

Preface To Manual For Non-Steady State Spreadsheet Analytical Model

Regional Board staff prepared the attached spreadsheet analytical model and model manual to assist in estimating Methyl Tertiary Butyl Ether (MTBE) and other oxygenates travel time to a downgradient receptor (usually a domestic supply well). The need for estimating the plume travel time is part of implementation of the Final Draft Guidelines for Investigation and Cleanup of MTBE and Other Oxygenates (Final Draft Guidelines) required by the State Water Resources Control Board. In order to implement the Final Draft Guidelines, the Los Angeles Regional Board staff have required responsible parties within the region to develop a site-specific conceptual model, in which the estimate of plume travel time is required.

The attached model is a non-steady state analytical model for one time instantaneous release situation. This model is posted at our website for users' convenience in compliance with Regional Board requirements. However, this model is NOT the only model that can be used to estimate the plume travel time. Other models are also available for the same purpose and may be utilized. If other models are applied, they will need to be evaluated on a case by case basis.

If you have any questions about the model, please contact Tom Shih at (213) 576-6729 or Yue Rong at (213) 576-6710.

MANUAL
FOR
NON STEADY STATE
SPREADSHEET ANALYTICAL MODEL
(FOR ONE TIME INSTANTANEOUS RELEASE)

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Manual for Non Steady State Spreadsheet Analytical Model

1. Introduction

The non-steady state analytical model presented in this manual is an analytical solution to a finite mass advection-dispersion partial-differential equation of organic contaminant transport processes in groundwater. The model contains one dimensional groundwater velocity, longitudinal and transverse dispersion, instantaneous contaminant discharge flux rate, and estimates of initial discharge time and concentration, under the non steady state condition. The analytical solution form is programmed into a Microsoft Excel spreadsheet. Since the concentration is a function of travel time in the model, the analytical model can be applied to estimate the plume travel time to a given distance for dissolved organic contaminant in groundwater. The use of the analytical model requires contaminant temporal concentration data at a minimum of one monitoring well, preferably a downgradient well from the source area. The groundwater temporal concentration data must show a reasonable “peak” pattern, in which contaminant concentration has increased and then decreased over time. The model is calibrated by adjusting four model-input parameters to fit the pattern of groundwater temporal concentration distribution at the monitoring well. The model after calibration is then used to predict the plume travel time to a given distance (e.g., to a drinking water well). Prior to applying the spreadsheet model and interpreting the model results, understanding of model assumptions and uncertainties associated with model calibration with field data is strongly advised.

2. Non Steady State Analytical Model

The non steady state analytical model is based on a finite mass advection-dispersion partial-differential equation for contaminant transport processes in groundwater as described below (Fried 1975):

$$\mathbf{a}_L u \frac{\partial^2 C}{\partial x^2} + \mathbf{a}_T u \frac{\partial^2 C}{\partial y^2} - u \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (1)$$

The Green function as the solution of this equation for the injection of a given amount of pollution at the origin is instantaneously:

$$C(x, y, t) = \frac{C_0 Q dt}{4 \mathbf{p} u t (\mathbf{a}_L \mathbf{a}_T)^{1/2}} \exp \left[-\frac{(x - ut)^2}{4 \mathbf{a}_L ut} - \frac{y^2}{4 \mathbf{a}_T ut} \right] \quad (2)$$

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Where,

$C(x,y,t)$ = Contaminant concentration in a down-gradient well at time t and located at x,y

C_0 = Initial concentration ($\mu\text{g/L}$)

Q = Rate of discharge (ft^2/year)

dt = Period of discharge (year)

C_0Qdt = Mass of discharge per unit depth ($\mu\text{g/ft}$)

u = Groundwater velocity (ft/day)

t = Time (day)

α_L = Longitudinal dispersivity (ft)

α_T = Transverse dispersivity (ft)

x = Distance parallel to the direction of groundwater flow (ft)

y = Distance perpendicular to the direction of groundwater flow (ft)

This non steady state analytical model assumes:

- (1) Non steady state (concentration is a function of time),
- (2) Initial mass discharged is finite and instantaneously introduced as a slug,
- (3) Homogeneous aquifer properties,
- (4) No change in groundwater flow direction and velocity,
- (5) The dispersion coefficients are constant and proportional to the velocity (dynamic dispersion regime), and
- (6) Contaminant natural degradation is not considered (e.g., no sorption or biodegradation).

