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EVALUATION OF EFFECTS THAT CAN MASK LOW DECAY RATES OF TCE IN AEROBIC GROUNDWATER PLUMES

Laura Daniels
Clemson University, ldaniels14@gmail.com

EVALUATION OF EFFECTS THAT CAN MASK LOW DECAY RATES OF TCE IN AEROBIC GROUNDWATER PLUMES

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Laura A. Daniels
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Accepted by:
Dr. Ronald Falta, Committee Chair
Dr. Brian Looney
Dr. James Castle
Dr. Larry Murdoch

ABSTRACT

Current methods for evaluating chlorinated solvent plumes often assume that no TCE degradation occurs under aerobic conditions. It is possible that decay rates with values greater than zero exist in these plumes, but this decay may be masked by effects of parameter values in zero-decay-rate models. This hidden decay can be identified by comparing the zero-decay-rate models with others that have been created with a decay rate greater than zero.

The results of this research and analysis show that it is possible to create matches between the zero-decay-rate models and models with greater than zero decay rates by adjusting model parameters other than the decay rates. The matches were closer and more easily achieved at lower decay rates than at higher ones, and increasing the number of spatial dimensions in which to match the models also increases the difficulty of creating the match. The matches are sensitive to time and do not maintain their similarity when they are examined at other discrete points in time. Time was the most important variable in making the distinction between the effects of degradation processes on the plume and those of physical processes, but the three-dimensional plume geometry is also an important factor. Because of the strong influence of time as a variable, it is crucial to collect plume data at different points in time to help constrain the models. Analysis of the results shows that it is indeed possible for rates of decay up to about 0.3 (yr^{-1}) to be masked by model parameter values and that this misinterpretation is more likely to occur in models with lower decay rates (such as 0.1 per yr) than in models with higher rates.

DEDICATION

To my precious husband and family:

I could not have gotten through it all without your support.

Thank you from the bottom of my heart. I love you.

ACKNOWLEDGMENTS

I would like to thank the professors, instructors, and teachers who have helped me over the years in my educational endeavors. Thanks especially to Dr. Ron Falta, my advisor and committee chair, and to the members of my committee: Dr. Brian Looney, Dr. Jim Castle, and Dr. Larry Murdoch. Your help and support made this work possible.

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LIST OF SYMBOLS AND NOMENCLATURE

cVOC .... chlorinated volatile organic compound

MNA .... monitored natural attenuation

TCE .... trichloroethene (trichloroethylene)

DNAPL .... dense non-aqueous phase liquid

NAPL .... non-aqueous phase liquid

EPA .... Environmental Protection Agency

MCL .... maximum contaminant level

MCLG .... maximum contaminant level goal

PCE .... tetrachloroethene

DCE .... dichloroethene

VC .... vinyl chloride

PAT .... pump and treat

USGS .... United States Geological Survey

AFB .... air force base

yr .... year

m .... meters

M .... mass (of TCE)

C .... concentration (of TCE)

C_0 .... original concentration (of TCE)

C_s .... concentration in source zone (of TCE)

k, λ, & "dr" .... first-order degradation rate (of TCE; yr^{-1})

t .... time

$t_{1/2}$ .... half-life

λ_s .... decay rate of source, not by dissolution

Q .... groundwater flow rate

R .... retardation coefficient

rxn(x, t) .... reaction rate of contaminant (+ or -)

List of symbols and nomenclature (continued)

α_L .... longitudinal dispersivity
α_T .... transverse dispersivity
α_V .... vertical dispersivity
v .... groundwater flow velocity (m/yr)
y .... yield coefficient
n .... number of plume zones
A .... cross-sectional area (m^2)
φ .... porosity of the matrix
x .... centerline position of advective front (m)
M_0 .... original mass (of TCE) (kg)
Γ .... Gamma; power function exponent
W .... source width (m)
D .... source depth (m)
V_D .... Darcy velocity (m/yr)
vMin .... minimum normalized stream tube velocity (m/yr)
vMax .... maximum normalized stream tube velocity (m/yr)
σ_v .... coefficient of variation of velocity field
X, Y, & Z .... the three dimensions in Cartesian space (m)
RMS .... root mean squared error
NRMS .... normalized root mean squared error
C_m or ($\overline{C}$) .... mean of base-case (TCE) concentrations

CHAPTER ONE

INTRODUCTION

1.1 Background

Large, dilute plumes of chlorinated volatile organic compounds (cVOCs) in groundwater present a specific set of remediation challenges [Looney, 2010]. These plumes generally occur in permeable aquifers and are often measured in units of miles due to their great spatial extent [Looney, 2012]. The aerobic (oxygen-rich), oligotrophic (organic carbon-poor) nature of these plumes causes difficulty when applying the existing remediation methods, which are largely designed for anaerobic conditions [Looney, 2010]. It is difficult to maintain conditions favorable to chemical reduction processes in these aerobic plumes due to the prevalence of electron acceptors, degradation processes within the aerobic plumes tend to be slow, and the plumes are often quite deep in the subsurface [Looney, 2012]. By showing that natural attenuation can occur in these large, dilute plumes of cVOCs, it is hoped that future remediation strategies at these sites may be designed to include Monitored Natural Attenuation (MNA) in the plume zones, which will save a great deal of expense over the life of the projects, save the sites from geological disruption caused by more invasive remediation techniques, and still be effective in reducing the groundwater concentrations of the cVOCs.

This project focuses specifically on the cVOC trichloroethylene (TCE). TCE, a dense non-aqueous phase liquid (DNAPL), is a non-flammable, colorless liquid with a subtly sweet smell that was first commercially produced in Europe in 1908 [Encyclopædia Britannica, 2013]. Current U.S. Environmental Protection Agency (EPA) drinking water standards require that levels of TCE in drinking water be less than the maximum contaminant level (MCL) of 5 μg/L (0.005 mg/L), and the EPA maximum contaminant level goal (MCLG) for this dangerous chemical is 0 μg/L [EPA, 2012]. Because it is a DNAPL, TCE is difficult and expensive to remove from soil and water and has the added hazard of volatilizing through overburden and into buildings [Hsiao et al., 2011].

Widespread use in degreasing applications, adhesives, dry-cleaning, as a base for commercial production of tetrachloroethylene (PCE), and (surprisingly) in decaffeination of coffee and removal of fats and waxes from wool and cotton has led to similarly widespread TCE-contamination of surface- and groundwater [Encyclopædia Britannica, 2013]. Known by the trade names "Triclene" and "Vitran," among others, TCE is released into the environment in the greatest amounts through evaporation from manufacturing facilities that use it as a degreaser [ATSDR, 1997]. A recent exhaustive study found that TCE can cause several types of cancer in humans through any route of exposure and it acts as a non-carcinogenic poison to the central nervous system, liver, kidneys, immune system, male reproductive system, and to embryos and fetuses of affected mothers [Chiu et al., 2013].

Degradation mechanisms known to exist for TCE under aerobic conditions are aerobic cometabolism and abiotic reactions with iron minerals [Looney, 2012]. Aerobic cometabolism of TCE produces no daughter products, occurs naturally at many sites, and has been found to be directly related to microbial population counts [Looney, 2012]. Abiotic reactions in aerobic plumes occur with iron-bearing minerals, such as pyrite, siderite, goethite, and magnetite (and others) and can result in half-lives of 4 to 6 years [He et al., 2009]. Along with physical dispersion and dissolution, aerobic cometabolism and abiotic reactions drive natural attenuation in aerobic plumes [B. Looney, personal communication, July 5, 2013].

TCE belongs to a family of chemicals known as the halogenated ethenes which have centrally located, double-bonded carbon atoms in their molecular structure and one or more atoms from the halogen group (in this case chlorine) attached to the carbon atoms as shown in Figure 1.1.1 [Peterson, 1999]. This family of chemicals forms a

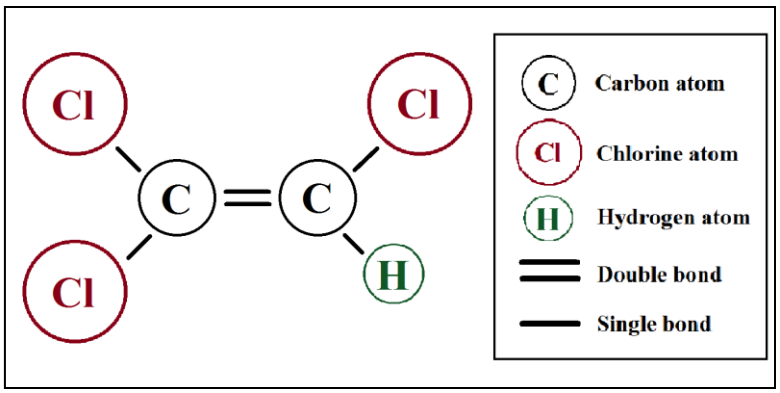


Figure 1.1.1: Molecular Structure of TCE modified from Peterson [1999]

degradation "chain" as dechlorination of the base compound occurs; from tetrachloroethene (PCE) with four chlorine atoms, to trichloroethylene (TCE) with three chlorine atoms and one hydrogen atom, to dichloroethene (DCE) with two chlorine atoms and two hydrogen atoms, to vinyl chloride (VC) with one chlorine atom and three hydrogen atoms, to ethene with no chlorine atoms and four hydrogen atoms, and finally to harmless ethane after hydrogenation increases the total number of hydrogen atoms from four to six as is shown in Figure 1.1.2 [ERM, 2006].

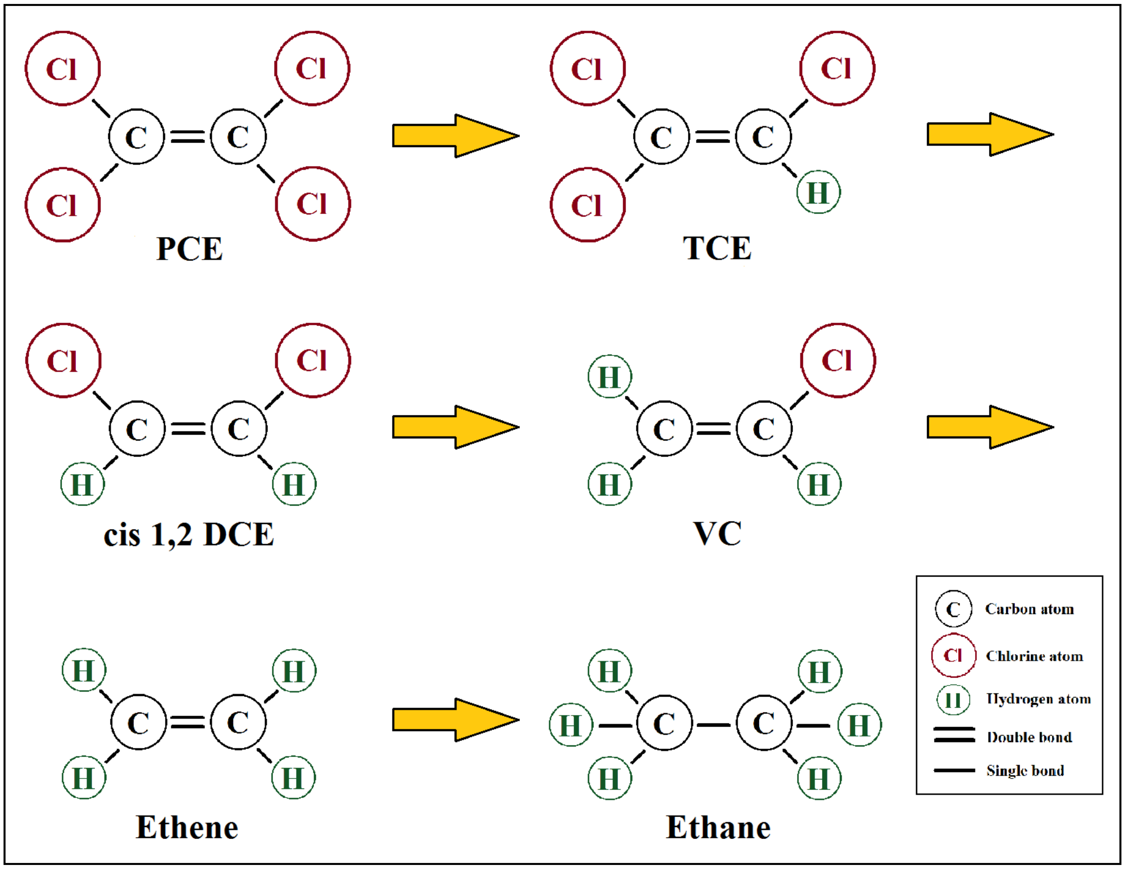


Figure 1.1.2: cVOC degradation chain modified from ERM [2006]

"Cometabolism" refers to the process by which microorganisms produce an enzyme or cofactor in their daily life process that has the fortunate side-effect of causing degradation of the cVOCs with the microorganisms not obviously benefiting from the actual degradation of the contaminant [Wiedemeier et al., 1999]. Cometabolism of TCE has been more frequently studied than has cometabolism of the other cVOCs in the series, and a wide range of microorganisms have been found to possess the ability to produce the enzymes necessary for the degradation of TCE [Alvarez-Cohen & Speitel, 2001]. These naturally occurring processes in aerobic plumes have a longer timeframe to total degradation and slower rates of decay than do the degradation processes associated with anaerobic plumes [Looney, 2010]. Not all of the cVOCs degrade by all of the different kinds of processes, and degradation can proceed by different mechanisms in aerobic or anaerobic zones of the plume [Wiedemeier et al., 1999]. Differences in the mechanisms of decay for aerobic versus anaerobic conditions is presented in Figure 1.1.3. As shown in the diagram, aerobic cometabolism of TCE produces no daughter compounds. In laboratory testing, aerobic cometabolism of TCE produced only CO_2 and stable compounds that are soluble in water [Little et al., 1988].

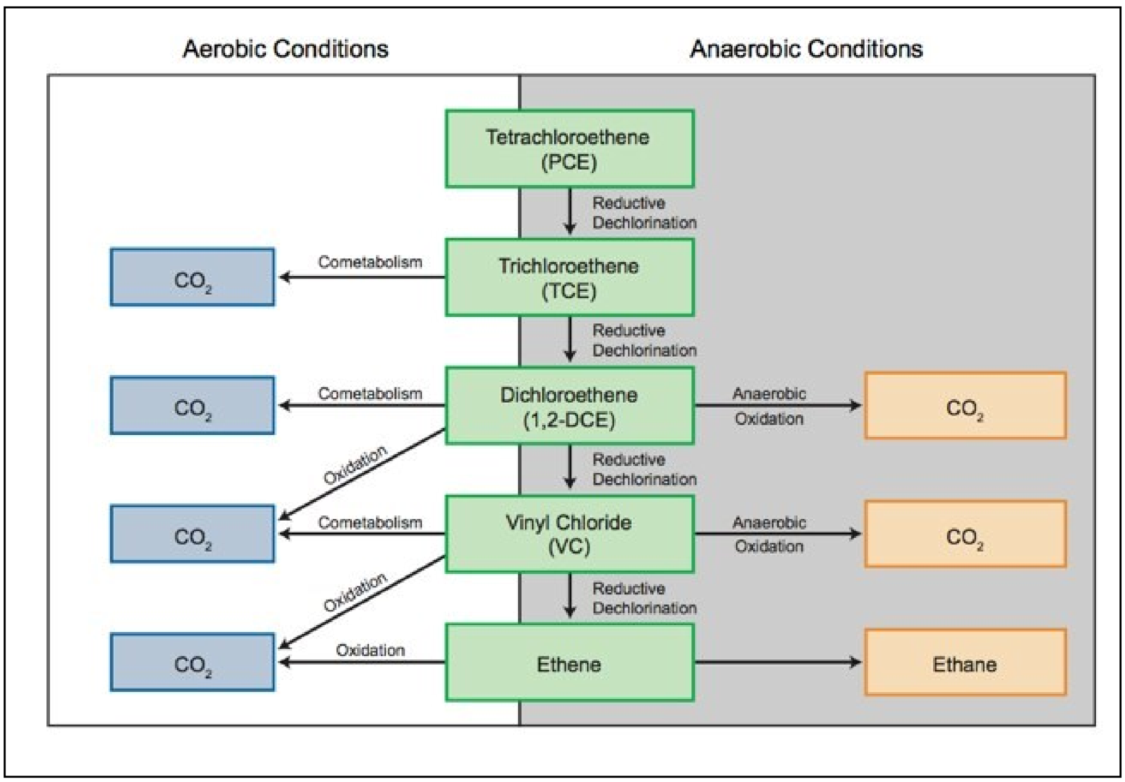


Figure 1.1.3: cVOC degradation series for aerobic & anaerobic conditions [Yan, 2009]

