DOMENICO

SPREADSHEET ANALYTICAL MODEL

MANUAL

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1.0   Introduction

Domenico analytical model (1987) presented in this manual is an analytical solution to the advection-dispersion partial-differential equation of organic contaminant transport processes in groundwater as shown in section below. The model contains one dimensional groundwater velocity, longitudinal, transverse, and vertical dispersion, the first order degradation rate constant, finite contaminant source dimensions, the steady state source condition, and the estimated concentration at the plume centerline. The analytical solution form is programmed into a Microsoft Excel spreadsheet. The analytical model is applied to estimate the plume length for dissolved organic contaminant in groundwater. The use of the analytical model requires contaminant spatial concentration data at a minimum of one source well and one to two downgradient wells. The groundwater data must show a reasonable plume pattern (i.e., contaminant concentration is highest in the source well and gradually decreasing in the downgradient monitoring wells). Model is calibrated by adjusting three model input parameters to fit groundwater concentration spatial pattern based on the spatial concentration distribution data. The model after calibration is then used to predict the horizontal plume length in groundwater. Prior to applying the spreadsheet model and interpreting the model results, understanding of model assumptions is strongly advised.

2.0   Domenico Analytical Model

The Domenico analytical model is based on the advection-dispersion partial-differential equation for organic contaminant transport processes in groundwater as described below (Domenico and Robbins 1985):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial x} \tag{1}$$

Where,

   C - contaminant concentration in groundwater (mg/L),
   t - time (day),
   v - groundwater seepage velocity (ft/day),
   x, y, z - coordinates to the three dimensions (ft),
   D_x, D_y, D_z - dispersion coefficients for the x, y, z dimensions (ft^2/day),
       respectively.

To solve equation (1) analytically, under conditions of the steady-state source and finite continuous source dimension with one-dimensional groundwater velocity, three-

dimensional dispersion, and a first order degradation rate constant, the analytical solution can be expressed as (Domenico 1987):

$$\frac{C_x}{C_0} = \exp\left\{\frac{x}{2\alpha_x}\left[1-\left(1+\frac{4\lambda\alpha_x}{\upsilon}\right)^{\frac{1}{2}}\right]\right\} erf\left[\frac{Y}{4(\alpha_y x)^{\frac{1}{2}}}\right] erf\left[\frac{Z}{4(\alpha_z x)^{\frac{1}{2}}}\right] \tag{2}$$

Where,

C_x - contaminant concentration in a downgradient well along the plume centerline at a distance x (mg/L),
C_0 - contaminant concentration in the source well (mg/L),
x - centerline distance between the downgradient well and source well (ft),
α_x, α_y, and α_z - longitudinal, transverse, and vertical dispersivity (ft), respectively,
$D_x = \alpha_x \times \upsilon$, $D_y = \alpha_y \times \upsilon$, $D_z = \alpha_z \times \upsilon$,
λ - degradation rate constant (1/day),
$\lambda = 0.693/t_{1/2}$ (where $t_{1/2}$ is the degradation half-life of the compound).
υ - groundwater velocity (ft/day),
Y - source width (ft),
Z - source depth (ft),
erf - error function,
exp - exponential function.

The Domenico Analytical Model assumes:

(1) The finite source dimension,
(2) The steady state source,
(3) Homogeneous aquifer properties,
(4) One dimensional groundwater flow,
(5) First order degradation rate,
(6) Contaminant concentration estimated at the centerline of the plume,
(7) Molecular diffusion based on concentration gradient is neglected,
(8) No retardation (e.g., sorption) in transport process.

Understanding model assumptions is crucial to simulate transport process for a specific contaminant in groundwater. For example, MTBE has a very low potential of being sorbed onto soil particles due to its low K_{oc} value and therefore the No. 8 assumption above may not be an influential factor. Whereas, PCE has relatively high retardation

potential and the model described in this manual needs to be modified before it can be applied for simulating PCE transport process in groundwater.

3.0 Estimation of Centerline Distance

One of the conditions for using Domenico Analytical Model is that the selected downgradient monitoring well must be along the plume centerline. In most contamination cases, downgradient monitoring wells may be off the centerline. In order to apply Domenico Analytic Model to these cases, the distance between these off-centerline wells and source wells must be converted to the centerline distance.

