a much longer period (12–24 hr or more). They also allow the use of multiple independent calculations of transmissivity from the same test: drawdown vs. time at the pumping and observation wells, drawdown vs. distance from the pumping well, and recovery after cessation of pumping. Pumping tests are more involved than slug tests, though [*Kruseman and de Ridder*, 1990, Ch. 2].

Various techniques are available for interpreting pump test data. The Cooper and Jacob method is commonly used. It is important to be aware of the assumptions and limitations of these methods. For instance, they include that the aquifer is confined, the well is fully penetrating, wellbore storage is negligible, and dimensionless time is small ($u < 0.1$). Acceptable solutions may be obtained if some of these assumptions are violated, but only under certain conditions that must be understood and justified.

A2.2. Representative Values for Local Rock Units

Aquifer testing may have been performed in other studies of sites in the area. The DEP regional files are a source of information for local hydraulic conductivity measurements. The US Geological Survey has published reports including hydraulic conductivity measurements and values used in groundwater models. Additional data may be found in the hydrogeology literature.

Low et al. [2002] presented hydraulic conductivity data for the geologic units found in southeastern Pennsylvania. Their hydraulic conductivity and transmissivity values were calculated from single-well aquifer tests or specific capacity tests of at least 1-hour duration. A modified Theis method was used to solve for the transmissivity. The authors assumed a constant value of the storage coefficient for each unit (~0.0002 for confined aquifers and ~0.007–0.2 for unconfined aquifers). The saturated thickness was defined as the borehole length less the depth to water to derive the hydraulic conductivity.

Low *et al.* used statistical methods to analyze the well data, and they calculated the quartile values for each population. The 25th percentile (P_{25}) and 75th percentile (P_{75}) values may be considered representative low- and high-range hydraulic conductivities. However, the published P_{90} and maximum values often greatly exceeded P_{75}, so it is not an upper bound.

A2.3. Reference Values

Representative hydraulic conductivities have been published in many hydrogeology textbooks. The values tabulated below are from *Domenico and Schwartz* [1998] (Table 3.2). "Likely minimum" and "likely maximum" values as well as selected other hydraulic conductivities are drawn from *Halford and Kuniansky* [2002]. Literature permeabilities are no substitute for site-specific data or regional studies. They may give guidance for ascertaining if results of well tests are reasonable and constrain the range of likely hydraulic conductivities when performing sensitivity tests and calibrating models.

Table A2.2. Typical minimum and maximum hydraulic conductivities

Material	K (ft/day)			
	Min	**Likely Min**	**Likely Max**	**Max**
Sediments				
Gravel	8×10^1	3×10^2	3×10^3	8×10^3
Sand–gravel mix	1×10^0	3×10^1	3×10^2	3×10^2
Coarse sand	2×10^{-1}	7×10^1	3×10^2	2×10^3
Medium sand	2×10^{-1}	2×10^1	7×10^1	2×10^2
Fine sand	5×10^{-2}	3×10^0	2×10^1	6×10^1
Silt, loess	3×10^{-4}	1×10^{-3}	1×10^{-1}	6×10^0
Till	3×10^{-7}	3×10^{-3}	3×10^{-1}	6×10^{-1}
Clay	3×10^{-6}	1×10^{-5}	1×10^{-4}	1×10^{-3}
Sedimentary Rocks				
Karst, reef limestone	2×10^{-1}	1×10^1	1×10^3	1×10^4
Limestone, dolomite	3×10^{-4}	4×10^{-3}	1×10^{-1}	2×10^0
Sandstone, medium grained	1×10^{-3}	1×10^0	1×10^1	8×10^1
Sandstone, fine grained	9×10^{-5}	1×10^{-3}	1×10^0	6×10^0
Siltstone	3×10^{-6}	1×10^{-5}	5×10^{-3}	4×10^{-2}
Shale	3×10^{-8}	1×10^{-7}	1×10^{-4}	1×10^0
Salt	3×10^{-7}			3×10^{-5}
Anhydrite	1×10^{-7}	1×10^{-7}	6×10^{-3}	6×10^{-3}
Crystalline Rocks				
Basalt	5×10^{-6}	3×10^{-2}	1×10^{-1}	1×10^{-1}
Permeable basalt	1×10^{-1}	1×10^0	1×10^2	6×10^3
Unfractured rock	8×10^{-9}	1×10^{-8}	6×10^{-5}	6×10^{-5}
Fractured rock	2×10^{-3}	5×10^{-2}	1×10^1	1×10^2
Weathered gabbro	1×10^{-1}	1×10^{-1}	1×10^0	1×10^0
Weathered granite	9×10^{-1}	1×10^0	1×10^1	2×10^1

Appendix 3.   Mechanical Dispersion

Dispersion is the process of mechanical mixing of a solute in groundwater. The origin of dispersion is the heterogeneity of aquifer permeability. This causes local velocities to be faster or slower than the average, and for the local direction of flow to vary from the overall potentiometric gradient. Dispersion causes spreading of the contamination forward of the advective front as well as laterally and vertically.

Dispersivity cannot be measured at the site; therefore, it must be a variable in the modeling. Nonetheless, there are some general guidelines and constraints on the magnitude of dispersivity. These are based on studies that have estimated the longitudinal dispersivity of conservative tracers in laboratory experiments and field investigations. Conservative tracers do not react, biodegrade, or adsorb, so their transport should be controlled by only advection and dispersion. A model is still used to elucidate the value of dispersivity from the lab or field data.