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 high solubility in water and therefore the No. 6 assumption above may not be an influential factor. Conversely, perchloroethylene (PCE) has a relatively high retardation potential and the model described in this manual need to be modified before it can be applied for estimating PCE transport process in groundwater. In addition, compare to other petroleum hydrocarbons, MTBE does not naturally degrade to a significant degree, and so dispersion is the primary mechanism for concentration reduction.

3. Uncertainties Regarding Initial Time (T_0) and Initial Mass (C_0) of Release

As in most contamination cases, the initial time of release (T_0) and the mass discharge (C_0Qdt) are usually unknown (although it could be estimated through model calibration using the spreadsheet analytical model format). It is thus difficult to determine the concentration of the mass discharge (C_0) because the typical rate of mass discharge Q and the period of mass discharge dt are also unknown. For instance, in this analytical model, the model parameter C_0Qdt or mass discharge per unit depth can be estimated through

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model calibration. However, since the typical rate and period of mass discharge are typically unknown, the estimation of the concentration of mass discharge (C_0) by dividing the mass discharge by its rate and period of discharge would generate large uncertainties that render the resulting C_0 meaningless. Fortunately, C_0 is not essential or necessary in our analysis and estimation of plume travel time.

The uncertainties associated with T_0 and C_0Qdt would affect the calibration of model input parameters for predicting plume travel time. As the model parameter sensitivity analysis indicates in the later section, the analytical model is much more sensitive to changes made to u than to C_0Qdt (see Table I). Furthermore, changes made to T_0 as well as groundwater velocity (u) would shift the time of the concentration peak on the x-axis in the plot of time versus concentration. The collective impact from T_0 and u would thus generate large uncertainties in the calibration of model-input parameters and the prediction of the plume travel time. This problem may be dealt with in two ways during the model calibration: (1) to obtain relatively accurate site-specific information regarding the initial time of release (e.g., time of underground tank leaking, or history of contaminant usage), or (2) to use a more conservative value of groundwater seepage velocity (faster), estimated by the range of groundwater velocities typically associated with certain soil types, formations, and hydrology. Since relatively accurate site-specific information regarding the time of release is generally unavailable or unknown, the latter approach is more useful and thus is the one applied in this model.

4. Spreadsheet Analytical Model

The analytical model can be applied to estimate the travel time to a receptor for contaminants in groundwater. Figure 1 shows the model setting. The monitoring well used to calibrate the model must be downgradient of the source. Figure 2 presents a flowchart of the analytical model application. Step one, groundwater monitoring data provide temporal concentrations at one downgradient well with known $C(T_i)$, T_i , X_1 , and Y_1 ($i = 1, \dots, n$) where $C(T_i)$ = concentration at downgradient well at time T_i , X_1 = the Cartesian coordinate of the downgradient well from the source area in the direction of groundwater flow, Y_1 = the Cartesian coordinate of the downgradient well perpendicular to direction of groundwater flow (Figure 1). T_0 is the initial time of contaminant release. T_1 is the time when groundwater-monitoring data were first obtained. The groundwater monitoring is conducted periodically. Since T_0 is usually unknown in most cases, T_1 or time of the first monitoring data point relative to T_0 will also be unknown. However, time T_2, \dots, T_n relative to T_1 is known. Thus an educated judgement for T_1 must be made first, and T_2, \dots, T_n are directly related to T_1 . Step two, the field data are plotted (T_i vs. $C(T_i)$, $i = 1, \dots, n$). Step three, the known $C(T_i)$, and T_i are used to choose values for model parameters α_L , u , T_1 , and C_0Qdt by trial and error to fit the data points on the plot generated in step two.