In this manual, an ellipse trigonometry method is used to convert an off-centerline distance to a centerline distance. The method is based on an assumption about the contaminant plume geometry, which can be described as an ellipse shape (Figure 1). This ellipse shape is idealized and assumed based on the observations that the plume migrates fastest along groundwater flow direction and the longitudinal dispersivity is greater than transverse dispersivity in general. This assumption is consistent with the shape in a similar study by Martin-Hayden and Robbins (1997).

Based on the assumption of the ellipse plume shape, the following offers the calculation of converting a distance from an off-centerline well to a centerline well. First, it is assumed that (1) the ellipse width = 0.33 ellipse length (since most studies assume α_y=0.33α_x) (the ellipse length/width ratio can be adjusted based on the field data collected from every individual site) and (2) the ellipse is the contaminant isoconcentration line.

The equation for an ellipse with a horizontal major axis:

$$\frac{X^2}{a^2} + \frac{Y^2}{b^2} = 1 \qquad\qquad (3)$$

Where, a = the length of the major axis, b = the length of the minor axis, a > b > 0. X and Y are the coordinates to the x and y dimension, respectively. If the source well is assumed at close to one end of the ellipse and one downgradient well located on the ellipse (see Figure 1) with an off-centerline distance L', given the angle θ, the centerline distance can be calculated as follows.

Since b = 0.33 × a, x_1 = Cos θ × L' − a, y_1 = Sin θ × L', where θ = the angle between off-centerline and centerline (θ < 90°) and 2a = the distance (x) between source well and projected downgradient centerline well on the isoconcentration line.

Therefore,

$$\frac{\left(Cos\,\theta\times L'-a\right)^2}{a^2}+\frac{\left(Sin\,\theta\times L'\right)^2}{\left(0.33\times a\right)^2}=1$$

$$\left(Cos\,\theta\times L'-a\right)^2+9.18\times\left(Sin\,\theta\times L'\right)^2=a^2$$

$$\left(Cos\,\theta\times L'\right)^2+9.18\times\left(Sin\,\theta\times L'\right)^2=2\times a\times Cos\,\theta\times L'$$

$$X=2a=\frac{Cos^2\theta\times L'+9.18\times Sin^2\theta\times L'}{Cos\,\theta}=L'(Cos\,\theta+9.18\times tg\,\theta\times Sin\,\theta) \qquad (4)$$
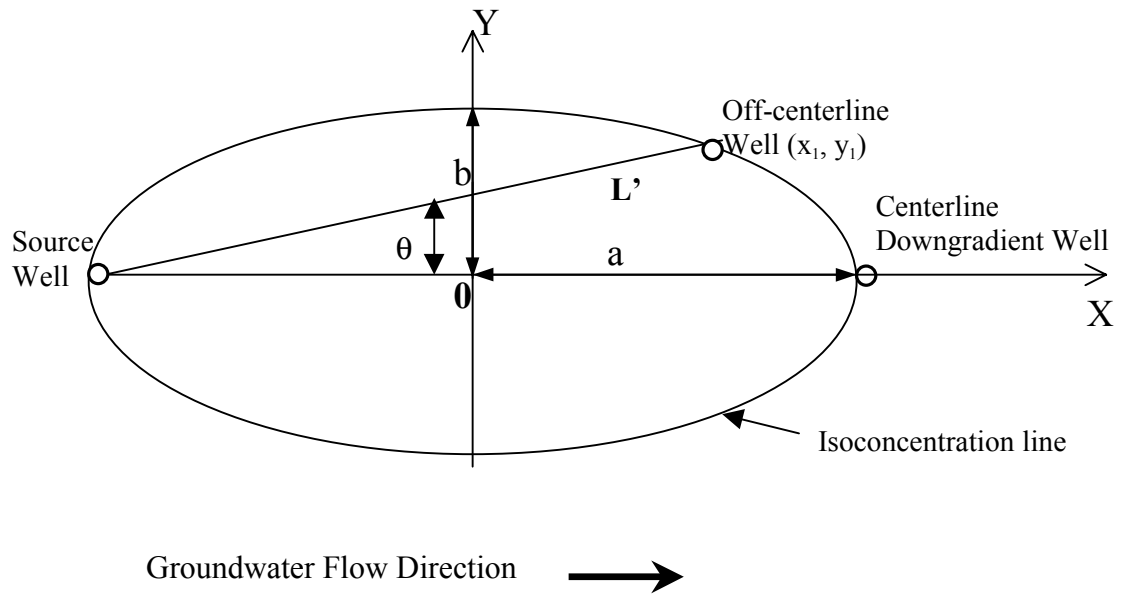
$$(\theta<90°)$$