For the purpose of this study, all of the different kinds of degradation taking place in the aerobic plumes will be referred to simply as “degradation” or “decay” due to the complex nature of the kinetics of the active processes which rely on chemical and environmental factors to proceed [Clement et al., 2000]. This project assumes that the degradation of the TCE in the plumes follows the first-order decay model. The formula for first-order decay, shown in Equation 1.1, is frequently applied when studying contaminant degradation [Wiedemeier et al., 1999].

$$C = C_0 e^{-kt} \tag{1.1}$$

Where: C = biodegraded concentration of TCE
C_0 = beginning concentration of TCE
k = decay rate of TCE
t = time

Equation 1.1 follows from the exponential relationship between the degradation rate and the TCE concentration [Wiedemeier et al., 1999]. It is sometimes helpful to express the rate constant in half-life notation using the formula in Equation 1.2 [Wiedemeier et al., 1999].

$$t_{1/2} = \frac{0.693}{k} \tag{1.2}$$

Where: $t_{1/2}$ = time of half-life
k = decay rate of TCE

There is a great deal of variability in the values of TCE aerobic decay half-lives reported in the literature, with some of the laboratory-derived values being higher than one would expect to find in the field (due to the greater ability to control and manipulate the experiments in the laboratory environment), and the decay rates are condition-dependent and can vary even within a single plume [Wiedemeier et al., 1999]. Table 1.1.1 shows values of TCE decay rates in units of yr^{-1} that were calculated from the first-order aerobic half-life values in Wiedemeier et al. [1999], which were gleaned from several sources in their literature review. The table also includes the estimated range of

First order aerobic half-life (years)	Rate Constants (1/yr)	Lab or Field	Reference
0.22-2.31	3.2-0.3	-	Aziz, 2002
>100	<0.007	F	Weidemeier, 1999
0.01	126.47	L	
0.19	3.67	L	
0.24	2.84	L	
0.1-0.25	7.67-2.81	L	
0.39	1.79	L	
0.39-0.58	1.79-1.20	L	
0.63-18.99	1.10-0.04	L	
0.32-0.95	2.18-0.73	F	
0.40-2.32	1.72-0.30	F	
0.50-0.58	1.39-1.20	F	
0.54-3.01	1.28-0.23	F	
0.63	1.10	F	
1	0.69	F	
1.19-1.73	0.58-0.40	F	
2.16	0.32	F	
2.40-4.22	0.29-0.16	F	
2.71-3.16	0.26-0.22	F	
3.8	0.18	F	
190	0.004	F	Clement, 2000
0.06-441	11.5-0.002	L	He et al., 2009

TCE Aerobic Decay Rates

Table 1.1.1: TCE aerobic decay rates from [Aziz et al., 2002], [Wiedemeier et al., 1999], [Clement et al., 2000], and [He, et al., 2009]

rate constants for TCE biodegradation from BIOCHLOR, a software package that is used to simulate remediation by means of natural attenuation [Aziz et al., 2002]. To produce this range of values, the BIOCHLOR model was calibrated with values from the BIOCHLOR database so that users would have reasonable field decay rate values [Aziz et al., 2002]. The "field" rate constant values in the table range from 0.18 to 2.18 (yr^{-1}) {a half-life range of 3.8 to 0.32 years}, which is relatively similar to the BIOCHLOR-estimated rate constant range of 0.3 to 3.2 (yr^{-1}) {a half-life range of 2.31 to 0.22 years}. Laboratory-measured rates in the table range from 1.10 to 126.47 (yr^{-1}) {a half-life range of 0.63 to 0.01 years}, which is a much greater range of values with a much shorter overall half-life than was reported for the field-derived values. In addition to the biodegradation rates in the table, the last set of rates are from laboratory studies of abiotic TCE degradation processes with iron-bearing minerals as discussed in He, et al. [2009]. In general, it has been found that rate constants derived from laboratory studies tend to be higher than those derived from studies conducted in the field [Suarez & Rifai, 1999]. It should be noted that the rates in this table may be greater than the aerobic rates of decay in real-world plumes because degradation rates are influenced by site-specific factors.

Current methods for evaluating aerobic plumes of chlorinated solvents often assume that no degradation occurs, other than physical processes such as dispersion and dilution [Looney 2010]. The methods employed in the remediation of chlorinated solvent plumes are expensive, can take projected centuries to clean the site, and have the potential to cause major mechanical disturbance in the geology of the treated site [Looney, 2010]. For example, studies conducted by the EPA on 19 sites where pump and treat (PAT) remediation methods were in use found that NAPLs at the sites could not be cleaned up by the PAT system and were the cause of the method not succeeding in remediating the sites in their originally projected time frames [Wiedemeier et al., 1999]. Though it is the most frequently utilized remediation strategy, PAT systems can sometimes take (projected) centuries to clean up a site to drinking water standards because of NAPL contamination, making the method expensive and impractical for some cases [Wiedemeier et al., 1999]. Monitored natural attenuation could be utilized in cases of large, dilute plumes of chlorinated solvents as a less expensive remediation option (or in addition to an existing remediation method) that could provide a means of closure for such EPA-designated sites [Looney, 2010].

Research is ongoing in the natural attenuation arena so that as it is better understood, this process can be thoughtfully applied as a legitimate remediation method for difficult NAPL-contaminated sites [Wiedemeier et al., 1999]. It is the aim of this study to be useful in the natural attenuation decision arena by analyzing, via mathematical modeling, first-order decay rates of TCE in aerobic groundwater plumes in the hopes of showing that it is possible for aerobic degradation of TCE to be occurring in these plumes.

The hypothesis of this research is that a decay rate of values greater than zero may exist in aerobic chlorinated solvent plumes and that this natural decay process can be used as an alternative remediation method to the more costly and disruptive remediation methods currently in use, such as the PAT systems mentioned earlier. An example of such a site exists in the form of a freshwater tidal wetland at Aberdeen Proving Ground in Maryland at which TCE is one of the primary parent contaminants [Lorah et al., 1997]. In a United States Geological Survey (USGS) study conducted at the site in 1992-1997 it was discovered that high rates of biodegradation of TCE were occurring in the thin layers of aerobic wetland sediment with half-lives due to methanogenic biodegradation as great as 2 to 7 days (and first-order degradation rates of 0.10 to 0.31 per day) [Lorah et al., 1997]. For cases such as this, it makes sense that monitored natural attenuation of the TCE could be favorable to upsetting the natural balance of the site with the installation of a disruptive remediation system, but that decision would depend on many other site-specific factors, including the immediate environmental impact of the TCE. Other sites for which monitored natural attenuation could be judiciously employed based on individual site conditions include those for which the contaminant source has been removed and the remaining contaminant plume is left in need of remediation, in sites where infrastructure would obstruct and preclude other forms of remediation, and at sites where the extant geology would interfere with the workings of traditional remediation methods (such as low permeability structures restricting the flow to a PAT system) [Wiedemeier et al., 1999].

1.2 Cases and strategy

When studying natural attenuation it is helpful to use a groundwater fate and transport model to make predictions about the movement of the contaminants and their degradation and to make estimates of the time it takes for the plume to exhibit an expected behavior [Wiedemeier et al., 1999]. There are many different types of analytical models to choose from, but REMChlor (Remediation Evaluation Model for Chlorinated Solvents) is the simulation program chosen for this project because it can address the plumes both spatially and temporally while remaining fairly simple to utilize, and it can produce exact results [Looney, 2010]. One of the assumptions inherent in the program is that biodegradation reactions in the plume are occurring as first-order reactions (as previously discussed) and can be described by Equations 1.1 and 1.2 [Falta, 2008]. Modeling the plume begins with a mass balance approach for contaminant flux into the groundwater from flow from the source zone and is described by Equation 1.3 [Falta et al., 2005a & Falta, 2008].

$$\frac{dM}{dt} = -Q(t)C_s(t) - \lambda_s M \qquad (1.3)$$

Where:
- M = mass of contaminant in the source zone
- C_s = dissolved contaminant concentration in the source zone
- λ_s = decay rate of the source, not by dissolution
- Q = flow rate of clean water through the source

This formula shows that the change in the mass of the contaminant in the source zone as time goes on is proportional to the flow of the contaminant ($Q(t)C_s(t)$) out of the source zone minus the amount of first-order degradation of the contaminant not due to the physical dissolution process ($\lambda_s M$), with the flow rate (Q) having a great deal of control over how much contaminant is released into the plume [Falta, 2008]. REMChlor considers the concentration of the contaminant in three dimensions (X, Y, and Z) in the plume and also in time. This is accomplished by using a three-dimensional governing equation that allows for variable reaction rates, which previous modeling applications have not, and is shown below in Equation 1.4 [Falta et al., 2005b and Falta, 2008].

$$R\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + \alpha_L v\frac{\partial^2 C}{\partial x^2} + \alpha_T v\frac{\partial^2 C}{\partial y^2} + \alpha_V v\frac{\partial^2 C}{\partial z^2} + rxn(x,t) \qquad (1.4)$$

Where:
R = retardation coefficient
$rxn(x,t)$ = reaction of the contaminant (+ or -)
α_L = longitudinal dispersivity
α_T = transverse dispersivity
α_V = vertical dispersivity
v = velocity of groundwater flow

This formula expresses the advection, dispersion in three dimensions, and the generation/degradation rate of the given contaminant. Advection, which is physical movement of the contaminant by groundwater flow, is described by the term ($v\frac{\partial C}{\partial x}$) while the next three terms ($\alpha_L v\frac{\partial^2 C}{\partial x^2}, \alpha_T v\frac{\partial^2 C}{\partial y^2}, \alpha_V v\frac{\partial^2 C}{\partial z^2}$) describe dispersion of the contaminant in three dimensions (α_L for longitudinal, α_T for transverse, and α_V for vertical) [Falta, 2008]. Dispersion causes the concentration of the contaminant in the groundwater to become less, but no actual change of mass of the contaminant is occurring [Wiedemeier et al., 1999]. The last term in the formula ($rxn(x,t)$) allows for the model to be run with various degradation (the term is negative) or generation (the term is positive) rates for the contaminant(s) in space and time in order to represent the possible real-world behavior of the dissolved substance(s) in the subsurface [Falta, 2008]. The reaction term ($rxn(x,t)$) is a generalized expression of the actual batch reaction terms that can form the degradation/generation portion of this governing equation for chemical species and their daughter products [Falta, 2008]. For example, if it were desired to model the behavior of four chemical species, A, B, C, and D, (which could be set to correspond to the cVOC degradation chain of PCE to TCE to DCE to VC) then the terms used in place of the general reaction term would be written as shown in Table 1.2.1 below [Falta, 2008]:

Chemical Species	Reaction Term
A	$-k_{A(n)}C_{A(n)}$
B	$y_{BA(n)}k_{A(n)}C_{A(n)} - k_{B(n)}C_{B(n)}$
C	$y_{CB(n)}k_{B(n)}C_{B(n)} - k_{C(n)}C_{C(n)}$
D	$y_{DC(n)}k_{C(n)}C_{C(n)} - k_{D(n)}C_{D(n)}$

Table 1.2.1: Batch Reaction Terms for ($rxn(x,t)$) in Governing Equation from [Falta, 2008]

where $y_{ij(n)}$ represents the yield coefficients for each reaction wherein a daughter product is generated, $k_{i(n)}$ represents the rate constants for the reactions taking place for each species, $C_{i(n)}$ represents the concentration of each species, and n represents the different zone(s) of the plume (in REMChlor there are three in space and three in time for a total of nine plume zones) in which the reaction(s) are occurring [Falta, 2008]. In each of the reaction terms for species B-D, the first portion of the expression ($y_{ij(n)}k_{j(n)}C_{j(n)}$) is positive and represents the generation of a daughter product, while in all four sets of terms the negative portion of the expression ($-k_{i(n)}C_{i(n)}$) describes the first-order degradation of the species [Falta, 2008]. Because this study focuses only on TCE with no daughter product generation occurring, the form of the reaction expression used in the governing equation for all zones of the plume is that of species A, $-k_{TCE(n)}C_{TCE(n)}$, where the reaction rate, k, corresponds to the chosen plume decay rate, λ, in each of the scenarios run for each of the three Cases. Because REMChlor can create models in space and time for the advection, dispersion, and first-order degradation of TCE, it will be possible to make comparisons between the models to study the spatial extent and concentrations of TCE that result from given conditions at chosen plume decay rates. The program will allow for reproducible results and multiple trials for each scenario at various rates of decay.

For this project, three types of groundwater plume behaviors were chosen for study: stable, growing-connected, and growing-disconnected. The "stable" plume designation applies to a groundwater plume that remains at approximately the same spatial extent (i.e. not increasing in size), has a slowly declining TCE concentration over time, and that has its contaminant mass present partially in both the source zone and the plume [Pate, 2010; Liang, 2009]. The "growing" plumes are in the process of expanding in spatial extent (migrating in the positive X-axis-direction) and are experiencing declining concentrations of TCE over time; the difference between them is that one of the growing plumes is still connected to its source zone (with contaminant mass present partially in the source zone and partially in the plume) while the disconnected plume has most of its contaminant mass in the plume and is no longer connected to its source zone [Liang, 2009]. The source zone for each of the three of the plume types is assumed to originate from a DNAPL release to the saturated zone with migration of the contaminant being caused by groundwater flow.

In this study, Case 1 presents a stable plume, one that is present and relatively unchanging for a long period of time that has been chosen as a base-case in REMChlor for study at six different decay rates. The DNAPL release to the subsurface is assumed to have occurred 60 years prior to the present day and the plume has had adequate time to migrate and develop into its current stable state. An extension of Case 1 is presented in Case 1b in which another stable plume, with the contaminant mass partially present in the source zone as well as in the plume is presented, but with a different set of base-case parameters that were taken from Liang [2009] and which is studied at three different plume decay rates. Once again, the DNAPL release to the subsurface is assumed to have occurred 60 years prior to the present day.

In Case 2, the plume type is Growing-Disconnected and it represents the scenario of a plume with increasing size over the study-time, with most of the contaminant mass in the plume, that is no longer connected to its contaminant source. The parameters for the base-case in Case 2 are taken from Liang [2009]. Upon running several trials of this Case in REMChlor and studying the results, it was decided that a period of 60 years from the time of DNAPL release (as was used in the first Case) was too long a period of time for plume development because of the much faster "washing-out" of the contaminants in this scenario. For this Case, then, the DNAPL release is assumed to have occurred 54 years prior to the present day instead of 60 years.

The final scenario is Case 3, in which the plume behavior is Growing-Connected and it represents a scenario with a plume of increasing spatial extent over the study-time, with part of the contaminant mass in the source zone and part of it in the plume, but that is still connected to its source zone. The parameters for the Case 3 base-case also originate from Liang [2009]. The DNAPL release for this Case is assumed to have occurred 60 years prior to the current date.

The times of DNAPL release to the subsurface in the scenarios described above, 60 years ago and 54 years ago, were chosen so that the models produced in this study would more closely resemble actual present-day cVOC plumes that were created at the height of TCE usage and improper disposal that occurred approximately that long ago.

The strategy for this project with each of these Cases is to create a base-case model with some given non-zero decay rate (0.1, 0.2, 0.3 etc. in units of yr^{-1}) and to then create a match-case model with a plume decay rate of zero with all the other parameters the same as in the base-case. Then for each match-case the parameters (those other than the plume decay rate) will be adjusted to cause the match-case model to coincide with the base-case model in the X- and Y-directions at a given time after initial contaminant release. The first manipulations applied were to the initial mass and concentration parameters (M_0 and C_0) to adjust the centerline plot along the vertical concentration axis. Next, the Darcy velocity and retardation factor (V_D and R) were manipulated to adjust the centerline plot along the horizontal X-direction axis. The longitudinal, transverse, and vertical dispersion terms (α_L, α_T, and α_V) were then manipulated in order to force the centerline and X-Y spatial plane plots to match. Successfully coordinating the match-case model with its plume decay rate of zero to the base-case models, which have non-zero plume decay rates, should show that it is possible for some amount of contaminant decay to be masked by the effects of physical dispersion.

CHAPTER TWO

OBJECTIVE

The objective of this research is to show that it is possible for degradation in aerobic chlorinated solvent plumes to be masked by model parameter values and to thereby be misinterpreted by zero-decay-rate models as dispersion.

CHAPTER THREE

METHODOLOGY: CREATION, MATCHING, & ANALYSIS OF MODELS

3.1 Creating the REMChlor models

The transport model for this research was REMChlor, Remediation Evaluation Model for Chlorinated Solvents, which can be downloaded from the Environmental Protection Agency (EPA) website [EPA, 2010]. REMChlor was used to simulate different scenarios for which the resulting output was processed in both Excel™ and Tecplot™ to produce chart-style comparisons of centerline TCE concentrations over longitudinal distance and two-dimensional contour plots of plume concentrations for the X-Y and X-Z spatial planes for each scenario.