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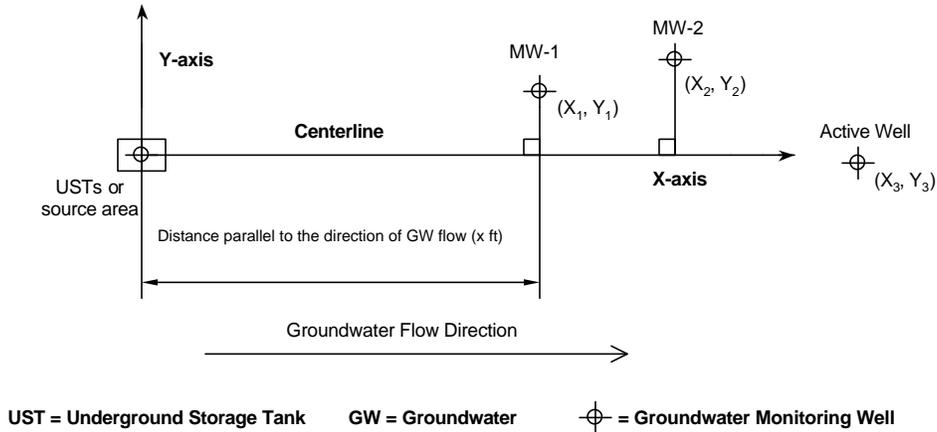


Figure 1. Plane View of Groundwater Monitoring System in Cartesian Coordinates

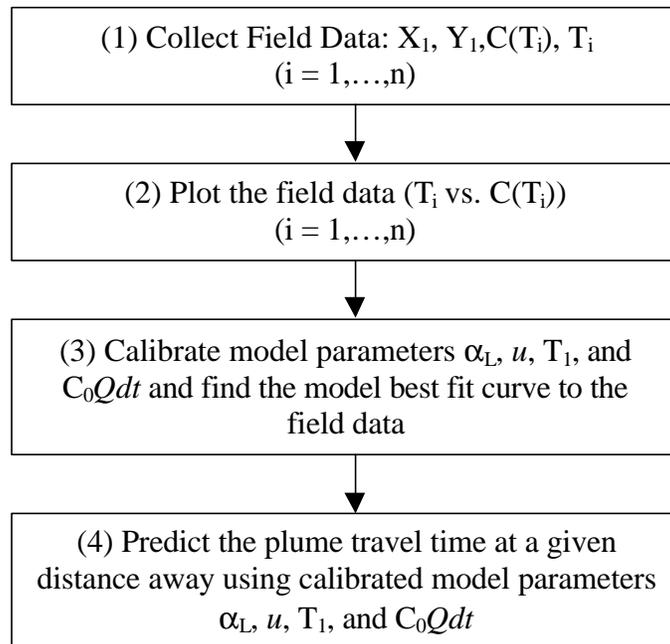


Figure 2. Non Steady State Analytic Model Flowchart

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Step four, the calibrated values of the parameters α_L , u , T_1 , and C_0Qdt are to be used to predict the travel time to a receptor (i.e. drinking water well) at a downgradient distance X .

The Non Steady State 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 provide $C(T_i)$ and T_i ($i = 1, \dots, n$) which are plotted ($C(T_i)$ vs. T_i). By trial and error method, the model parameters α_L , u , T_1 , and C_0Qdt are altered within the reasonable ranges until a best-fit curve to the temporal concentration distribution field data is visually identified (see example in Figure 4, Section 7). For example, changes made to T_1 and groundwater velocity (u) would shift the time of the concentration peak curve on the x-axis in the plot of time versus concentration; changes made to α_L would primarily affect the spreading of the curve; and changes made to C_0Qdt would affect the height of the curve. After a “best-fit” curve is established, the calibrated values of α_L , u , T_1 , and C_0Qdt are used to predict the travel time t at a down-gradient distance X . An example of Excel spreadsheet is demonstrated in Tables V and VI, Section 7.

5. Sensitivity Analysis

A sensitivity analysis is conducted for the Non Steady State 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 respective “baseline” cases. The sensitivity analysis results, as presented in Table I, indicate that model output t (time for plume to reach 5 $\mu\text{g/L}$ in down-gradient receptor) is relatively sensitive to model input parameters α_L , u , and C_0Qdt . Consequently, these three parameters are used to calibrate the model by changing the values of these parameters to fit in the field data.