Figure 1. Plane view of regular plume geometry and groundwater monitoring system

4.0   Spreadsheet Analytical Model

The analytical model can be applied to estimate the plume length for organic contaminant in groundwater. Figure 2 presents a flowchart of the analytical model application. First, groundwater monitoring data provide concentrations at the source well and at one or two downgradient wells (known C_0, C_1, and X_1, where C_1 = downgradient well concentration, X_1 downgradient well distance from the source well). Second, the ellipse trigonometry method is used to convert the off-centerline distance to centerline distance. Third, the field data are plotted on semi-logarithmic chart (C_1/C_o vs. X_1). Fourth, the known C_0, C_1, and X_1 are used to choose values for model parameters α_x, v, and λ by trial and error to fit the data points on the plot generated in step three. Fifth, the calibrated values of the parameters α_x, v, and λ are to be used to predict the concentration C_x at a downgradient distance x. The distance x is the plume length at the plume centerline.

Model Flowchart

(1) Collect Field Data: C_o, C_1, X_1, dh/dx,

(2) Convert X_1 to centerline distance

(3) Plot the field data on semi-logarithmic chart C_1/C_o vs. X_1

(4) Calibrate model parameters α_x, v, and λ and find the model best fit line for the field data

(5) Predict plume length x at a given concentration (e.g., C_x=5 µg/L) using calibrated α_x, v, and λ
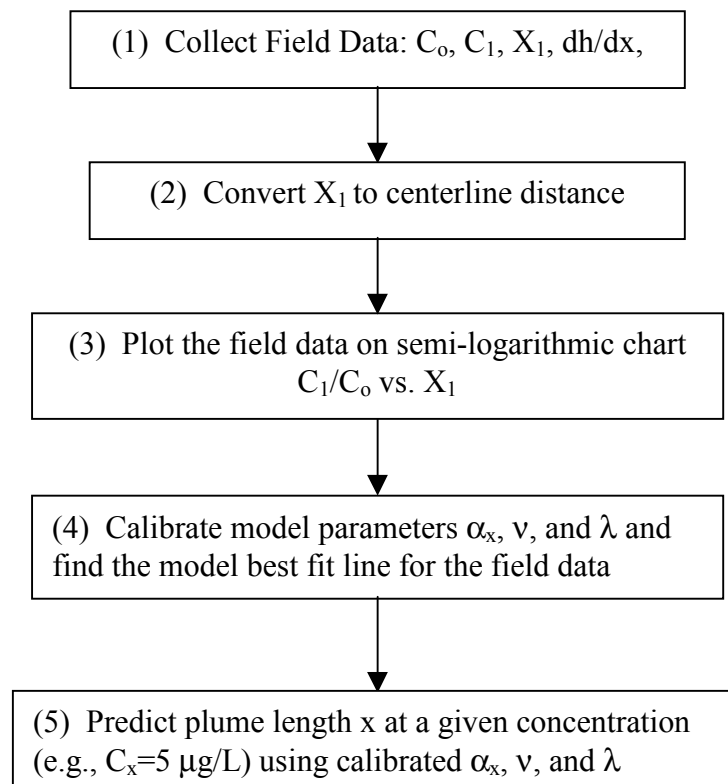
Figure 2. Domenico Analytic Model Flowchart

The Domenico Analytical Model solution form has been programmed into a user-friendly spreadsheet in Microsoft Excel (version 7.0). The groundwater monitoring data from a specific site are used to determine C_0, C_1, X_1, C_2, and X_2, which are plotted on a semi-logarithmic chart (C_1/C_o vs. X_1, C_2/C_o vs. X_2, etc.). By trial and error method, the model parameters α_x, v, and λ are altered within the reasonable ranges until a best fit curve to the spatial concentration distribution field data is identified. A plot is used to visually fit the field data (see example in Figure 4, Section 7.0). After a "best fit" curve is established, the calibrated values of α_x, v, and λ are used to predict the concentration C_x at a downgradient distance x. The distance x is the plume length at the plume centerline. An example of Excel spreadsheet is demonstrated in Table 6, Section 7.0.

5.0 Sensitivity Analysis

A sensitivity analysis is conducted for the Domenico Analytical Model in the same way as presented in Rong et al. (1998). Model runs under the condition of varying input parameter values, one at a time, within reasonable ranges. Then model outputs from various input values are compared with the "baseline" cases. The sensitivity analysis results, as presented in Table 1, indicate that model output is sensitive to model input parameters α_x, v, x, and λ. Coincidentally, these four parameters are used to calibrate the model by changing the values of these parameters to fit in the field data.