The calculations in REMChlor begin with a mass balance of the source zone (which was presented as Equation 1.3) that is shown below as Equation 3.1 [Falta et al., 2005a & Falta, 2008]:

$$\frac{dM}{dt} = -Q(t)C_s(t) - \lambda_s M \tag{3.1}$$

Where: M = mass of contaminant in the source zone
C_s = dissolved contaminant concentration in the source zone
λ_s = decay rate of the source, not by dissolution
Q = flow rate of clean water through the source

This means that the discharge of contaminant from the source zone, as a mass varying over time, is dependent upon the flow rate of clean water through the source, the concentration of contaminant that can dissolve over that period of time, the contaminant mass that remains in the source, and the decay rate of the contaminant in the source by other means than dissolution [Falta, 2008]. These other causes of decay of the source contaminant could be the result of a natural process such as sorption, biodegradation, chemical reduction, chemical oxidation, aerobic cometabolism, or a combination of these mechanisms [Falta, 2008].

The relationship between the mass of contaminant in the source and the amount of it that is discharged from the source can be described by Equation 3.2 [Rao et al., 2001; Rao & Jawitz, 2003; Parker & Park, 2004; Zhu and Sykes, 2004; Falta et al., 2005a; Falta, 2008]:

$$\frac{C_s(t)}{C_0} = \left[\frac{M(t)}{M_0}\right]^{\Gamma} \tag{3.2}$$

Where:
M_0 = original mass of contaminant in the source zone
C_0 = original dissolved contaminant concentration in the source zone
Γ = controls proportion of source discharge to source mass

Gamma (Γ) has been shown through theoretical analysis to vary widely, but for the purpose of this study it was decided to assign Γ a value of 1, which indicates a 1:1 relationship between source discharge and source mass [Falta, 2008]. This linear relationship between the source discharge and the source mass when Γ is equal to one is supported by studies conducted by Rao & Jawitz [2003], by Parker & Park [2004] and by Newell et al. [2006]. The effect of smaller and larger values of Γ on the source discharge/source mass relationship is best illustrated in a diagram from the REMChlor User's Manual, shown in Figure 3.1.1. It follows that if remediation is done on the source zone, then the source zone discharge is reduced linearly if the Gamma value is one [Newell et al., 1996; Parker & Park, 2004; Zhu and Sykes, 2004; Falta, 2008].

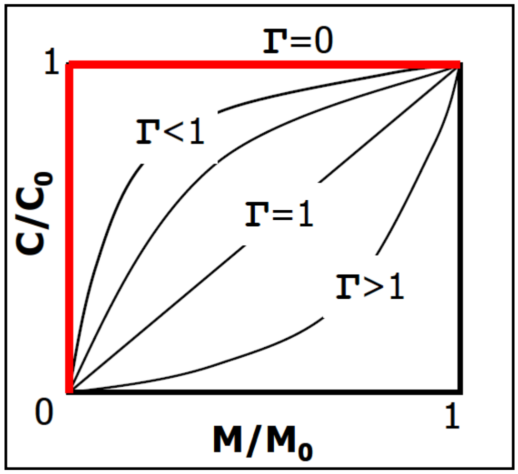


Figure 3.1.1: Source discharge/source mass relationship under control of Gamma [Falta, 2008]

Having REMChlor run the calculations with Γ=1 results in the exponential decrease of both contaminant mass in the source zone and contaminant discharge from the source zone over time, which is a behavior that has been documented under field conditions at sites contaminated with chlorinated solvents [Newell & Adamson, 2005; McGuire et al., 2006; Newell et al., 2006; Falta, 2008]. However, by using a value of one for Γ, a situation is created where the source always exists at some mass and concentration, though small, even after very long periods of time [Falta, 2008]. When Γ is assigned a value of 0, it indicates a source that is relatively stable that releases a continuous amount of TCE [Newell & Adamson, 2005; McGuire et al., 2006; Newell et al., 2006; Falta, 2008]. A value of between 0.5 and 2 is used for Gamma in most situations, but because of the variable nature of Γ and the range of effects it can cause in the models, it was decided for this project to assign a value of 1 to Γ to represent exponential decay of the source that one might expect to see occurring naturally in a given environment due to dissolution [Newell & Adamson, 2005; McGuire et al., 2006; Newell et al., 2006; Falta, 2008].

For the plume portion of the model, REMChlor utilizes a three-dimensional governing equation for the dissolved concentration of the contaminant(s), shown below in Equation 3.3 [Falta et al., 2005b and Falta, 2008]:

$$R\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + \alpha_L v\frac{\partial^2 C}{\partial x^2} + \alpha_T v\frac{\partial^2 C}{\partial y^2} + \alpha_V v\frac{\partial^2 C}{\partial z^2} + rxn(x,t) \qquad (3.3)$$

Where: R = retardation coefficient
$rxn(x,t)$ = reaction rate of the contaminant (+ or -)
α_L = longitudinal dispersivity
α_T = transverse dispersivity
α_V = vertical dispersivity
v = velocity of groundwater flow

The reaction rate of the contaminant, expressed by the term, $rxn(x,t)$, accounts for chemical and biological processes that can cause generation or destruction of the contaminant in question within the plume [Falta, 2008]. As explained before in the Introduction and as shown in Table 1.2.1, the reaction term for this study is equivalent to the expression: $-k_{TCE(n)}C_{TCE(n)}$ because this study focuses exclusively on the contaminant, TCE, without its daughter products. The partial differential terms on the right side of the equal sign express advection and contaminant dispersion in three dimensions; longitudinal in X-, transverse in Y-, and vertical in Z-directions [Falta, 2008]. REMChlor links Equation 3.3, the governing equation for concentration of dissolved contaminant in the plume, to Equation 3.1, the source zone mass balance, via Equation 3.2, the power function relationship between mass of the contaminant in the source zone and how much of it is discharged. This linkage results in the formula shown in Equation 3.4 that describes the mass flux of contaminant discharging from the source zone into the plume [Falta et al., 2005b and Falta, 2008]:

$$\frac{Q(t)C_s(t)}{A} = \left[\varphi v C(t) - \varphi \alpha_L v \frac{\partial C(t)}{\partial x}\right]_{x=0} \tag{3.4}$$

Where: A = area of contaminant flux into groundwater
φ = porosity of the matrix through which flow occurs

Equation 3.4 is a flux boundary condition set by the term $x = 0$ that guarantees that the rate at which contaminants are entering the groundwater flow from the source zone is the same as the rate at which those same contaminants are migrating into the contaminant plume [van Genuchten & Alves, 1982 and Falta, 2008]. Contaminant mass flux into the groundwater from the source zone is restricted to only the area described by A which is in a vertical orientation perpendicular to flow [Falta et al., 2005b and Falta, 2008].

REMChlor requires the input of values for a specific set of parameters in order to make the necessary calculations for each model [Falta, 2008]. These values are entered into fields in the program's graphical user interface, shown in Figure 3.1.2, which is comprised of seven categorical areas: Source Parameters, Source Dimensions, Source Remediation, Transport Parameters, Simulation Parameters, Cancer Risk, and Decay Rates in both time and distance. Because this thesis is predominantly an examination of factors affecting rates of decay, the Cancer Risk section was not utilized. The Source Parameters section for each of the models consists of Source Concentration of TCE (C_0 at time zero in g/L), Mass of TCE (M_0 at time zero in kg), and Gamma (Γ) which is a dimensionless value [Falta, 2008]. The Source Dimensions are described by Source Width and Source Depth, both in meters [Falta, 2008]. Also included in this section are Darcy Velocity (V_D in m/yr) and Porosity (φ) [Falta, 2008].

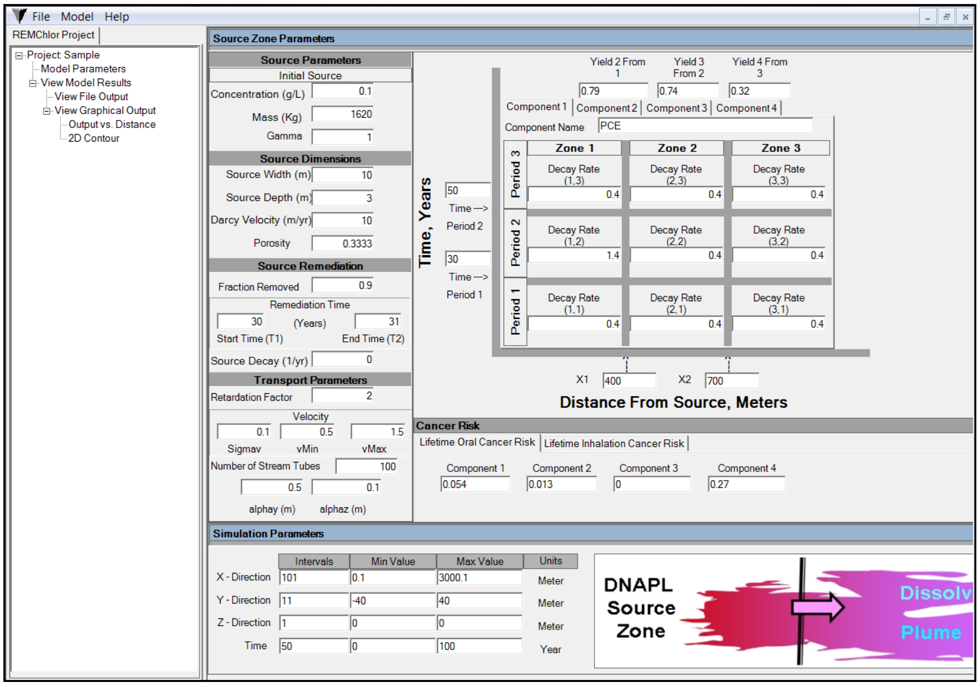


Figure 3.1.2: Parameter value entry screen in REMChlor program [Falta, 2008]

Because the focus of this study is on plume decay, fields in the Source Remediation section were kept at values of zero. However, much of the parameter adjustment for the purpose of creating better model fit in the different scenarios was applied in the next section: Transport Parameters. Retardation Factor (R), a dimensionless parameter, is estimated from the fraction of organic carbon in the subsurface and from the organic carbon partition coefficient [Falta, 2008]. Because it describes adsorption in the subsurface, higher R values cause chemical dispersion to be hindered while lower values allow for a greater amount of contaminant transport [Anderson & Woessner, 1992].

There are six fields under the subheading "Velocity" within the Transport Parameters section. The Number of Stream Tubes value determines the number of longitudinal "pathways" used by REMChlor to perform the calculations in which higher values yield smoother-looking results but take greater amounts of time for the program to run [Falta, 2008]. The terms vMin, and vMax describe the minimum and maximum values for normalized stream tube velocity, should not be negative values, and are closely related mathematically to Sigmav (σ_v), the "coefficient of variation of velocity field" [Falta, 2008]. Sigmav (σ_v) is a critical factor when manipulating the parameters in attempts to produce matches between pairs of models and is intimately linked to a scale-dependent longitudinal dispersivity (α_L) [Falta, 2008].

The results of the calculations that define the relationship between σ_v and α_L are best viewed in tabular format as shown in Table 3.1.1. In REMChlor, longitudinal dispersivity (α_L) is a scale-dependent value where "x" represents distance along the centerline of the plume [Charbeneau, 2000; Falta, 2008].

α_L	σ_v
x/200	0.1
x/100	0.14142
x/50	0.2
x/20	0.31623
x/10	0.44721

Table 3.1.1: Longitudinal dispersivity (α_L) correspondence to Sigmav (σ_v) [Falta, 2008]

The last two fields in the Transport Parameters section are for "alphay" (α_T) and "alphaz" (α_V), in meters, which represent transverse and vertical dispersivity respectively [Falta, 2008]. The value of α_T is typically one tenth (or less) the value of α_L, while α_V is typically one one-hundredth (or less) of α_L [Falta, 2008]. Because the values of α_T and α_V depend on the value of the scale-dependent α_L, they often are also scale dependent in nature, though there were certain scenarios in this study for which the transverse and vertical dispersivity were adjusted beyond their normal ranges of values for purposes of fitting the model pairs. Using these guidelines, it was possible to estimate input values for the manipulation of α_T and α_V which allowed for fine-tuning a better fit in the model-matching.

The final, largest section of the main project screen is for inputting values for the "Plume Decay Rates and Yield Coefficients" which are applicable both spatially and temporally [Falta, 2008]. Because of the narrow scope of this project, where only one component with no daughter products is of interest (namely TCE), the yield coefficient fields were not utilized in the modeling. The nine fields in this section allow for the entry of first-order decay rates with units of per year (yr^{-1}), to simulate realistic site conditions in both time and space [Falta, 2008]. For the purpose of this thesis, all nine fields were assigned the same value for each "base-case," where the decay rate was an assumed non-zero value, and for each "match-case," where the fields were all set to zero. By holding many of the parameter values equal as appropriate between models, it was hoped that the results of the applied parameter changes would be more easily visible during the ongoing analysis.

3.2 Plume centerline concentration

The centerline of each plume is defined as the longitudinal distance of the plume at the exact center of the plume, which is the “Y=0 and Z=0” location on the Cartesian X-Y spatial plane. After running each model in REMChlor, the resultant output file was exported into Excel™ for centerline TCE concentration analysis. The procedure to create the centerline plots began by selecting the desired time: 60 years in all Cases except for Case 2: Growing-Disconnected, which required a value of 54 years due to its quick washing-out period. These year values were selected to represent TCE spills that would have occurred 60 (and 54) years ago so that the models at these times would approximate the potential present-day characteristics of the resultant contaminant plumes. For each Case, comparison had to be made for sets of “model pairs,” each consisting of a “base-case” in which the plume decay rate was set at a fixed value and a “match-case” in which the plume decay rate was set to zero. Specific parameters in the match-case were then adjusted manually in an attempt to force the match-case to coincide with the base-case.

The matching process was performed systematically by first creating the base-case plot, then the first match-case plot with no values changed from the base-case scenario except for the plume decay rates having been set to zero. Observation of the differences between the curves led to further estimations of parameter values with the intent of causing the difference between the curves to become less and less over multiple repetitions of the process. The parameters most useful in producing matches between the model pairs, and thus the most often manipulated, were initial concentration (C_0), initial mass (M_0), Darcy velocity (V_D), retardation factor (R), and the dispersion terms: α_L, α_T, and α_V. The value of these parameters each had a direct effect on the geometry and position of the centerline curve. With repeated manipulation of these variables and much patience, it was possible to achieve some almost-exact matches for many of the centerline plots, as is shown in Figure 3.2.1. The centerline matches were all plotted on semi-log charts which have a linear scale for the X-axis to measure centerline distance in meters and a base-10 logarithmic scale for the Y-axis to better represent the relationship between the first-order exponentially-decaying TCE concentrations for each model pair. The figures and charts in this project all use “dr” to represent the TCE degradation rate (also written as k or λ) from various contributing sources.

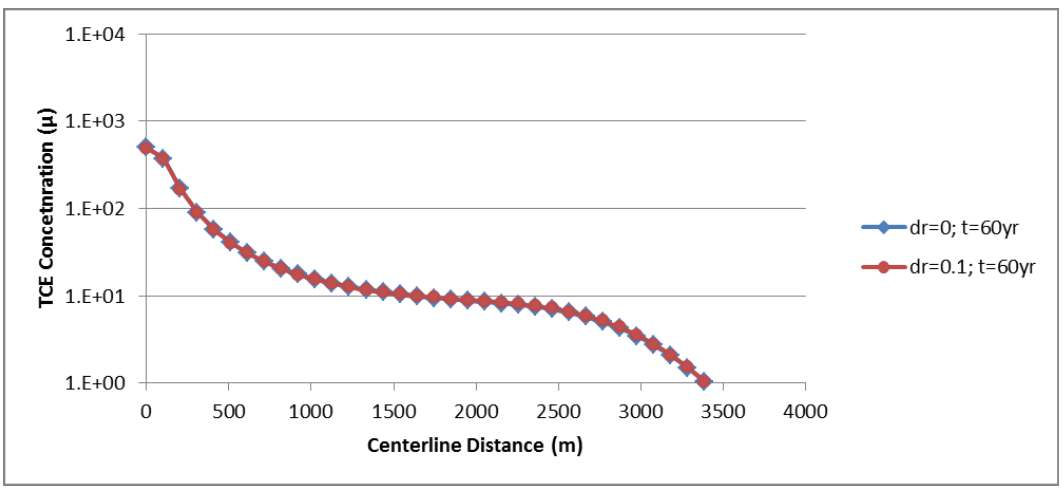


Figure 3.2.1: Example of a near-perfect match between base-case and match-case curves in Microsoft Excel™

3.3 Two-dimensional contour plots

The third computer program integral to the successful completion of this research is Tecplot™, a powerful program with many capabilities concerning the plotting of data in two- and three-dimensions. Tecplot™ was used to plot two-dimensional map-view-style contour plots of the plumes to show how they were affected by changes in the transverse and vertical dispersivity parameters (α_T and α_V). This made it possible to match the plumes graphically in the transverse direction as well as in the longitudinal direction so that the matches were made in two dimensions.