6. Model Input Parameters

6.1. Dispersivity (α_L)

One of the primary parameters that control the fate and transport of a contaminant is dispersivity of the aquifer. Non steady state analytical model uses longitudinal (α_L) and transverse (α_T) 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 reported in studies. Most of existing studies traditionally use α_T as a fraction of α_L . For this relationship, we only calibrate α_L , which

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relates α_T . Table II is a summary of the two-dimensional dispersivity values obtained from literature reviews.

Table I. Sensitivity Analysis Results for Non Steady State Analytical Model

<i>Input Parameter</i>	<i>Factor of Input Change from Baseline</i>	<i>Model Output t (years)</i>	<i>Factor of t Difference from Baseline</i>	<i>Relative Sensitivity S</i>
α_L (ft)				0.038
1 (baseline)	---	24.4	---	
0.1	0.1	26.3	1.08	
4	4.0	22.7	0.93	
u (ft/day)				0.404
0.1 (baseline)	---	24.4	---	
0.15	1.5	16.4	0.67	
0.05	0.5	49.3	2.02	
0.5	5.0	4.9	0.20	
x (ft)				0
150 (baseline)	---	24.4	---	
300	2.0	24.4	1.00	
500	3.3	24.4	1.00	
y (ft)				0
0 (baseline)	---	24.4	---	
10	N/A	24.4	1.00	
20	N/A	24.4	1.00	
C_0Qdt ($\mu\text{g}/\text{ft}$)				0.025
50 (baseline)	---	24.4	---	
10	0.2	25.2	1.03	
100	2.0	24.1	0.99	

Note: Relative sensitivity (S) is calculated using the following equation:

$$S = \left(\left(\frac{df}{f} \right) \left(\frac{x}{dx} \right) \right)$$

Where x and f are baseline input and model output values, dx and df are input and model output range, respectively.

6.2. Groundwater Velocity (*u*)

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:

$$u = K \times \frac{dh}{dx} \times \frac{1}{n_e} \tag{3}$$

Where,

- u* - 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 (i.e., pumping test or slug test), to estimate groundwater velocity, the lithologic boring logs can be evaluated to identify predominant aquifer materials needed to estimate hydraulic conductivity and effective porosity to be consistent with value ranges from published references (see Tables III and IV).

Table II. Dispersivity Values In Literature

<i>Dispersivity Values</i>	<i>Reference</i>
$\alpha_L = 0.1 X$ $\alpha_T = 0.33 \alpha_L$	Gelhar and Axness (1981)
$\alpha_L = 0.1 X$ $\alpha_T = 0.1 \alpha_L$	Gelhar et al. (1992)
$\alpha_L = 14 - 323$ (ft) $\alpha_T = 0.13 \alpha_L$	USEPA (1996)
$\alpha_L = 16.4$ (ft) $\alpha_T = 0.1 \alpha_L$	Martin-Hayden and Robbins (1997)
$\alpha_L = 0.33 - 328$ (ft) $\alpha_T = 0.1 \alpha_L$	AT123D (1998)

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X = distance to the downgradient well (ft), α_L = longitudinal dispersivity (ft), and α_T = transverse dispersivity (ft).

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

<i>Material</i>	<i>Hydraulic Conductivity, ft/day</i>			
	<i>Todd 1980</i>	<i>Bouwer 1978</i>	<i>Freeze & Cherry 1979</i>	<i>Dawson & Istok 1991</i>
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 IV. Total Porosities and Effective Porosities of Well-sorted, Unconsolidated Formations

<i>Material</i>	<i>Diameter (mm)</i>	<i>Total Porosity (%)</i>	<i>Effective Porosity (%)</i>
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

7. Case Study

A case study example is included in this manual to demonstrate the modeling procedures for estimating MTBE plume travel time. The case study is a real case from an underground storage tank (UST) site in the City of Los Angeles, California. Figure 3 depicts the site layout (USTs, dispenser islands, buildings, and well locations) and site groundwater contour map with gradient and approximate direction of groundwater flow. The modeling procedures are described in detail as the following steps:

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Step 1:

Find the groundwater contour map for the site. Identify the area of the USTs, dispenser islands, piping, or any other likely sources of release that will be designated as the source area. Locate one or two down-gradient well(s) along or in close proximity to the centerline with sufficient data that show a temporal trend of increasing followed by decreasing MTBE groundwater concentration.