6.0 Model Input Parameters

As indicated in sensitivity analysis, model input parameters α_x, v, and λ would have great impacts on model output. Therefore, selections of these parameters have great effects to the model outcome. This section provides a summary of those parameter values from available references.

6.1 Dispersivity (α_x)

One of the primary parameters that control the fate and transport of contaminant is dispersivity of the aquifer. Domenico Analytic Model uses longitudinal (α_x), transverse (α_y), and vertical (α_z) dispersivities to describe the mechanical spreading and mixing caused by dispersion. The spreading of a contaminant caused by molecular diffusion is assumed to be small relative to mechanical dispersion in groundwater movement and is ignored in the model. Various dispersivity values have been used in previous studies. Table 2 is a summary of the three dimensional dispersivity values in literatures.

Table 1. Sensitivity Analysis Results for Domenico Analytical Model

Input Parameter	Factor of Input Change from Baseline	Model Output C_w (µg/L)	Factor of C_w Difference from Baseline
α_x (ft)			
1 (baseline)	-	5	-
4	4	1	0.2
0.1	0.1	50	10
v (ft/day)			
0.1 (baseline)	-	5	-
0.5	5	1,020	204
0.05	0.5	0.008	0.0016
x (ft)			
670 (baseline)	-	5	-
335	0.5	268	53.6
1,000	1.49	0.13	0.026
Y (ft)			
20 (baseline)	-	5	-
10	0.5	3	0.6
30	1.5	7	1.4
Z (ft)			
5 (baseline)	-	5	-
1	0.2	1	0.2
10	2	10	2
λ (1/day)			
0.001 (baseline)	-	5	-
0.002	2	0.0076	0.00152
0.0005	0.5	139	27.8

6.2   Groundwater Velocity (ν)

Groundwater velocity in the geologic material is controlled by hydraulic conductivity, hydraulic gradient in the vicinity of the study area, and effective porosity of the geologic material. Based on the Darcy's Law, the average groundwater velocity can be calculated using the following equation:

$$v = K \times \frac{dh}{dx} \times \frac{1}{n_e} \qquad (5)$$

Table 2. Dispersivity Values In Literature

Dispersivity Values	Reference
$\alpha_x = 0.1\ X$ $\alpha_y = 0.33\ \alpha_x$ $\alpha_z = 0.056\ \alpha_x$	Gelhar and Axness (1981)
$\alpha_x = 0.1\ X$ $\alpha_y = 0.1\ \alpha_x$ $\alpha_z = 0.025\ \alpha_x$	Gelhar et al. (1992)
$\alpha_x = 14 - 323$ (ft) $\alpha_y = 0.13\ \alpha_x$ $\alpha_z = 0.006\ \alpha_x$	USEPA (1996)
$\alpha_x = 16.4$ (ft) $\alpha_y = 0.1\ \alpha_x$ $\alpha_z = 0.002\ \alpha_x$	Martin-Hayden and Robbins (1997)
$\alpha_x = 0.33 - 328$ (ft) $\alpha_y = 0.1\ \alpha_x$ $\alpha_z = 0.1\ \alpha_x$	AT123D (1998)

X = the distance to the downgradient well (ft), α_x = the longitudinal dispersivity (ft), α_y = the transverse dispersivity (ft), α_z = the vertical dispersivity (ft).

Where,

ν - Groundwater velocity (ft/day)
K - Hydraulic conductivity (ft/day)
dh/dx - Hydraulic gradient (ft/ft)
n_e - Effective porosity (dimensionless)

The groundwater hydraulic gradient can be determined from field data. The hydraulic conductivity and effective porosity are also preferably obtained from site-specific testing. The hydraulic conductivity and effective porosity are mainly affected by the geologic material grain size. In cases where site-specific data are absent, to estimate groundwater velocity, the lithologic boring logs can be analyzed and hydraulic conductivity and effective porosity can be estimated to be consistent with value ranges from published references (see Tables 3 and 4).