Many options exist within the program that can be used to create contour plots with a variety of line styles and color schemes to aid in clarifying visualization of both the transverse X-Y and vertical X-Z plots. An example of one of the X-Y plots is shown in Figure 3.3.1 below with optional grid lines turned on and with the plume contour intervals and color scheme chosen for this project.

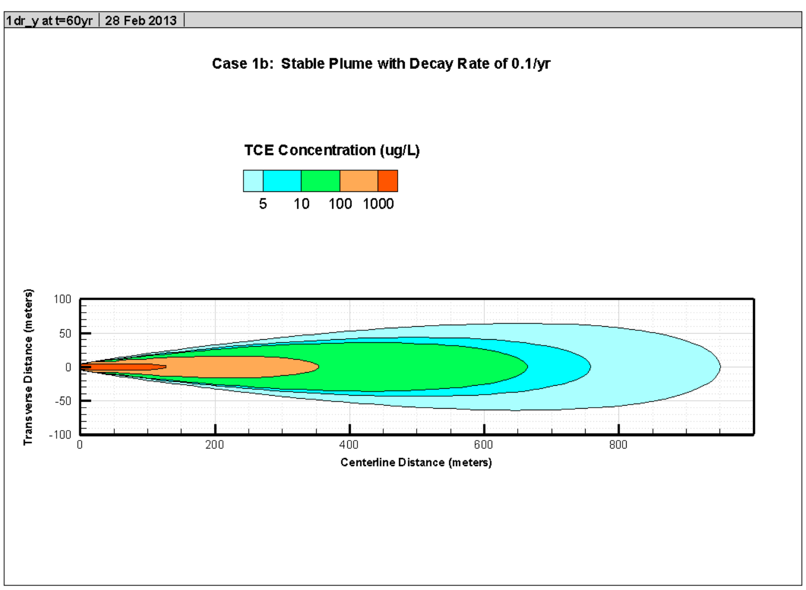


Figure 3.3.1: Example of Tecplot™ working environment; origin of all of the X-Y and X-Z plots

3.4 Graphical analysis of model matches

The easiest and fastest way to make an interpretation of the variance between the models was to plot them and then visually inspect them for goodness-of-fit. In some respects this visual qualification of the matches was most likely sufficient to show that it was indeed possible to coax the models into apparent similarity without further mathematical quantification of the variance between the models. This process was executed by plotting the data in its appropriate X-, Y-, or Z-spatial plane and printing the results at matching scales. Comparing the pairs that were similar allowed for recognition of slight differences in the models that had to be corrected by manipulating the input parameters.

It was decided that matching the centerline curves above the "non-detect" value of 1 μg/L was more important than attempting to force the curve to match below this cutoff value. This decision led to matches that look good at levels above 1 μg/L, but that sometimes vary substantially below 1 μg/L as is shown in Figure 3.4.1.

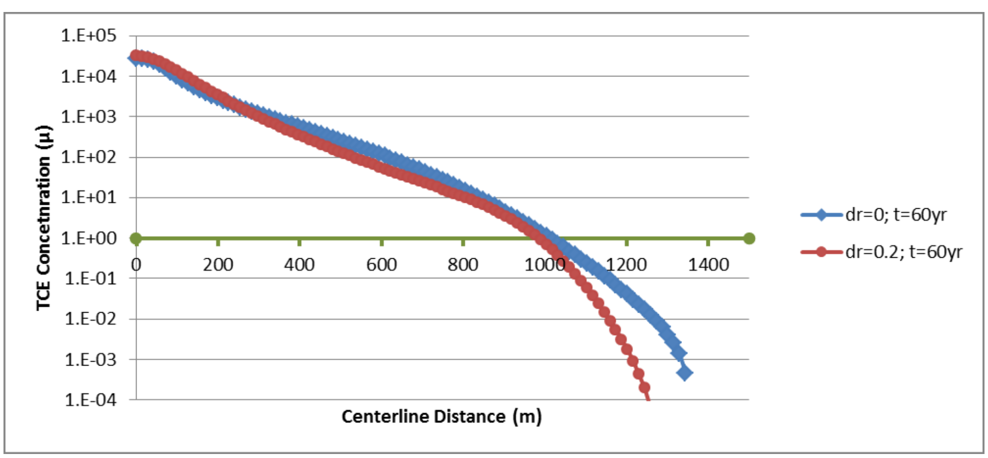


Figure 3.4.1: Example of centerline plot behavior in relation to assumed non-detect limit at 1μg/L

Model matches in the Y- and Z-directions were also compared visually. In order to account for the lower limit in the X-Y and X-Z spatial planes, it was necessary to assign a cutoff contour value of 1μg/L. The other contours were assigned values based on logarithmic intervals (10, 100, 1000 μg/L) to better coincide with the semi-log centerline plots, and it was decided to also include a contour line to represent a concentration of 5μg/L for the TCE MCL.

3.5 Statistical analysis of model matches

Statistical analysis of the data began with organization of the various parameter values for each pair of matched models. Tabular collection of parameters and their respective changes in value was carried out after each curve and plot match was accomplished. From these small tables, shown as needed for quick reference in the Results section, a more comprehensive table was created for side-by-side comparison of all of the relevant parameter values for all of the Cases: the Parameter Comparison Master Table which can be found in Appendix A as Table 4.2.1.

Statistical quantification of the variance between the model results was performed upon the conclusion of the comparisons between the centerline plots, the X-Y plane plots, and the X-Z plane plots using a root mean squared error (RMS) method. There exist a multitude of methods for performing statistical analysis of data sets, but the RMS method was chosen for its simplicity and for the fact that it describes average error in the data sets [Anderson & Woessner 1992]. Because the TCE concentration values were studied in logarithmic scale in this project, it was decided to perform these calculations with the base-10-log values of each of the concentrations in place of "$C_{1\&2}$" in Equation 3.5. This resulted in statistical comparison values that made much more sense when compared with the results of the graphical analysis than did the results of the non-logarithmic calculations. The formula for calculating the root mean squared error (RMS) is:

$$RMS = \sqrt{\left[\frac{\sum_{i=1}^{n}(C_{2,i} - C_{1,i})^2}{n}\right]} \quad (3.5)$$

Where: n = the number of data points in the column
C_2 = log of concentration value in the match-case
C_1 = log of concentration value in the base-case
i = the summation index during the calculation

This particular formula is reformatted from Anderson & Woessner [1992] and was applied to the data sets in multiple steps within the Excel™ worksheets for each matched-model pair. These calculations were performed for all three dimensions (X, Y, and Z) for all of the matched model pairs, and the complete, tabulated results are shown in Tables 4.2.2, 4.2.3, and 4.2.4 in Appendix B. Abbreviated versions of these comprehensive tables are shown as needed in the Results section.

After further research of the RMS method, the decision was made to normalize the RMS to the mean log concentration of the base-case for each model pair. The procedure employed in Excel™ to execute and normalize this calculation for all matched-model pairs in the centerline, X-direction consisted of a sequence of five steps:

1. subtraction and squaring of values in the two "log of concentration" columns
2. summation of the resultant column
3. the square root was taken of (the summation divided by the number of values in the column)
4. resultant value was divided by the mean log concentration of the base-case column ($\overline{C}$) which resulted in the normalized root mean squared error (NRMS)
5. NRMS value was then multiplied by 100 to read as a percentage of deviation

Reformatted from Janssen & Heuberger [1995], the normalized root mean squared error formula applied to the data was written this way:

$$NRMS = \frac{RMS}{\overline{C}} \tag{3.6}$$

Where: $\overline{C}$ = the mean of the base-case log concentration column

There were several sound reasons to use the Normalized Root Mean Squared error (NRMS) method for studying the variance between the models instead of utilizing the unmodified Root Mean Squared error method (RMS). The first and most obvious reason is of course that it was necessary to somehow show mathematically the relationship, if any, between and among the models [Janssen & Heuberger, 1995]. The RMS can be used to express variance between and among two or more models on an individual level to show the spread of the data points in standard-deviation-style, but it is sensitive to "outlying" values in the data set [Janssen & Heuberger, 1995]. Normalizing the RMS by dividing it by the mean value of the data set for the model in question averages out any wildcard data points so that comparisons can be more easily understood [van Ruijven et al., 2009]. The value resulting from the NRMS is between zero and infinity in which zero indicates a perfect fit and higher values represent increasing randomness [van Ruijven et al., 2009]. Further understanding of the meaning of the resultant NRMS value can be gained by multiplying it by 100, which results in a percentage of variance that can be used to further gauge the similarity of the models to each other [van Ruijven et al., 2009].

CHAPTER FOUR

RESULTS

4.1 Graphical analysis results

Three sets of ranking charts, located in Appendix C, were developed to aid in the visual comparison of the centerline, transverse, and vertical plots. These charts are divided into two sets, one for each of the two chosen study times: the first set at 60 (54) years and the second at 40 (34) years. The goodness of fit in each of the plots was evaluated visually and each set of plots were then ranked from 1 to 13 (because there are 13 pairs of models to compare) where the ranking of 1 designates the best fit and 13 designates the poorest fit. NRMS values from the statistical analysis are included on these charts, and they generally agree with the graphical analysis results. Table 4.1.14 shows the graphical analysis rankings for the centerline (X-direction) plots, Table 4.1.15 shows the rankings for the transverse (X-Y spatial plane) plots, and Table 4.1.16 shows the rankings for the vertical (X-Z spatial plane) plots.

Case 1: Stable plume

The “stable” plume designation applies to a groundwater plume that remains at approximately the same spatial extent (i.e. not expanding or shrinking) with a slowly declining TCE concentration over time and that has its contaminant mass present partially both in the source zone and in the plume [Pate, 2010; Liang, 2009]. In this Case six different plume decay rate values were chosen for the match-cases to determine if the data could be matched to plots made with plume decay rates of zero by manipulation of certain other parameter values. The parameters for the base-case other than decay rate are held the same for the six examples in this Case and are shown in Tables 4.1.1 through 4.1.6 as they are discussed in order in this section. For each model in this Case, the original TCE concentration (C_0) is 0.1 g/L, the original TCE mass (M_0) is 1000 kg, the Darcy velocity (V_D) is 30 m/yr, the retardation factor (R) is 2.0, the longitudinal dispersivity (α_L) is approximated as x/100, the transverse dispersivity (α_T) is approximated as x/1,000, the vertical dispersivity (α_V) is approximated as x/10,000, porosity of the matrix (φ) is assigned a value of 0.3, the source width (W) is 10 m, and the source depth (D) is 3m.

The chosen plume decay rates for each model pair are respectively 0.1, 0.2, 0.3, 0.4, 0.5, and 1.0 (in units of yr^{-1}) which cause a significant amount of degradation of the TCE in the plume when compared with the rates from Wiedemeier et al. [1999] Aziz et al. [2002] and Clement et al. [2000] shown in Table 1.1.1 in the Introduction. These rates correspond to half-lives which are respectively 6.93, 3.47, 2.31, 1.73, 1.39, and 0.69 years, which are quite fast when compared with the half-lives from the literature review. The model pairs were matched at 60 years from time of initial release of TCE. A question arose as to whether the plumes would match as well at an earlier point in each of their histories. This question was answered by holding all the parameter values the same as they were for the final 60-year matches and plotting the 40-year data to create corresponding plots of the plumes at that earlier time. A total of twelve each of centerline plots, transverse plots, and vertical plots were compared for visual similarity in this Case.

Plume decay rate = 0.1 yr^{-1}

corresponding half-life of 6.93 years

The centerline chart shown in Figure 4.1.1 illustrates the match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.1 for the base-case and 0 for the match-case. This almost-perfect match (ranked #1 of 13 in Table 4.1.14) was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.1. In order to create the best match in both the X-

Case 1: Stable plume with hypothetical parameter values (model pair 1)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.1	0
C_0 (g/L)	0.1	0.0048
M_0 (kg)	1000	171.5
V_D (m/yr)	30	45
R	2	2.99
α_L (m)	x/100	x/100
α_T (m)	x/1,000	x/1,000
α_V (m)	x/10,000	x/10,000
φ	0.3	0.3
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.1: Comparison of base-case and final match-case parameter values (model pair 1)

and Y-directions, the parameters were manipulated in a series of 118 trials to produce the centerline match and its corresponding transverse (X-Y) match. C_0 was reduced from 0.1 to 0.0048 g/L and M_0 was decreased from 1000 to 171.5 kg in the match-case to move the centerline curve to an overall lower concentration. V_D was increased from 30 to 45 m/yr and R was increased from 2 to 2.99 to force the match-case centerline curve to the appropriate length in the X-direction. The shape of the match-case centerline curve was approximately the same as that of the base-case curve so the α_L value was not changed.

The transverse dispersivity value, α_T, had to be increased very slightly to create a match between the base- and match-case plumes in the X-Y spatial plane (Figures 4.1.2a & b) by causing a slight widening in the Y-direction of the match-case plume. This increase in α_T from the base-case value of 0.001 to the match-case value of 0.00101 was small enough to not have an impact on the value shown in Table 4.1.1 (which was x/1000), though it did enhance the match of the plumes in the transverse plots shown in Figures 4.1.2a & b. The transverse and vertical dispersivity values are very closely related and scale-dependent so the α_V value was also increased very slightly, in the same manner as for α_T, which seemed to have little effect on the vertical centerline plots in Figures 4.1.3a & b. Because the three dispersivity values remained unchanged for the most part, the two most important parameter changes that forced this match were the large changes made to C_0 and M_0. These changes in mass and concentration gave the match-case curve the same source concentration as in the base-case curve, as shown in Figure 4.1.1, but caused the match-case curve to be decreased in concentration over the length of the plume so that the two curves coincided.

This matched model pair has the best similarity of all the matches produced in this study (Figure 4.1.1). The gray curve in the figure, labeled "dr=0; original parameters," shows the original position on the chart of the match-case curve before any parameter manipulation was applied. The blue curve represents the match-case centerline TCE concentration after the parameter value manipulations and the red curve represents the base-case TCE concentrations along the centerline. The overall effect of the parameter manipulations was to move the match-case curve down the chart along the concentration

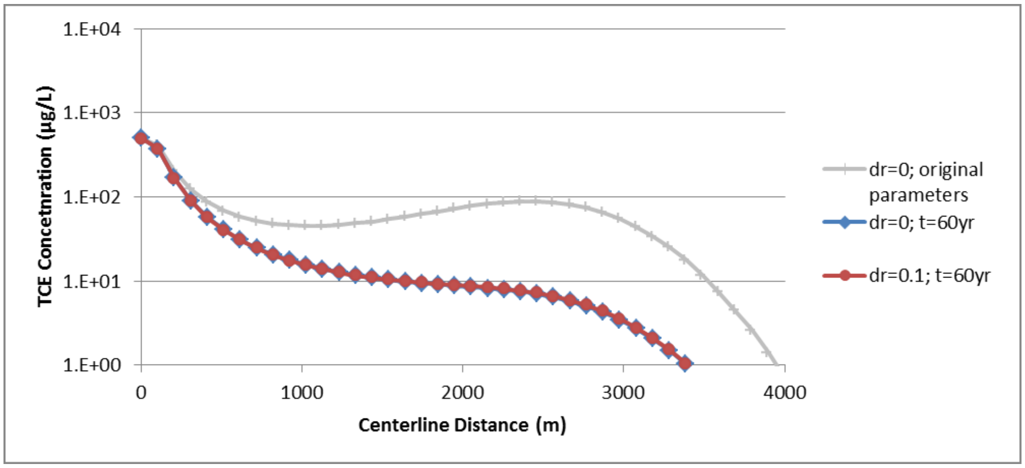
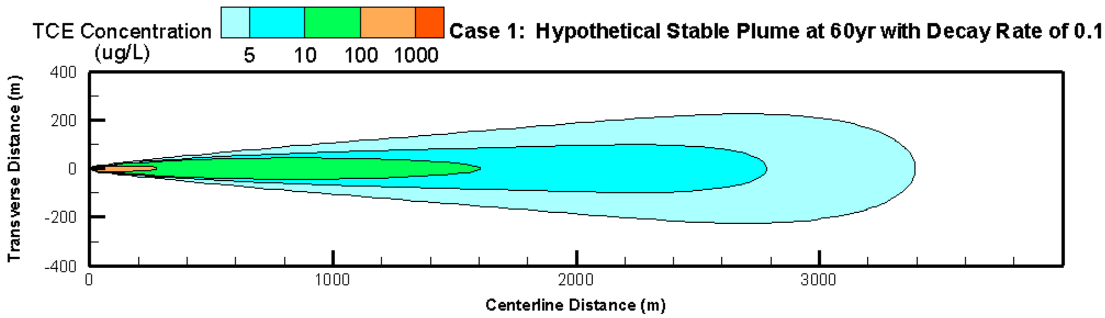


Figure 4.1.1: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 60yr

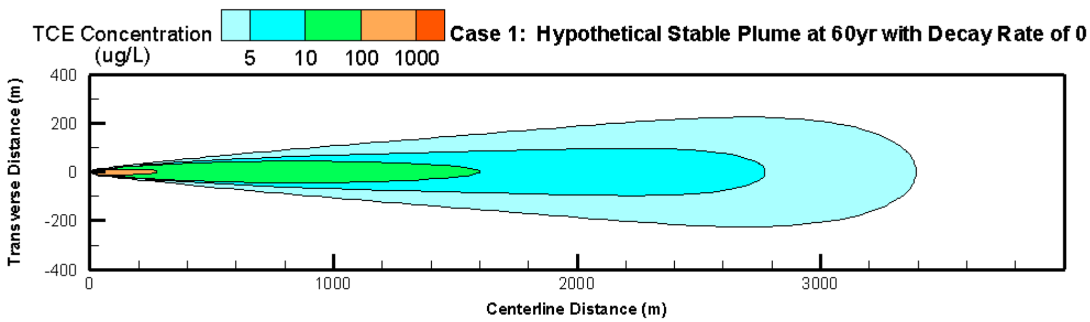
axis and to shorten it in the X-direction to fit the length of the base-case curve.