Figure A3-1 shows compiled longitudinal dispersivity estimates [*Schultze-Makuch*, 2005]. As dispersivity is understood to be a function of transport scale, the data are plotted against the estimated length scale for each site. Results for unconsolidated (blue circles) and bedrock (green squares) aquifers are shown, although there is no apparent distinction between them in terms of the magnitude or trend of dispersivity. Note that both axes are logarithmic. Very little data are available for distances of ~1000 ft or greater.

Clearly there is a lot of scatter in the data, reflecting the complex, localized processes that cause dispersion. Several authors have proposed equations for longitudinal dispersion as a function of scale. These all pass through the clustered data, but none of them account for the range of possible dispersivities at a given transport distance. Two common relationships are the 10% rule (i.e., dispersivity is one-tenth the scale, shown by the solid black line) and *Xu and Eckstein's* [1995] formula (dashed curve). The latter relationship is $\alpha_x = 2.7[\log(0.3x)]^{2.4}$ (in units of feet). Other equations are given by *Neuman* [1995] and *Schultze-Makuch* [2005].

The field data demonstrate that dispersivity virtually never exceeds 100% of the scale length, and 10% of scale is a representative relationship. However, there is commonly a two order-of-magnitude range in dispersivity observed at a given scale, and this needs to be considered when calibrating fate-and-transport models. The 10% rule is a reasonable starting point, but sensitivity testing must account for variations of 5–10 times around this value.
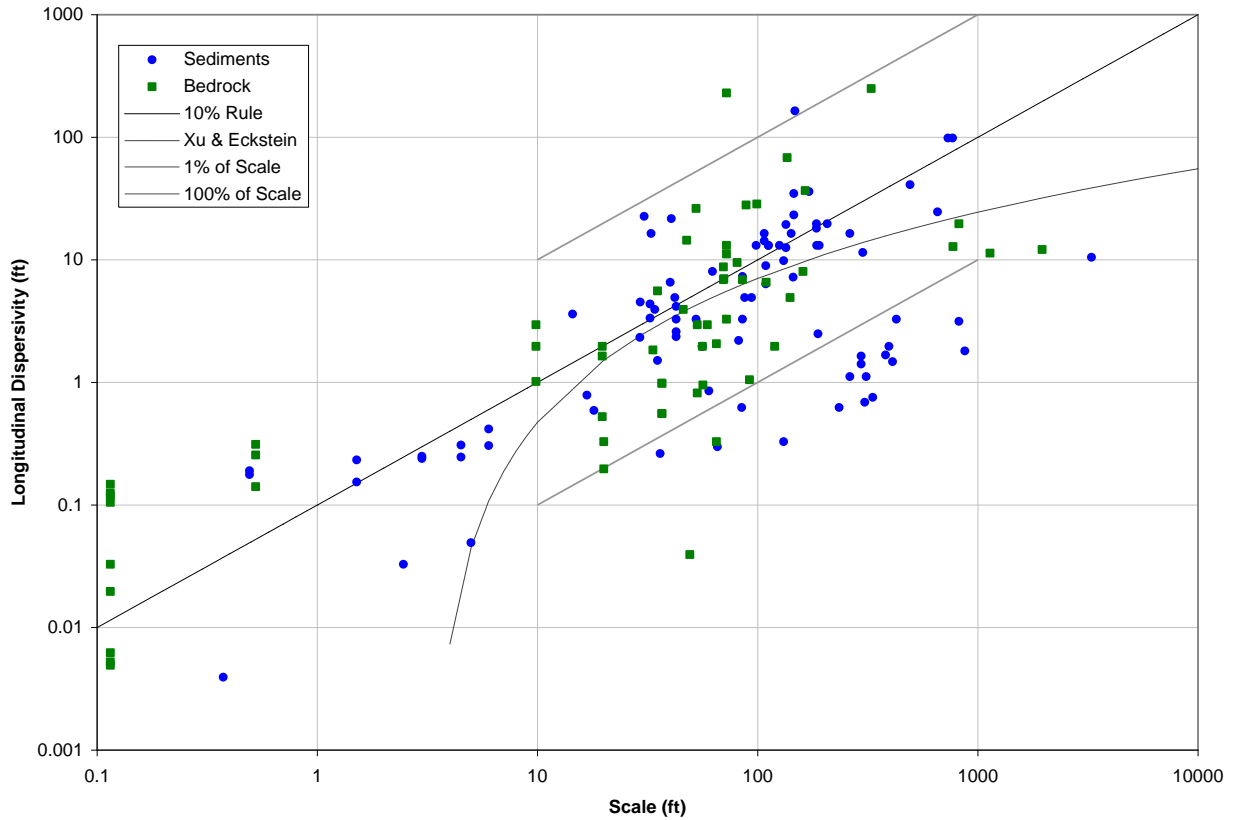
Figure A3-1. Plot of dispersivity versus scale data compiled by *Schultze-Makuch* [2005]. Two common relationships, the "10% Rule" (solid) and *Xu and Eckstein's* [1995] equation (dashed) are plotted for comparison.

Appendix 4. Example Problems

Example A4.1. Quick Domenico applied to a UST corrective action site.

Example A4.2. Bioscreen-AT applied to a petroleum site with source decay.