Table 3. Hydraulic Conductivity Range for Various Classes of Geologic Materials

Material	Hydraulic Conductivity, ft/day			
	Todd 1980	Bouwer 1978	Freeze & Cherry 1979	Dawson & Istok 1991
Gravel	$5 \times 10^2 - 1 \times 10^3$	$3 \times 10^2 - 3 \times 10^3$	$3 \times 10^2 - 3 \times 10^5$	$3 \times 10^3 - 3 \times 10^5$
Coarse Sand	1×10^2	$7 \times 10^1 - 3 \times 10^2$	$3 \times 10^{-2} - 3 \times 10^3$	
Medium Sand	4×10^1	$2 \times 10^1 - 7 \times 10^1$		$3 - 3 \times 10^3$
Fine Sand	10^1	$3 - 2 \times 10^1$		$3 \times 10^{-2} - 3$
Silt and Clay	$10^{-3} - 3 \times 10^{-1}$	$3 \times 10^{-8} - 3 \times 10^{-2}$	$3 \times 10^{-7} - 3 \times 10^{-3}$	$3 \times 10^{-6} - 3 \times 10^{-1}$

Table 4. Total Porosities and Effective Porosities of Well-sorted, Unconsolidated Formations

| Material	Diameter (mm)	Total Porosity (%)	Effective Porosity (%)
Gravel			
Coarse	64.0 – 16.0	28	23
Medium	16.0 – 8.0	32	24
Fine	8.0 – 2.0	34	25
Sand			
Coarse	2.5 – 0.5	39	27
Medium	0.5 – 0.25	39	28
Fine	0.25 – 0.162	43	23
Silt	0.162 – 0.004	46	8
Clay	<0.004	42	3

Source: Roscoe Moss Company, 1990

6.3   Degradation Rate Constant (λ)

Table 5 lists degradation constant and half-life for various hydrocarbon compounds in soil and groundwater (Howard, et al., 1991).

7.0   Case Study

A case study example is included in this manual to demonstrate the modeling procedures for estimating MTBE plume length. The case study is a real case from an underground storage tank site in the City of Los Angeles, California. Figure 3 shows the site layout and
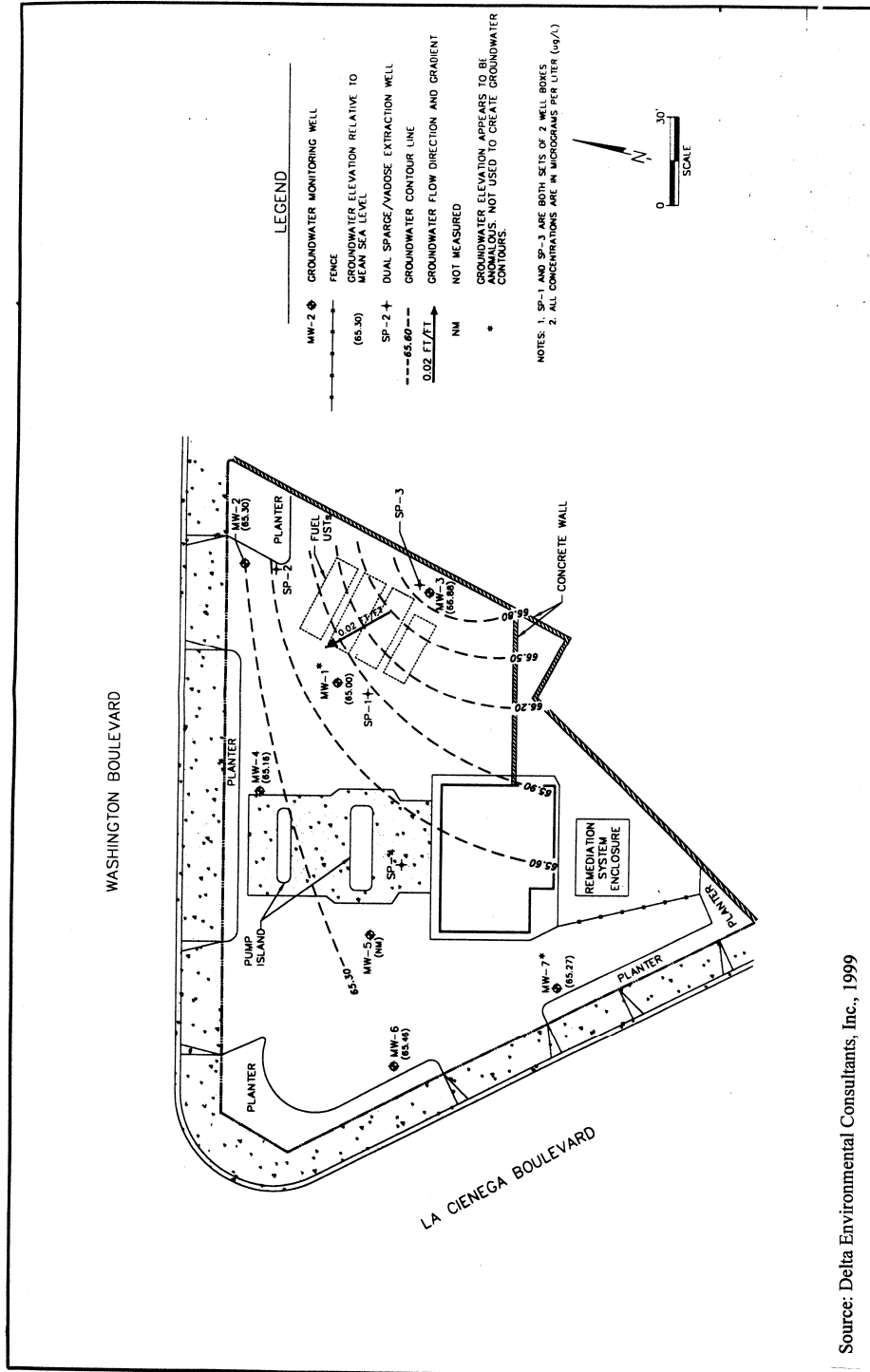
Source: Delta Environmental Consultants, Inc., 1999