During the process of producing the centerline match it was necessary to manipulate the parameters to arrive at the best possible manually-derived match in the transverse, Y-direction as well. This was achieved primarily by adjusting the value of α_T, the transverse dispersivity parameter, and then plotting the resulting data in the X-Y spatial plane to produce a map-view-style depiction of the plume. As stated earlier, the increase in the value of α_T was too small to have an impact on the reformatted value presented in Table 4.1.1 (i.e. x/1000). Figure 4.1.2a shows the contour plot depiction of the base-case plume plot while Figure 4.1.2b shows that of the match-case; both at 60 years. This match, much like the centerline match for this particular pair, was nearly perfect and was ranked #1 of 13 in Table 4.1.15.

It was recognized that manipulation of the dispersivity parameters could be causing unnoticed changes in the vertical spatial plane of the plumes. It was decided to make contour plots of vertical slices of the plumes along their centerlines so that any effects in the X-Z plane could be compared. No attempt was made (in any of the Cases) to force matches in the vertical direction, but the plots in this scenario show decent similarity (ranked #1 of 13 in Table 4.1.16) between the concentration contours of the plumes (Figures 4.1.3a & b).



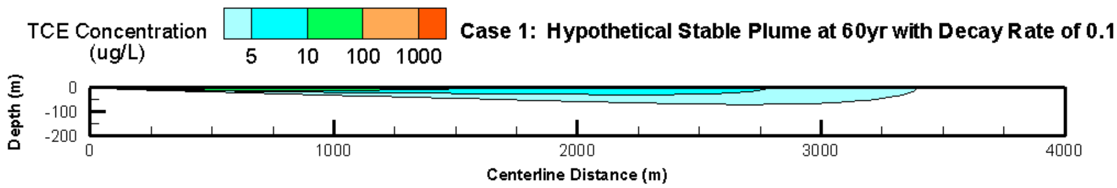
(a) base-case



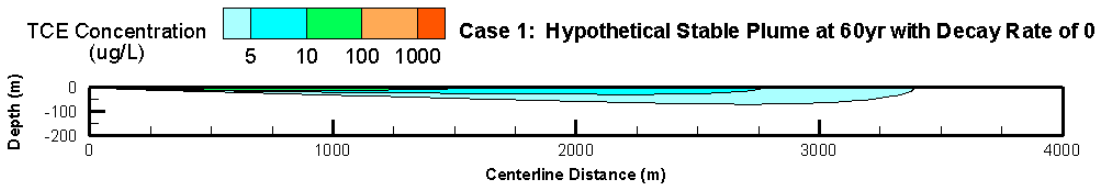
(b) match-case

Figures 4.1.2a & b: Transverse plot pair at 60yr with base-case decay rate of 0.1 and match-case decay rate of 0

This almost perfect match in both the centerline and X-Y plots and the fortunate (but not forced) match in the X-Z plot serve to show that it is possible to match the base-case (λ=0) to the match-case (λ=0.1 yr^{-1} and $t_{1/2}$=6.93 yr) at 60 years from the time of the original TCE release by manipulation of the other parameters as explained above.



(a) base-case



(b) match-case

Figures 4.1.3a & b: Vertical plot pair at 60yr with base-case decay rate of 0.1 and match-case decay rate of 0

Without any further manipulation of the parameter values, the centerline, transverse and vertical plots were made again using data produced by REMChlor for each of the plumes at 40 years from the time of the initial contaminant release. This comparison is necessary to determine if the match exists for other points in time or if time can serve as another variable that will add an extra layer of discrimination that could aid in developing more realistic model parameters. The centerline plot at 40 years, Figure 4.1.4, shows that the overall TCE concentration for the base-case curve at 40 years is higher than that of the match-case curve at 40 years, most likely because of the large reduction in C_0 and M_0 values, as discussed earlier. The geometry and length of the curves are both very similar, but if a match for this model pair were desired at 40 years, additional manipulation of parameters would be necessary. This comparison was ranked #6 of 13 in Table 4.1.14 in the 40-year comparison section. Based on the behavior of the match-case curve in the 60-year manipulations, it might be that lowering M_0 and C_0 in the

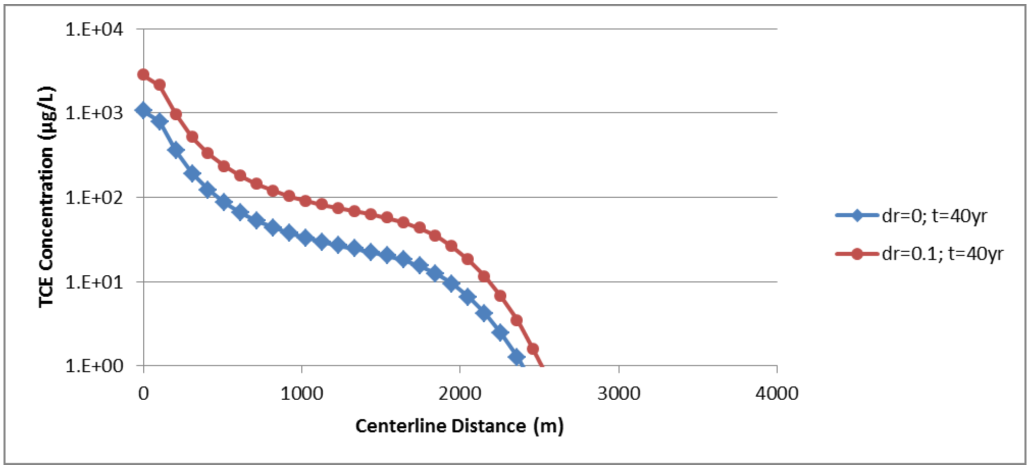
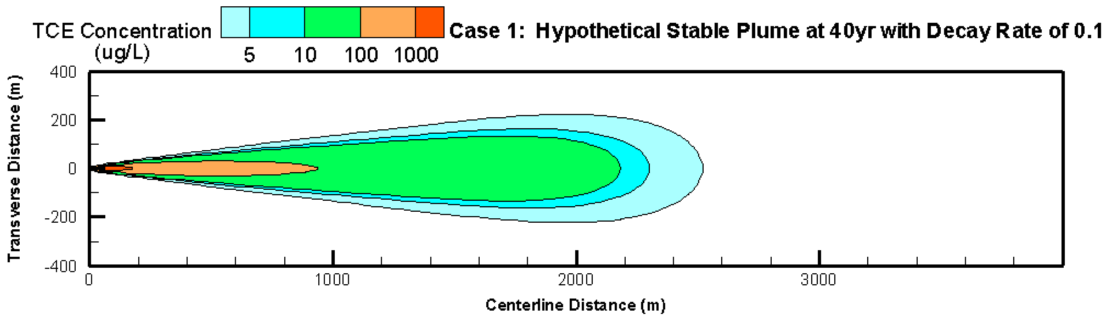


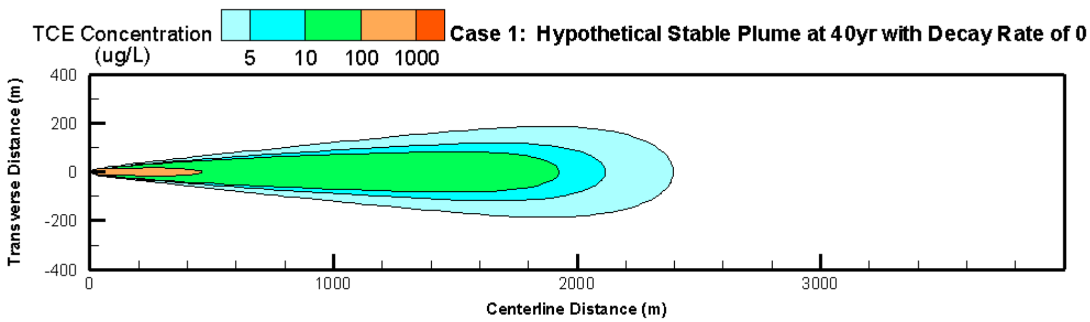
Figure 4.1.4: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 40yr

40-year comparison could result in increased similarity for the 40-year pair. The 60-year match would probably suffer, though, from this additional change in parameter values.

Transverse and vertical plots were produced to show the 40-year plumes in the X-Y and X-Z spatial planes, Figures 4.1.5a & b and Figures 4.1.6a & b respectively. The transverse plots (ranked #4 of 13 in Table 4.1.15) show that the 40-year base-case plume has a greater expanse and higher set of TCE concentrations than the 40-year match-case plume. The vertical plots (ranked #2 of 13 in Table 4.1.16) show that the base-case plume has a greater expanse of higher concentrations of TCE over its vertical extent than does the match-case plume. If a match were desired between these plumes in either of these spatial planes at 40 years, changes could be made to the dispersion terms, but it would upset the 60-year match.

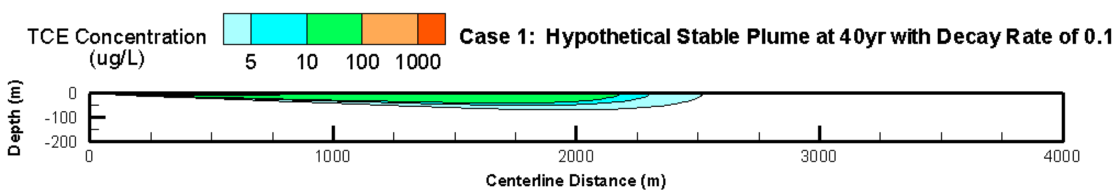


(a) base-case

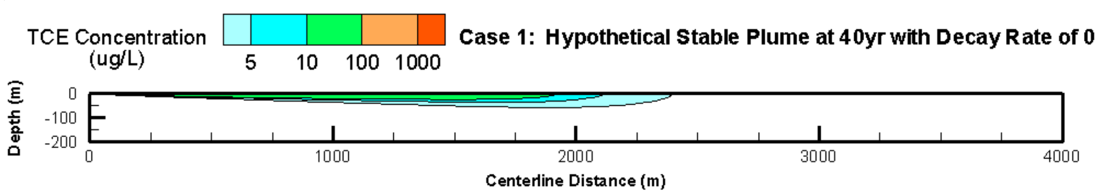


(b) match-case

Figures 4.1.5a & b: Transverse plot pair at 40yr with base-case decay rate at 0.1 and match-case decay rate at 0



(a) base-case



(b) match-case

Figures 4.1.6a & b: Vertical plot pair at 40yr with base-case decay rate of 0.1 and match-case decay rate of 0

The comparisons of the base-case to match-case centerline and X-Y plots (and to some degree the unforced X-Z plots) at 40 years, without further manipulation of the parameters chosen during the 60-year match-making, show that a match does not exist between the base- and match-case at 40 years unless more parameter manipulation is applied. This additional manipulation in order to force the 40-year match would likely upset the 60-year match so the conclusion could be drawn for this model pair with this particular set of parameters that if a match were desired for multiple points in time over the life of the plume then a different matching-procedure would be necessary.

Plume decay rate = 0.2 yr^{-1}

Corresponding half-life of 3.47 years

This centerline chart (Figure 4.1.8) describes the manipulated match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.2 for the base-case and 0 for the match-case. The match was developed along with the X-Y match for this Case by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.2, and required a total of 47 trials to produce the centerline

Case 1: Stable plume with hypothetical parameter values (model pair 2)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.2	0
C_0 (g/L)	0.1	0.0004
M_0 (kg)	1000	1000
V_D (m/yr)	30	31
R	2	2.6
α_L (m)	x/100	x/50
α_T (m)	x/1,000	x/1,111
α_V (m)	x/10,000	x/11,110
φ	0.3	0.3
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.2: Comparison of base-case and final match-case parameter values (model pair 2)

match and its corresponding transverse (X-Y spatial plane) match. It was possible to move the curve down the chart slightly along the concentration axis by significantly lowering the value of C_0 (from 0.1 to 0.0004 g/L) while maintaining the base-case value of 1,000 kg for M_0. The source equation, Equation 3.2 in the Methodology chapter, describes the proportional relationship between the source concentration and contaminant mass and can help to explain why C_0 can be so drastically reduced for matching purposes, as was done in this scenario, and still make physical sense. As discussed in the

Methodology chapter, the proportionality constant, Γ, was assigned a value of 1 in this study. When Γ=1 and the source decay rate is 0 (λ_s=0) a special situation occurs in the calculations where the source concentration (C_s) equation can be simplified to an exponential decay formula as shown below in Equation 4.1 [Falta, 2008; Newell et al., 1996; Parker & Park, 2004; Zhu & Sykes, 2004]:

$$C_s(t) = C_0 e^{\frac{QC_0}{M_0}t} \tag{4.1}$$

Where:
- Q = groundwater flow rate
- C_0 = original dissolved contaminant concentration in the source zone
- M_0 = original mass of contaminant in the source zone
- t = time

Figure 4.1.7 shows a plot of data from Case 1 (at plume decay rate of 0.1 yr^{-1} at a distance from the source zone of X=0.1 meters, over the interval of time from 2 to 100 years after initial contaminant release) in which the red base-case curve begins its decay at a higher source concentration than does the blue match-case curve. The

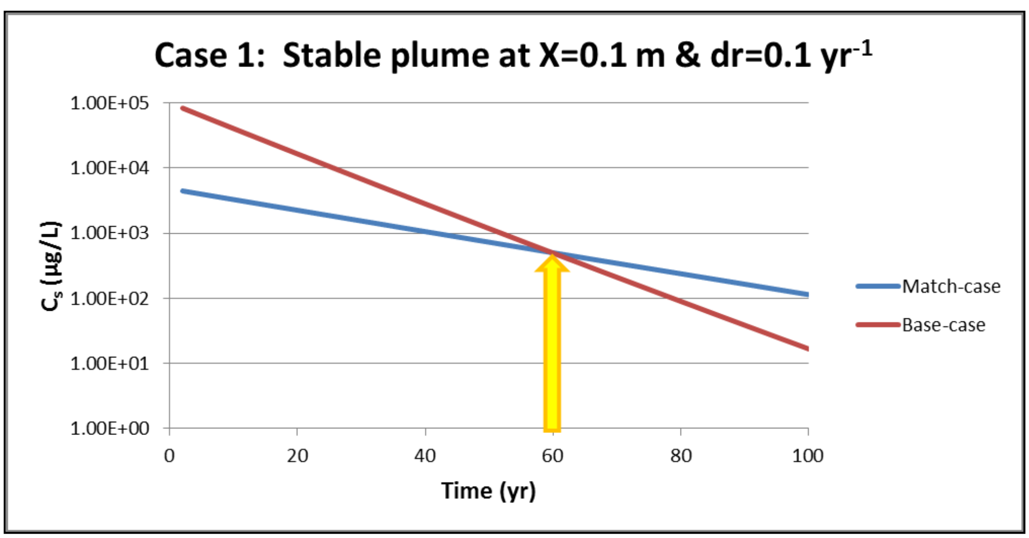


Figure 4.1.7: Example of source concentration proportionality versus time

proportionality described by the source equation causes the curves to eventually cross at some point in time; in this case at 60 years. The space between the two curves while the time is less than 60 years represents the variation in the mass portion of Equation 4.1 as the value of C_0 changes. Because the curves intersect at 60 years it is possible to manipulate the match for the model pair at that particular point in time with that particular low value of C_0 in the match-case. The match would not be possible at an earlier time on the plot with the same value of C_0. This may also help to explain the behavior of the model-pair at 40 years (shown later in Figures 11 through 13a & b) in which the base-case models are at an overall higher concentration and greater length in the X-direction than are the match-case models. Furthermore, it is not possible to know exactly the concentration and mass values that were actually present in the initial TCE release, which makes the guidance of the source equation very useful in estimating a realistic proportion for those parameters in the model.