As shown on Figure 3, the groundwater flow direction is towards south-southwest with a gradient of 0.029 ft/ft. The USTs are the suspected source of release. Monitoring well MW-15 is directly downgradient of the source area, and has 10 quarters of MTBE groundwater concentration data with a “peak” pattern of MTBE temporal groundwater concentration. The boring logs for these monitoring wells indicate that soil materials are composed predominantly of fine and silty sand.

Step 2:

Measure the distance between the source area and the downgradient well. Measure the distance perpendicular to the direction of groundwater flow (if any). Tables V and VI are the case field data entry and model parameter entry, respectively.

Table V. Field Data Entry

<i>Case Name: ABC Company</i> <i>Address: XYZ Blvd., Los Angeles, CA</i> <i>Case ID Number: 12345678910</i>		
<i>Well No.</i>	<i>Distance X (ft)</i>	<i>Distance Y (ft)</i>
MW-15	160	0

<i>Down-gradient well at Time T_i</i>	<i>Concentration $C(T_i)$ (mg/L)</i>	<i>Time (day)</i>
T_1	380	565
T_2	2200	655
T_3	3800	745
T_4	4270	835
T_5	3100	895
T_6	540	1015
T_7	210	1098
T_8	81	1201
T_9	57	1261
T_{10}	0.5	1351

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The actual field monitoring data provides the time (month, day, year) and the corresponding MTBE groundwater concentration. Hence, the real time between the monitoring events is known, and can be linked together by adding the difference in time elapsed between monitoring events from the previous event. For example, three months or one quarter had elapsed between T_1 and T_2 , and then $T_2 = T_1 + 90$ (days), and so on. However, field-monitoring data would not typically provide information on the initial time of release (T_0). Consequently, T_1 from the above data entry is unknown and an educated judgement for T_1 must be made first. Here, we choose $T_1 = 565$ days to start with. T_1 will be readjusted during the model calibration.

Table VI. Spreadsheet Model Parameter Entry

<i>Parameter</i>	<i>Notation</i>	<i>Value</i>	<i>Unit</i>
X axis dispersivity	α_L	1.7	ft
Y axis dispersivity	α_r	0.561	ft
Groundwater velocity	u	0.20	ft/d
Mass discharged per Unit depth	C_0Qdt	2.38E8	mg/ft
Rate of discharge	Q	25	ft ² /yr
Discharge duration	dt	8.33E-2	yr
Concentration of mass discharged	C_0	4.03E6	µg/L
Distance parallel to direction of GW flow (DG Well 1)	X_1	160	ft
Distance perpendicular to direction of GW flow (DG Well 1)	Y_1	0	ft
Distance parallel to direction of GW flow (DG Well 2)	X_2	N/A	ft
Distance perpendicular to direction of GW flow (DG Well 2)	Y_2	N/A	ft
Distance parallel to direction of GW flow (drinking water well)	X_3	1000	ft
Distance perpendicular to direction of GW flow (drinking water well)	Y_3	0	ft

The choice of parameter values in Table VI is dependent upon the “best-fit” with field data plot by trial-and-error. For the best fitting in the plot, experience is needed. Parameters α_L , u , and C_0Qdt as in boldface are those “fitting” parameters. The general guidance on how the model parameters are calibrated is provided in Section 4 of this manual (page 5). Changes made to groundwater velocity u and T_1 would shift horizontally the model predicted and the field measured peak, respectively, in the plot of concentration versus time. As was discussed in Section 3 on uncertainties, the approach of using a more conservative value of groundwater seepage velocity that is estimated by the range of groundwater velocities typically associated with certain soil types, formations, and hydrology will be used in this model to estimate the groundwater seepage velocity. The

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estimated u will then be used to readjust T_1 until the model best-fit curve is established relative to the measured field data.