Figure 3. Site map for sample case

the site groundwater contour map. The modeling procedures are described in details as the following steps:

Step 1:

Find one source monitoring well (usually in the source area with highest MTBE concentration) and one to two downgradient well(s) along or close to the centerline with decreasing MTBE concentrations.

As shown on the Figure 3, the groundwater flow direction is towards northwest with a gradient of 0.02 ft/ft. The monitoring well MW-3 had the highest MTBE concentration (25,000 µg/L). Monitoring wells MW-1 and MW-4 are downgradient wells with declining MTBE concentrations (3,600 µg/L and 67 µg/L, respectively). The boring logs for these monitoring wells indicate that soil materials are predominantly poorly graded sands.

Step 2:

Measure the distance between the source well and the downgradient wells; measure the off-centerline angle if any. Use the ellipse trigonometry method presented in this manual to estimate centerline distance. Use equation (4): given L' = 90 ft, θ = 15°,

$$X = L'(Cos\theta + 9.18 \times tg\theta \times Sin\theta)$$
$$= 102 \text{ (ft)}$$

 Fill out the form below:

Case Name:	Source Well	Downgradient Wells	
	MW-3	MW-1	MW-4
MTBE Concentration [µg/L]	25,000	3,600	67
Distance to Source Well [ft]	-	45	90
Off-centerline Angle θ [degree]	-	0	15
Centerline Distance to Source Well [ft]	-	45	102

Step 3:

    A. Open the Microsoft Excel file "Domenico," (included in this manual)
    B. Use "distance" sheet to calculate centerline distance to source well,
    C. Use "MTBE" sheet to find the best-fit curve on the plot of concentration versus distance:

- Enter case information: case name, address and ID
- Enter case data: $C_0 = 25,000$ µg/L, $X_1 = 45$ ft, $C_1 = 3,600$ µg/L, $X_2 = 102$ ft, $C_2 = 67$ µg/L
- Manipulate model parameters (α_x: $0.35 – 4$ ft, v: $0.01 – 0.5$ ft/day, and λ: $0.1 – 0.001$ /day) to find best-fit curve (Based on references in Table 2, the following value ranges are used in this case study: $\alpha_x = [0.35$ ft, 4 ft$]$, $\alpha_y = [0.33\alpha_x, 0.65\alpha_x]$, $\alpha_z = 0.056\alpha_x$) (see Table 6 for model data entry and Figure 4 for plot)
- Record plume parameters after the "best fit" curve is established

$\alpha_x = \underline{4}$ ft; $\lambda = \underline{0.008}$ 1/day; $v = \underline{0.25}$ ft/day; dh/dx $= \underline{0.02}$ (ft/ft)

    D. Change distance X value until $C_x = 5$ µg/L
    E. Record X value: MTBE plume length $X = \underline{183}$ ft
    F. Save the file

8.0   Troubleshooting for the Spreadsheet Analytical Model

Trouble 1: By changing the values of either α_x, v, or λ, the model calculation and curve on the chart do not response.
Solution: Go to "Add-In" option in Excel under the "Tools" menu bar and select the "Analysis Toolpak."

Trouble 2: Some field data do not show on the chart
Solution: Change the Y axis range by double clicking the Y axis, and add one or two more decimals for minimum range in Scale sheet.

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