V_D and R were manipulated together and their values slightly increased (V_D changed from 30 to 31 m/yr and R from 2 to 2.6) to stretch the match-case curve in the X-direction so that the initial decline in the match-case curve would more closely match that of the base-case curve. In order to force the match-case curve into a pattern of quicker decay, the value of α_L was increased from x/100 to x/50. The change in value for α_T from x/1,000 to x/1,111 and in α_V from x/10,000 to x/11,110 was necessary to force the match-case plume width in the Y-direction to match that of the slightly narrower base-case plume, as shown Figures 4.1.9a & b. This slight decrease in the value of α_V

seemed to have a negligible effect on the vertical extent of the plume as shown below in Figures 4.1.10a & b.

This matched model pair has relatively good similarity as shown in Figure 4.1.8

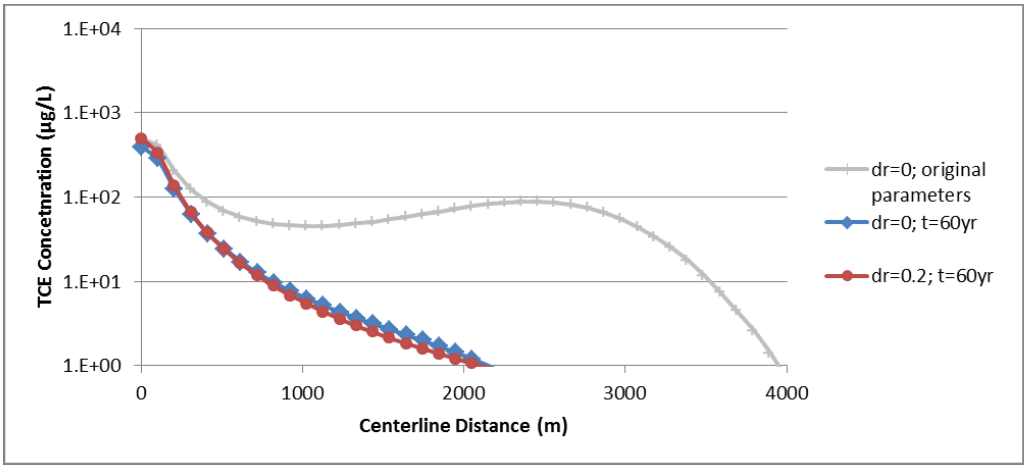
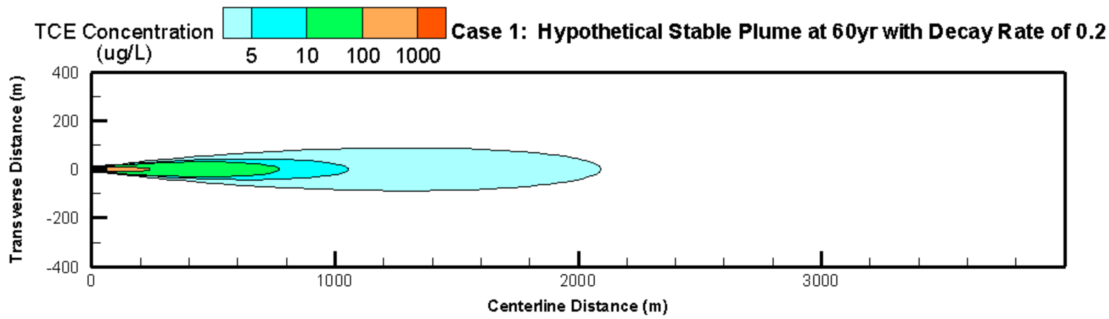


Figure 4.1.8: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 60yr

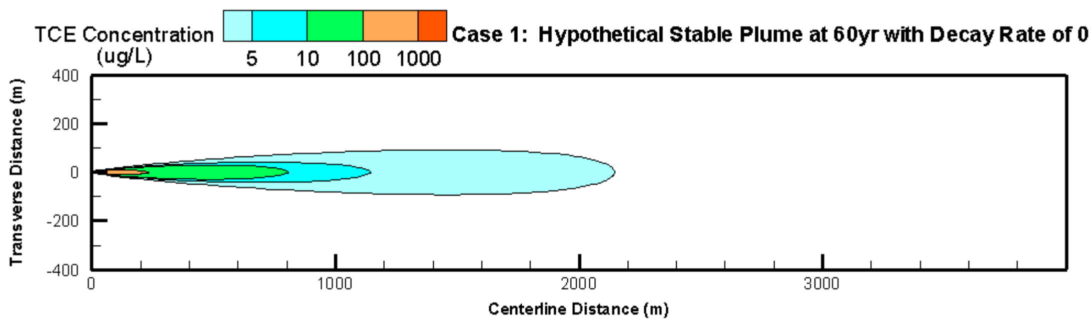
and was ranked #3 of 13. The gray curve in the figure, labeled "dr=0; original parameters," shows the original position on the chart of the match-case curve before any parameter manipulation was applied. The blue curve represents the match-case centerline TCE concentration after the parameter value manipulations and the red curve represents the base-case TCE concentrations along the centerline. The overall effect of the parameter manipulations was to stretch the match-case curve along the X-direction and to move it down the chart along the concentration axis to force it to match the base-case curve between the X values of 0 and approximately 2100 meters.

The transverse plots were created by adjusting the value of α_T and plotting the resulting data in the X-Y spatial plane to produce a map-view-style depiction of the plume. Figure 4.1.9a shows the contour plot depiction of the base-case plume plot while

Figure 4.1.9b shows that of the match-case; both at 60 years. This match, as was the centerline plot, is quite close for this pair of plumes and was ranked #6 of 13.



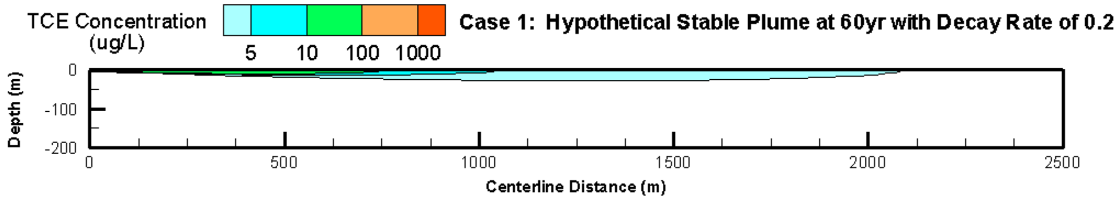
(a) base-case



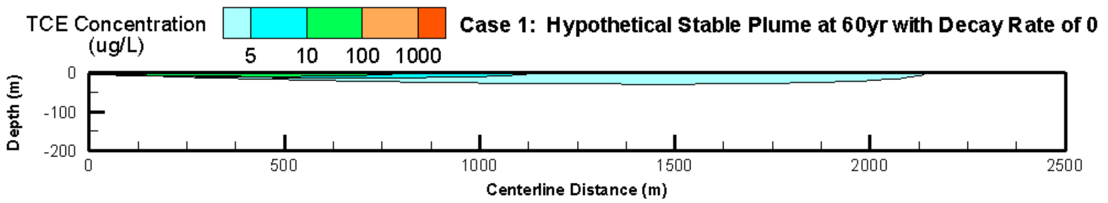
(b) match-case

Figures 4.1.9a & b: Transverse plot pair at 60yr with base-case decay rate of 0.2 and match-case decay rate of 0

Contour plots of vertical slices of the plumes were made along their centerlines so that any effects in the X-Z plane could be compared. No attempt was made to force matches in the vertical direction, but the plots show a high degree of similarity (ranked #6 of 13) in both the placement of the concentration contours and the overall shape and spatial extent of this model pair as shown in Figures 4.1.10a & b.



(a) base-case



(b) match-case

Figures 4.1.10a & b: Vertical plot pair at 60yr with base-case decay rate of 0.2 and match-case decay rate of 0

This almost perfect match in both the centerline and X-Y plots and the similar (unforced) match in the X-Z plot serve to show that it is possible to match the base-case (λ=0) to the match-case (λ=0.2 yr^{-1} and $t_{1/2}$=3.47 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above.

Without any further manipulation of the parameter values, the centerline, transverse, and vertical plots were made again using data produced by REMChlor for each of the plumes at 40 years from the time of the initial contaminant release. The centerline plot, Figure 4.1.11, shows that the overall TCE concentration for the base-case curve at 40 years is higher than that of the match-case curve at 40 years. The geometry and length of the curves are both fairly similar with a ranking of #7 of 13, but if a match for this model pair were desired at 40 years, additional manipulation of parameters would be necessary. Based on the behavior of the match-case curve in the 60-year manipulations, it might be possible that lowering M_0 and C_0 in the 40-year comparison could result in increased similarity for the 40-year pair.

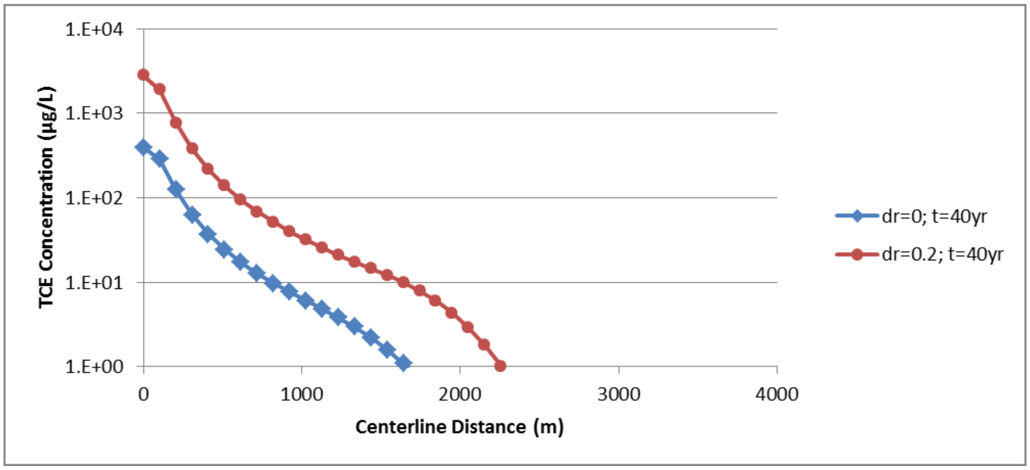
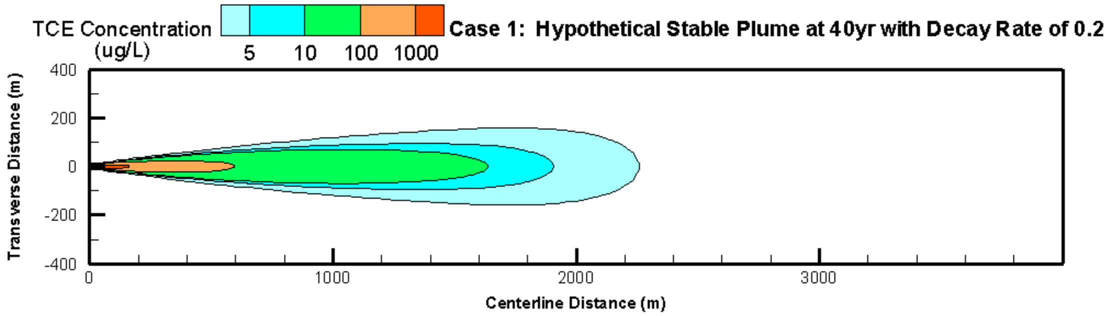


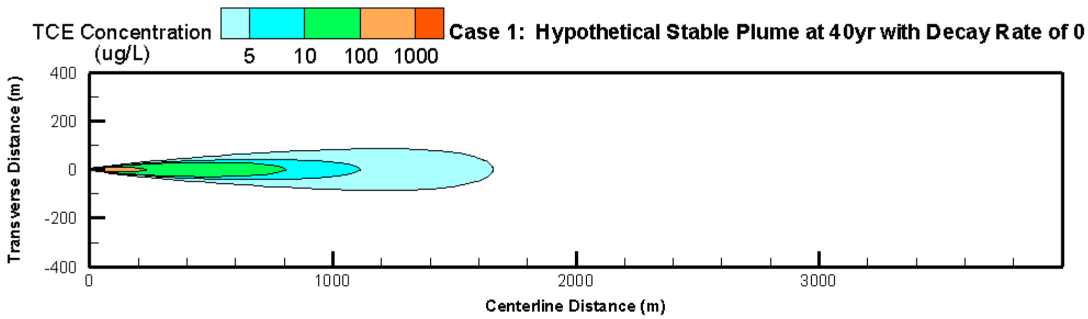
Figure 4.1.11: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 40yr

Transverse and vertical plots were produced to show the 40-year plumes in the X-Y and X-Z spatial planes, Figures 4.1.12a & b and Figures 4.1.13a & b respectively. The transverse plots (ranked #8 of 13 at 40 years) show that the 40-year base-case plume has a much greater expanse of TCE concentrations than does the 40-year match-case plume. The vertical plots (ranked #9 of 13 at 40 years) show that the base-case plume has a much greater expanse of higher concentrations of TCE over its vertical extent than does the match-case plume. If a match were desired between these plumes in the transverse or vertical directions at 40 years, changes could be made to the dispersion terms to force the match, but it would certainly upset the 60-year match.

The comparisons of the base-case to match-case centerline and X-Y plots at 40 years show that there is no match between the base- and match-case at 40 years unless more parameter manipulation is applied. Additional manipulation in order to force the 40-year match would upset the 60-year match which shows that time must be a key variable in creating the matches.

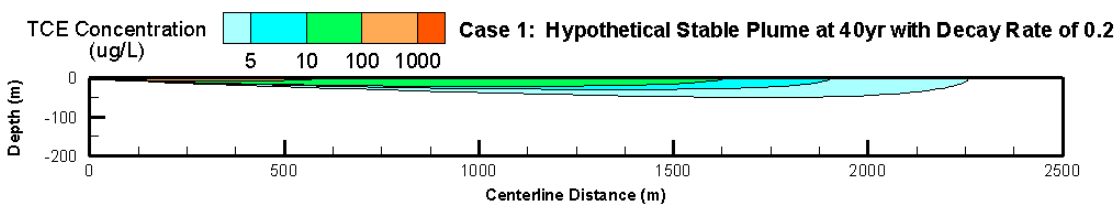


(a) base-case

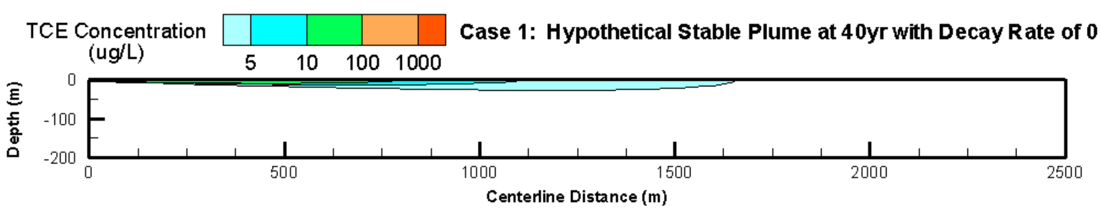


(b) match-case

Figures 4.1.12a & b: Transverse plot pair at 40yr with base-case decay rate of 0.2 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.13a & b: Vertical plot pair at 40yr with base-case decay rate of 0.2 and match-case decay rate of 0

Plume decay rate = 0.3 yr⁻¹

corresponding half-life of 2.31 years

This centerline chart (Figure 4.1.14) describes the manipulated match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.3 for the base-case and 0 for the match-case. At a decay rate of 0.3, making the curves match became more difficult, the result of which is a less exact pairing between the curves. The centerline match was developed along with its corresponding X-Y plane match for this Case through a series of parameter adjustments in the match-case in a total of 31 trials. Table 4.1.3 shows the final values of the parameters after their manipulation

Case 1: Stable plume with hypothetical parameter values (model pair 3)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.3	0
C_0 (g/L)	0.1	0.0004
M_0 (kg)	1000	1000
V_D (m/yr)	30	13.5
R	2	3.2
α_L (m)	x/100	x/10
α_T (m)	x/1,000	x/1,667
α_V (m)	x/10,000	x/16,670
φ	0.3	0.3
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.3: Comparison of base-case and final match-case parameter values (model pair 3)

was completed. It was possible to move the curve down the chart slightly along the concentration axis by lowering the value of C_0 from 0.1 to 0.0004 g/L while maintaining the base-case value for M_0, 1,000 kg. V_D was decreased from 30 to 13.5 m/yr and R was increased from 2 to 3.2 in order to control the length of the match-case curve in the X-direction to more closely match that of the base-case curve. It was necessary to increase the value of α_L (from x/100 to x/10) to force the match-case curve into a much more steeply declining pattern, one of quicker decay, like that of the base-case curve. The change in value for α_T from x/1,000 to x/1,667 and in α_V from x/10,000 to x/16,670 was required to force the match-case plume width in the Y-direction to match that of the slightly narrower base-case plume as shown in Figures 4.1.15a & b. This slight decrease in the value of α_V seemed to have a negligible effect on the vertical extent of the plume as is shown below in Figures 4.1.16a & b.