Changes made to α_L and C_0Qdt affect primarily the height and spreading, respectively, of the model prediction curve. Initial values for α_L and C_0Qdt are entered first in order to “match” the spreading and height of the model prediction curve to the observed field data. In any case, groundwater seepage velocity u should be estimated first, with the other parameters (i.e., T_1 , α_L , and C_0Qdt) to follow. Repeat this sequence until the best-fit model prediction curve to the field data is obtained. The range of values for the calibration of these parameters is derived from literature sources and appears in the Cell next to the model parameters in the Microsoft Excel Spreadsheet File.

Step 3:

- A. Open the Microsoft Excel file “Non Steady State Analytical Model” (Included in this manual).
- B. Use “MTBE” sheet to find the best-fit curve on the plot of time vs. MTBE concentration:
 - Enter case information: case name, address and ID.
 - Enter case data: $X_1 = 160$ ft, $Y_1 = 0$ ft, $C(T_1) = 380$ $\mu\text{g/L}$, $T_1 = 565$ days, $C(T_2) = 2200$ $\mu\text{g/L}$, $T_2 = 655$ days, $C(T_3) = 3800$ $\mu\text{g/L}$, $T_3 = 745$ days, and so on (see Table V). Enter an initial temporary value for T_1 . T_1 will be modified to fit the field data during the model calibration process. This can be done by entering the formula into the excel worksheet. In this case, click on cell F23 to enter the formula for T_2 . A formula of “= F22 + 90” should be displayed in the formula bar. Change the default value 90 to whatever the difference in time in days between the two monitoring events. Repeat the same procedure for all subsequent monitoring events, replacing the part of the formula of “= F22” with F23, F24, F25, and so on to correspond to the previous monitoring event.
 - Manipulate model parameters α_L , u , C_0Qdt , and T_1 to find best-fit curve. The general guidance on how these parameters affect the curve shape is provided in Section 4 of this manual (page 5). Table VI shows the spreadsheet model data entry and Figure 1 of the Microsoft Excel Spreadsheet File shows the plot of field data versus model fitting curve. The model parameters are in bold fonts in Table V and VI, and they are in cells colored in red in the Microsoft Excel Spreadsheet File. The

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field data are in cells colored in pink. Based on references in Table II and the approximate ratio of the contaminant plume width to its length, the following value ranges are used in this case study: $\alpha_L = [0.1 \text{ ft}, 10 \text{ ft}]$, $\alpha_T = [0.33\alpha_L, 0.65\alpha_L]$. For instance, from the contaminant (i.e. TPHg, benzene, or MTBE) isoconcentration plots, the width of the plume for this particular case is approximately one-third of its length. Based on this finding, the value of $0.33*B2$ is entered into Cell B3. Cells E1-E8 and F1-F8 contains the soil types and the range of groundwater velocities typically associated with. Based on the soil boring logs, the predominant soil type is a combination of fine and silty sand. Apply conservative groundwater velocity values associated with these two soil types. In this case, the resulting range of groundwater velocity should be from 0.1 ft/day to 0.5 ft/day, corresponding to the conservative groundwater velocity values associated with the two soil types.

- The first step in the calibration process should consist of narrowing down the groundwater velocity u . Apply an initial value of $u = 0.5$ ft/day. It can be adjusted downwards (with the constraint of minimum u value of 0.1 ft/day) later in the process of obtaining the best-fit model curve to the observed field data. As the time versus concentration plot for the model prediction curve (Figure 1 in Excel Spreadsheet File) is shifted to the left of the field data curve, T_1 has to be readjusted (decreased). A value of 80 days is entered. Compare to the model prediction curve, the field data curve has significantly more spreading. Readjust α_L (increasing α_L has the effect of increasing the spreading of the curve). An initial maximum value of 10 ft is entered. The height of the model prediction curve is now much less than field data curve. Readjust C_0Qdt (increase). An initial value of 1,250 g/ft is entered. Compare the two curves. The field data curve still has greater spreading. Now decrease the groundwater velocity. With everything else being equal, decreasing the groundwater velocity has the effect of “allowing more time for dispersion” and thus indirectly affects (increase) the spreading of the time versus concentration curve. Repeat the same procedure as above (i.e. readjust u , T_1 , α_L , and lastly C_0Qdt) until the best-fit model prediction curve to the observed field data curve is established.
- Record plume parameters after the “best-fit” curve is established:

$$\alpha_L = \underline{1.7} \text{ ft}; u = \underline{0.20} \text{ ft/day}; C_0Qdt = \underline{238} \text{ g/ft}; T_1 = \underline{565} \text{ days}$$