It was not possible to create as "perfect" a match with this model pair at the decay rate of 0.3 as it was in the previous pairings at decay rates of 0.1 and 0.2 as is shown in Figure 4.1.14. This centerline chart was ranked #11 of the 13 total 60-year centerline

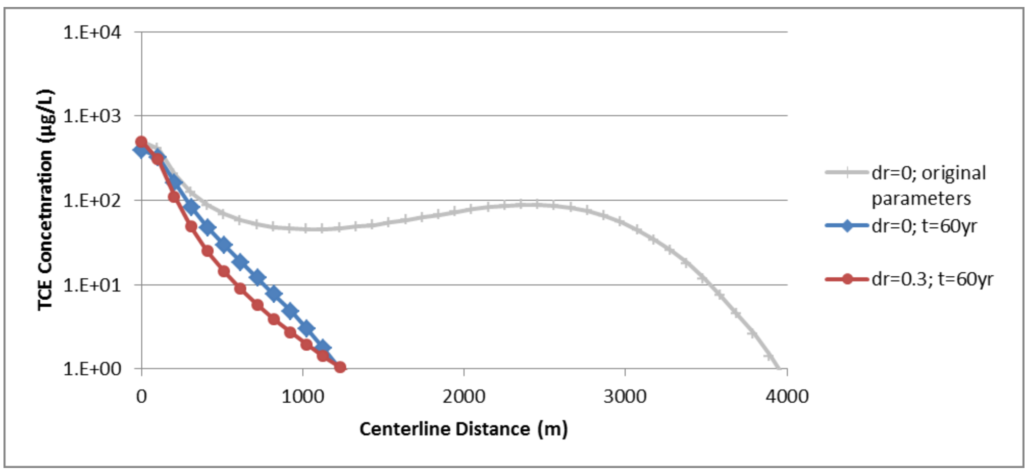
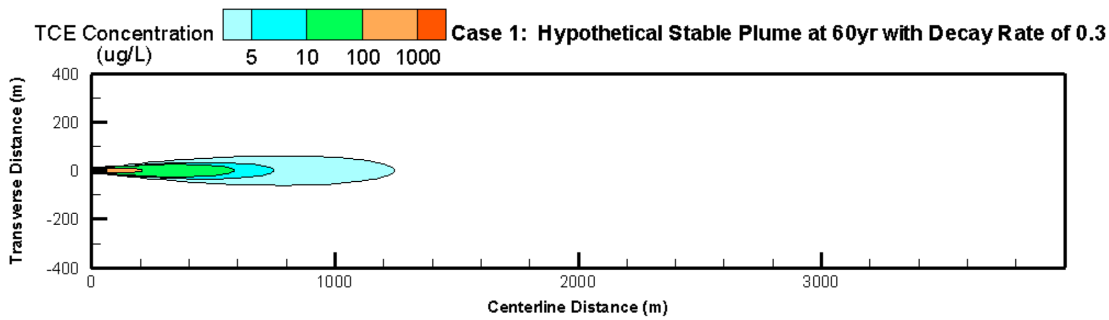


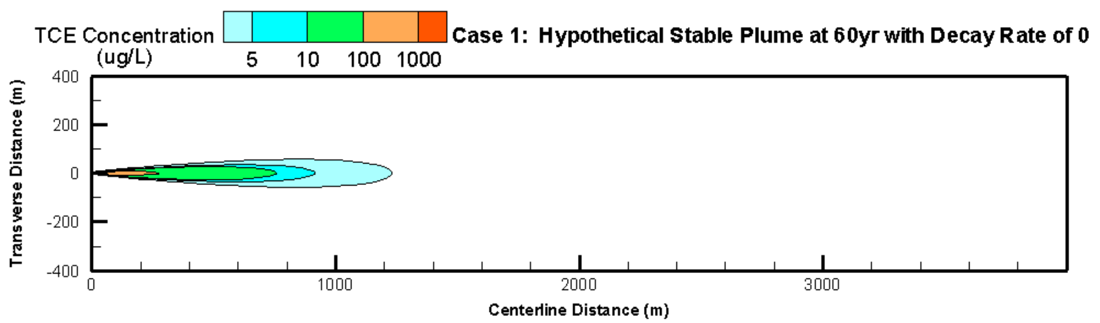
Figure 4.1.14: Centerline plot for base-case (dr=0.3) and match-case (dr=0) at 60yr

plots. The overall effect of the parameter manipulations was to stretch the match-case curve in the X-direction and to move it down the chart along the concentration axis to force it to match the base-case curve between the X values of 0 and approximately 1200 meters.

The transverse plume plot was created by adjusting the value of α_T, as stated earlier, and then plotting the resulting data in the X-Y spatial plane. Figure 4.1.15a shows the contour plot depiction of the base-case plume plot, while Figure 4.1.15b shows that of the match-case; both at 60 years. This match was ranked #10 of 13 due to differences that exist in the plumes' concentration contour placement and overall size.



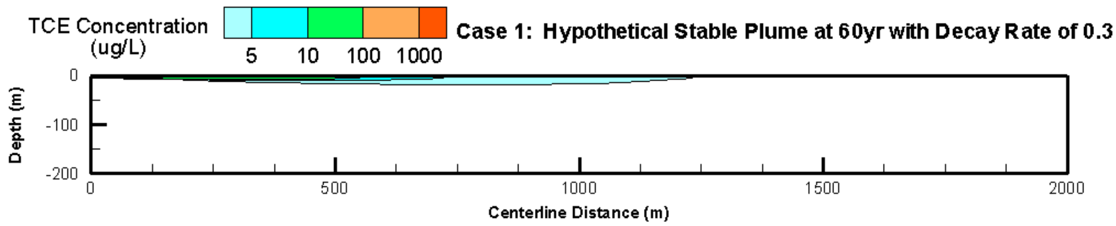
(a) base-case



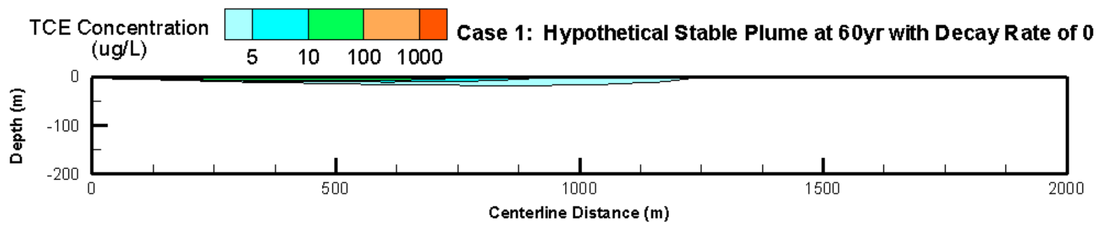
(b) match-case

Figures 4.1.15a & b: Transverse plot pair at 60yr with base-case decay rate of 0.3 and match-case decay rate of 0

Contour plots were made of vertical slices of the plumes along their centerlines with no attempts made at causing them to match. In spite of this, the vertical plume plots are a fair match and were ranked #5 of 13. Concentration contour placement within the vertical slices of the plumes, though, does not display the same amount of similarity between the base- and match-case plumes as is shown in Figures 4.1.16a & b.



(a) base-case



(b) match-case

Figures 4.1.16a & b: Vertical plot pair at 60yr with base-case decay rate of 0.3 and match-case decay rate of 0

The centerline, transverse, and vertical plots were made again without further parameter manipulation for each of the plumes at 40 years from the time of the initial contaminant release. The centerline plot, Figure 4.1.17 (ranked 12 of 13 at 40 years), shows that the overall TCE concentration for the base-case curve at 40 years is higher than that of the match-case curve at 40 years. The geometry of the curves is not similar this time, and a distinct divergence of the curves occurs at approximately 800 meters along the X-axis. If a match were desired for this model pair at 40 years, additional parameter manipulation would be necessary. Based on the behavior of the match-case curve in the 60-year manipulations, it is possible that lowering the values of M_0 and C_0 in the 40-year comparison could result in better overall similarity for the pair. It would further be necessary to increase the value of α_L to help stretch the match-case curve into a more intensely decreasing behavior between the X values of 0 and 1000 meters.

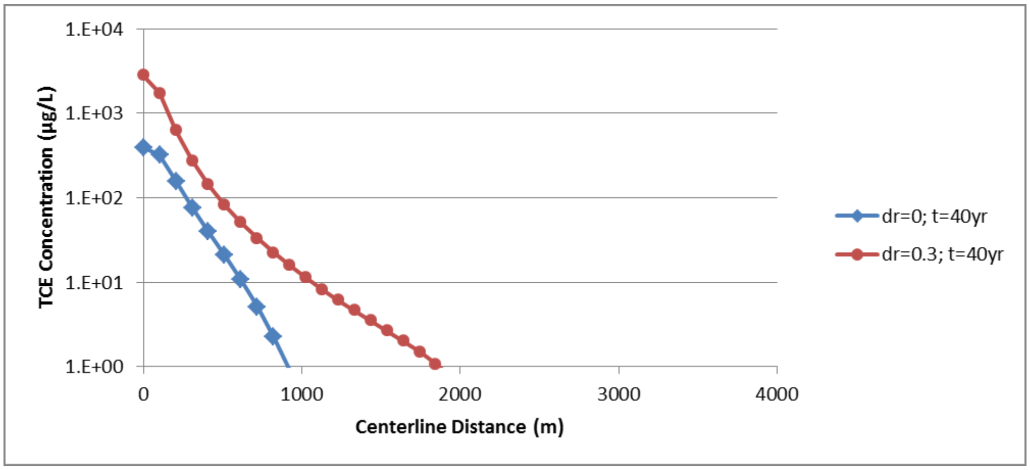
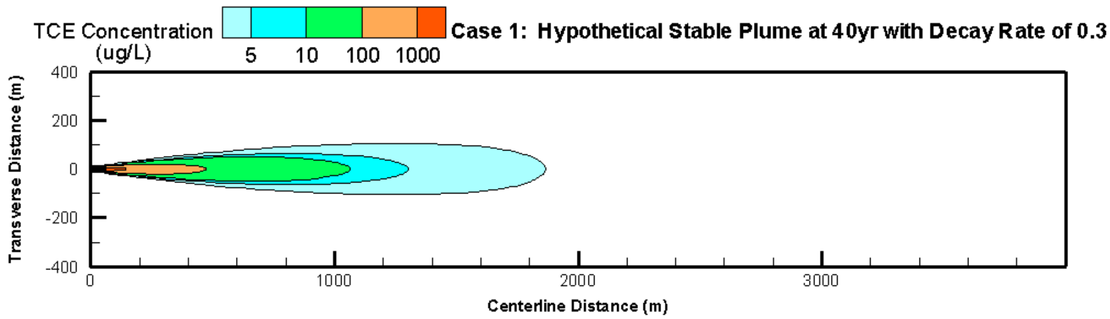
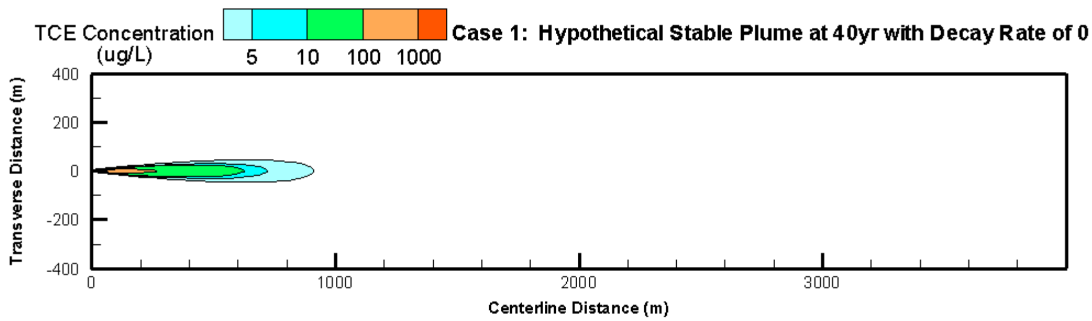


Figure 4.1.17: Centerline plot for base-case (dr=0.3) and match-case (dr=0) at 40yr

Transverse and vertical plots were created to show the 40-year plumes in the X-Y and X-Z spatial planes, shown in Figures 4.1.18a & b and Figures 4.1.19a & b respectively. The transverse plots show that the 40-year base-case plume has a much greater expanse and set of TCE concentrations than does the 40-year match-case plume, which led to a ranking of #9 of 13. The vertical plots show that the base-case plume has a much greater expanse and higher TCE concentrations over its vertical extent than does the match-case plume and was ranked #10 of 13 at 40 years. If a match were desired between these plumes in the transverse or vertical directions at 40 years, changes could be made to the dispersion terms, in addition to those changes already mentioned for the centerline plot at 40 years, to force the match, but it would destroy the match that was forced between the plumes at 60 years.

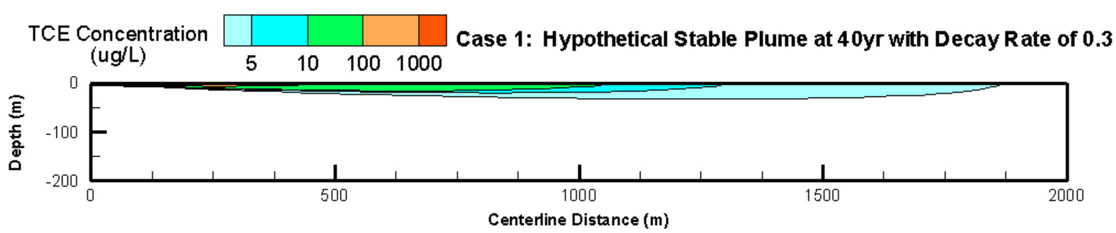


(a) base-case

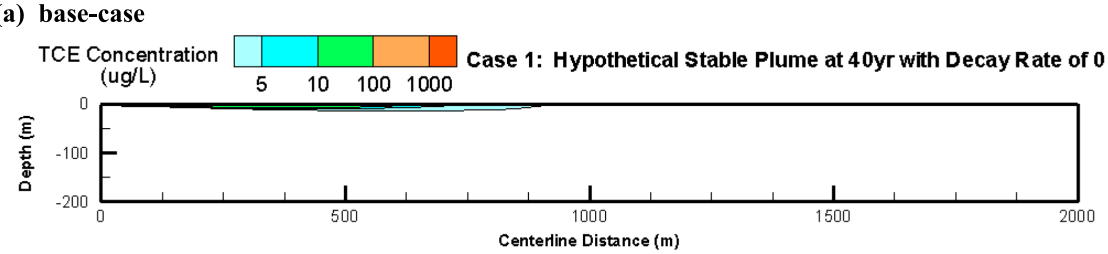


(b) match-case

Figures 4.1.18a & b: Transverse plot pair at 40yr with base-case decay rate of 0.3 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.19a & b: Vertical plot pair at 40yr with base-case decay rate of 0.3 and match-case decay rate of 0

The comparison of the base-case to match-case centerline and X-Y plots (and to some degree the unforced X-Z plots) at 40 years, without further manipulation of the parameters chosen during the 60-year match-making, show that there is no match between the base- and match-case at 40 years unless more parameter manipulation is applied. The conclusion for this model pair with the parameters shown in Table 4.1.3 is that time has a definite effect on the match at different points in the plume's history.

Plume decay rate = 0.4 yr^{-1}

corresponding half-life of 1.73 years

Figure 4.1.20 describes the manipulated match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.4 for the base-case and 0 for the match-case. This set of plots displays the same type of behavior as those created with a decay rate of 0.3 with the lack of similarity of the matched pair being much more exaggerated at the 0.4 decay rate. This match was developed along with the X-Y match for this Case by a series of parameter adjustments in the match-case in a total of 12 trials. Table 4.1.4 shows the beginning and final values of the parameters. It was possible to

Case 1: Stable plume with hypothetical parameter values (model pair 4)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.4	0
C_0 (g/L)	0.1	0.0004
M_0 (kg)	1000	1000
V_D (m/yr)	30	10
R	2	3.4
α_L (m)	x/100	x/10
α_T (m)	x/1,000	x/1,428
α_V (m)	x/10,000	x/14,280
φ	0.3	0.3
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.4: Comparison of base-case and final match-case parameter values (model pair 4)

move the curve down the chart slightly along the concentration axis by lowering the value of C_0 from 0.1 to 0.0004 g/L while maintaining the base-case value for M_0, 1,000 kg. V_D was lowered from 30 to 10 m/yr and R was raised from 2 to 3.4 to control the length of the match-case curve in the X-direction to more closely match that of the base-case curve. The value of α_L was increased from x/100 to x/10 to force the match-case curve into a much more steeply declining pattern, one of quicker decay, like that of the base-case curve. The change in value for α_T from x/1,000 to x/1,428 and in α_V from x/10,000 to x/14,280 was necessary to force the match-case plume width in the Y-direction to match that of the slightly narrower base-case plume, as shown in Figures 4.1.21a & b. The slight decrease in value of α_V seemed to have a negligible effect on the vertical extent of the plume as shown in Figures 4.1.22a & b.