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- C. Change distance X value in Cell B14 of this spreadsheet model (X_3 in Table IV) to correspond to the distance to the receptor (e.g., a drinking water well). In this case, a hypothetical downgradient distance of 1,000 ft is entered.
- D. Record the time at which the MTBE plume front first appears (i.e., when MTBE concentration is greater than 5 $\mu\text{g/L}$). The time is shown in Cell B18. The maximum MTBE concentration predicted to appear in the drinking water well and the associated time at which it appears is shown in Cell B16 and B17, respectively. Alternatively, the time when the MTBE plume first becomes greater than 5 $\mu\text{g/L}$ can also be found by looking up the column AE and scrolling down to locate the cell where MTBE concentration first becomes greater than 5 $\mu\text{g/L}$. Then go across the Microsoft EXCEL worksheet horizontally to locate the corresponding time in column G. This should be the same value reported in Cell B18. Repeat the same procedure to record the time when MTBE concentration reaches its maximum. This should be the same number reported in Cell B17. The Microsoft EXCEL worksheet shows that given the monitoring data at MW-15, it would take approximately 4,200 and 5,000 days for the MTBE plume to travel and to reach maximum, respectively, in the downgradient drinking water well 1,000 feet away. An approximate estimate for this time can also be obtained through visualizing Figure 3 in EXCEL file.
- E. Save the file.

8. Troubleshooting for the Spreadsheet Analytical Model

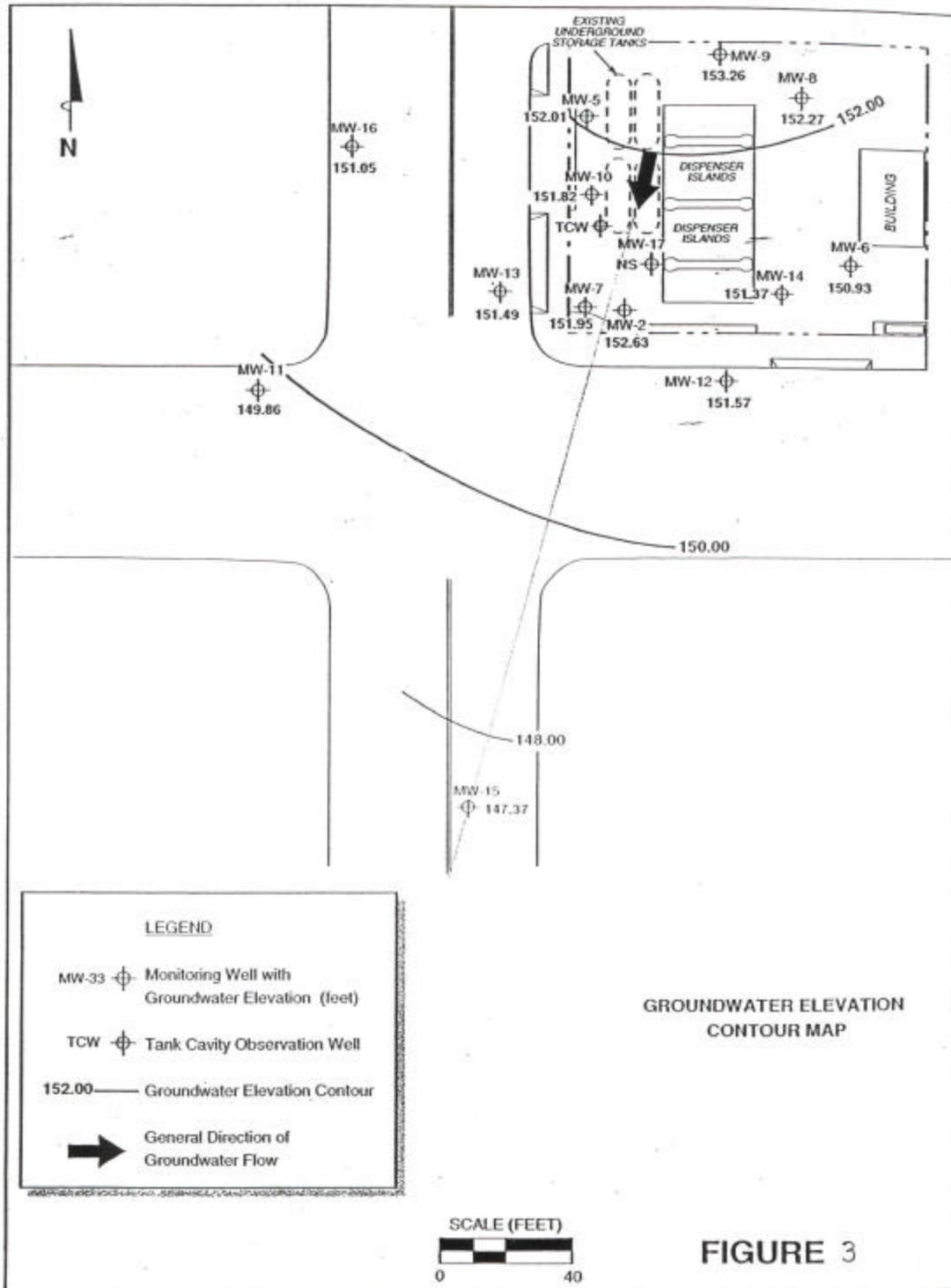
Trouble 1: Some field data do not show on the chart.

Solution: Change the Y-axis range by double clicking the Y-axis, and add one or more digits for maximum range in Scale sheet.

Trouble 2: The predicted plume travel times do not show on the chart.

Solution: Change the X-axis range by double clicking the X-axis, and add one or more digits for maximum range in Scale sheet.

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9. References

AT123D, Reference Guide and User's Guide (Version 3.0) 1998. General Sciences Corporation, 4600 Powder Mill Road, Suite 400, Beltsville, MD 20705.

Bouwer, H. 1978. *Groundwater Hydrology*. McGraw-Hill Book, New York, 448 pp.

Dawson, K.J. and Istok, J.D. 1991. *Aquifer Testing – Design and Analysis of Pumping and Slug Tests*. Lewis Publishers. Chelsea. 344 pp.

Environmental Applications, Inc., 1998, Quarterly Groundwater Monitoring Report – First Quarter 1998.

Freeze, R.A. and Cherry, J.A. 1979. *Groundwater*. Prentice-Hall, Inc., Englewood Cliffs, NJ 07632. 604 pp.

Fried, J. J. 1975. *Developments in Water Science. Groundwater Pollution: Theory, Methodology, Modeling and Practical Rules*. American Elsevier, New York, 132 pp.

Gelhar, L.W. and Axness, C.L. 1981. *Stochastic analysis of macrodispersion in three-dimensionally heterogeneous aquifers*. Report H-8. Hydraulic Research Program. New Mexico Institute of Mining and Technology, Socorro, NM 87801.

Gelhar, L.W., Welty, C. and Rehfeldt, K.R. 1992. A critical review of data on field-scale dispersion in aquifers. *Water Resources Research* **28(7)**:1955-1974.

Martin-Hayden, J.M. and Robbins, G.A. 1997. Plume distortion and apparent attenuation due to concentration averaging in monitoring wells. *Ground Water* **35(2)**:339-346.

Rong, Y., Wang, R.F., and Chou, R. 1998. Monte Carlo simulation for a groundwater mixing model in soil remediation of tetrachloroethylene. *Journal of Soil Contamination* **7(1)**:87-102.

Roscoe Moss Company 1990. *Handbook of Ground Water Development*. John Wiley and Sons, New York. 493 pp.

Todd, D.K. 1980. *Ground Water Hydrology*. John Wiley and Sons, New York.

United States Environmental Protection Agency (USEPA) 1996. Soil screening guidance: technical background document E-25pp EPA/540/R-95/128, PB96-963502.