It was not possible to create a "perfect" match with this model pair at the decay rate of 0.4 as it was in the pairings at decay rates of 0.1 and 0.2, as shown in Figure 4.1.20, so this centerline chart was ranked #10 of 13. The overall effect of the parameter

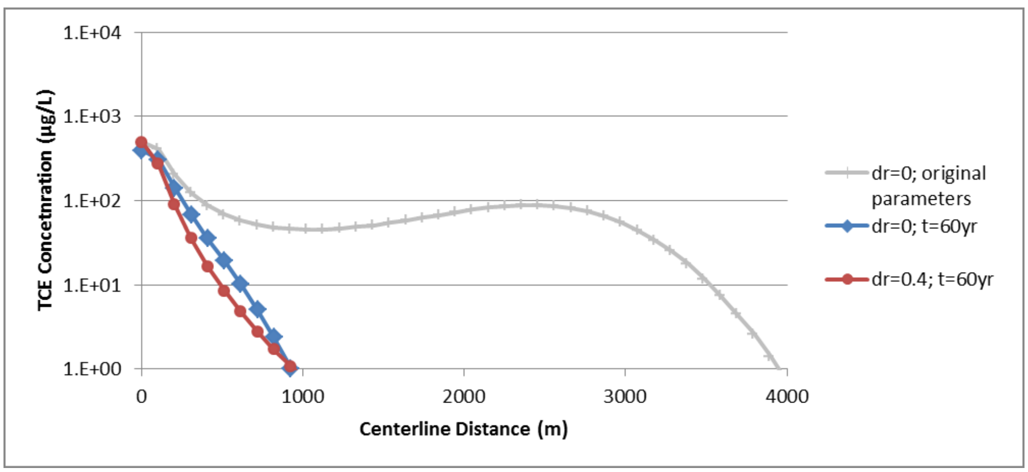
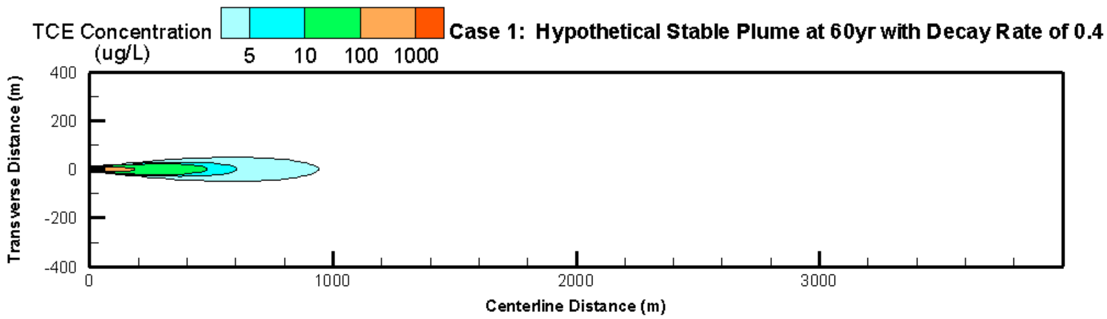


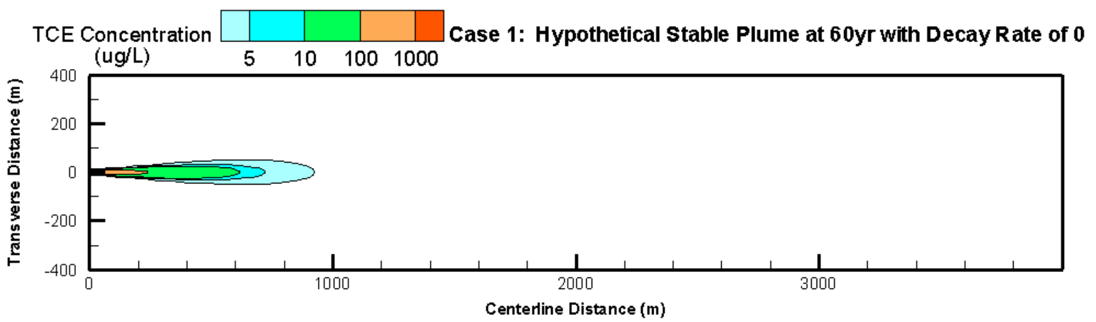
Figure 4.1.20: Centerline plot for base-case (dr=0.4) and match-case (dr=0) at 60yr

manipulations was to stretch the match-case curve along the X-direction and to move it down the chart along the concentration axis to force it to match the base-case curve between the X values of 0 and approximately 1000 meters.

The transverse plume plots were made by adjusting the value of α_T, as stated above, and plotting the resulting data in the X-Y spatial plane. Figure 4.1.21a shows the contour plot depiction of the base-case plume plot, while Figure 4.1.21b shows that of the match-case; both at 60 years. This match was ranked #11 of 13 mainly because of its concentration contour differences.



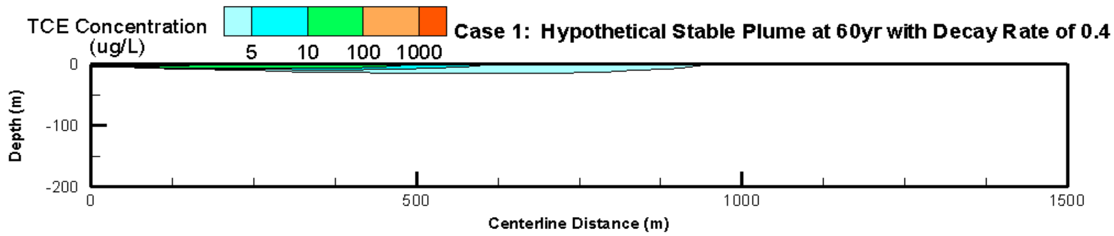
(a) base-case



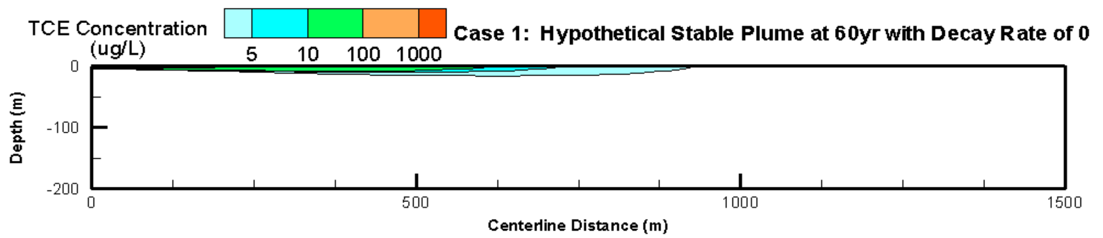
(b) match-case

Figures 4.1.21a & b: Transverse plot pair at 60yr with base-case decay rate of 0.4 and match-case decay rate of 0

Vertical contour plots were made along the plume centerlines so that any effects in the X-Z plane could be compared. The vertical plots show that the plumes are relatively similar in this dimension, but with differences in concentration contour placement, as is shown in Figures 4.1.22a & b (ranked of #3 of 13).



(a) base-case



(b) match-case

Figures 4.1.22a & b: Vertical plot pair at 60yr with base-case decay rate of 0.4 and match-case decay rate of 0

The comparisons in both the centerline and X-Y plots and the unforced match in the X-Z plot show that it is possible to make a decent match between the base-case (λ=0) and the match-case (λ=0.4 yr^{-1} and $t_{1/2}$=1.73 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above.

The centerline, transverse, and vertical plots were made again (using the same input data) for each of the plumes at 40 years from the time of the initial contaminant release. The centerline plot, Figure 4.1.23, shows that the overall TCE concentration for the base-case curve at 40 years is higher than that of the match-case curve at 40 years, and was ranked #11 of 13. The geometry of the curves is not similar this time and a distinct divergence of the curves occurs at approximately 600 meters along the X-axis. Lowering the values of M_0 and C_0 in the 40-year comparison could possibly result in better overall similarity for the pair. To cause the plot to match at 40 years, it would be necessary to increase the value of α_L to help force the match-case curve into a more

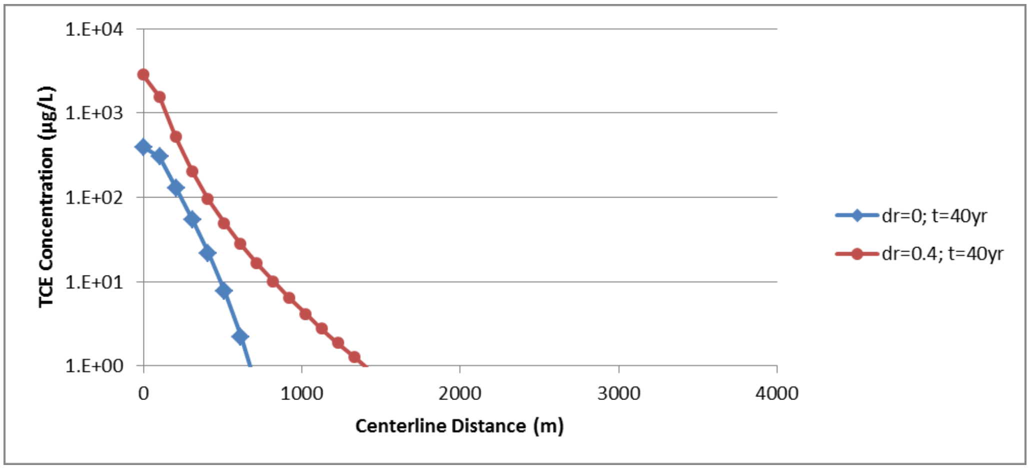
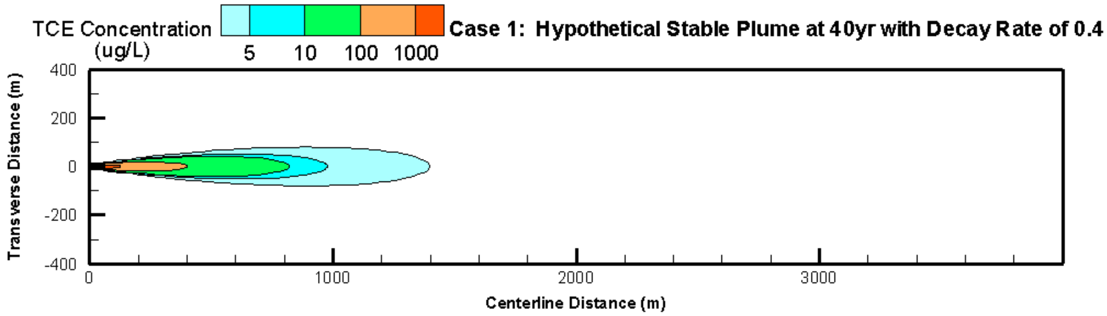


Figure 4.1.23: Centerline plot for base-case (dr=0.4) and match-case (dr=0) at 40yr

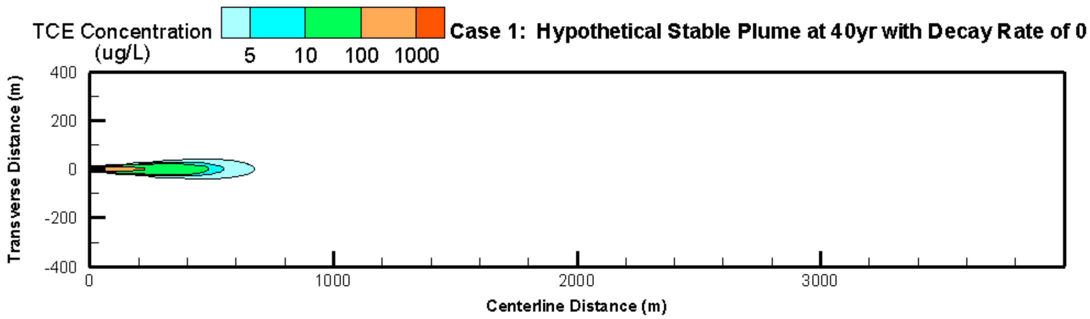
intensely decreasing behavior between the X values of 0 and 600 meters, but the 60-year match would probably be unmade by these manipulations.

Transverse and vertical plots show the 40-year plumes in the X-Y and X-Z spatial planes in Figures 4.1.24a & b and Figures 4.1.25a & b respectively. The transverse plots, ranked #13 of 13, show that the 40-year base-case plume is not well-matched by the corresponding match-case plume.

The vertical plots show that the base-case plume has a much greater expanse and higher TCE concentrations over its vertical extent than does the match-case plume, which resulted in a ranking of #11 of 13 at 40 years. If a match were desired between these plumes in the transverse or vertical directions at 40 years, changes could be made to the dispersion terms, in addition to those changes already mentioned for the centerline plot at 40 years, to force the match, but doing so would damage the 60-year match.

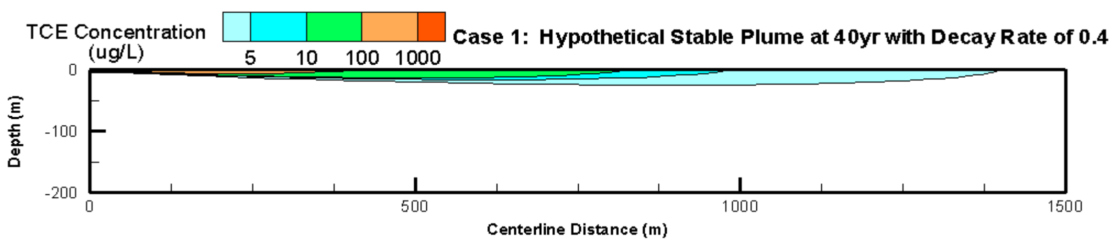


(a) base-case

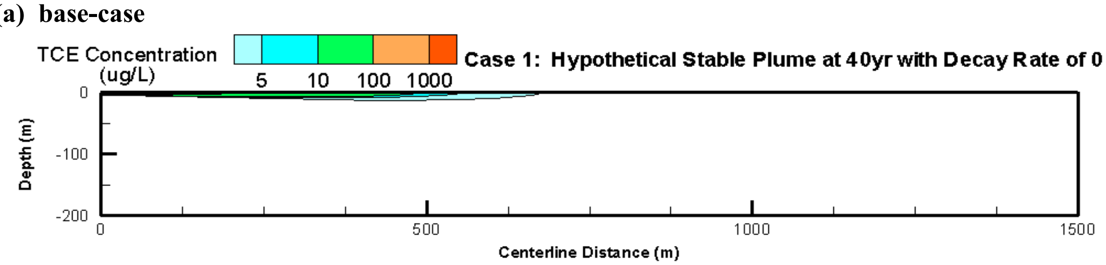


(b) match-case

Figures 4.1.24a & b: Transverse plot pair at 40yr with base-case decay rate of 0.4 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.25a & b: Vertical plot pair at 40yr with base-case decay rate of 0.4 and match-case decay rate of 0

Plume decay rate = 0.5 yr^{-1}

corresponding half-life of 1.39 years

The chart shown in Figure 4.1.26 describes the match (ranked #8 of 13) along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.5 for the base-case and 0 for the match-case. This pairing requires a stretch of the imagination to call a "match" since the two curves are in geometric opposition to each other in the plot. This model pair required a total of 7 trials to produce the centerline match along with its corresponding transverse match. Table 4.1.5 shows the beginning

Case 1: Stable plume with hypothetical parameter values (model pair 5)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.5	0
C_0 (g/L)	0.1	0.0004
M_0 (kg)	1000	1000
V_D (m/yr)	30	8.5
R	2	3.7
α_L (m)	x/100	x/10
α_T (m)	x/1,000	x/1,667
α_V (m)	x/10,000	x/16,670
φ	0.3	0.3
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.5: Comparison of base-case and final match-case parameter values (model pair 5)

and final values of the parameters for this set of trials. It was possible to move the curve down the chart slightly along the concentration axis by lowering the value of C_0 from 0.1 to 0.0004, while maintaining the base-case value for M_0. V_D was decreased from 30 to 8.5 m/yr and R was increased from 2 to 3.7 to control the length of the match-case curve in the X-direction to more closely match that of the base-case curve. The value of α_L was increased from x/100 to x/10 to force the match-case curve into a much more steeply declining pattern, one of quicker decay, like that of the base-case curve. The change in value for α_T from x/1,000 to x/1,667 and in α_V from x/10,000 to x/16,670 was necessary to force the match-case plume width in the Y-direction to match that of the slightly narrower base-case plume as shown in Figures 4.1.27a & b. The slight decrease in value of α_V seemed to have a negligible effect on the vertical extent of the plume as is shown in Figures 4.1.28a & b.

It was not possible to create a very close match with this model pair at the decay rate of 0.5 as is shown in Figure 4.1.26. The overall effect of the parameter

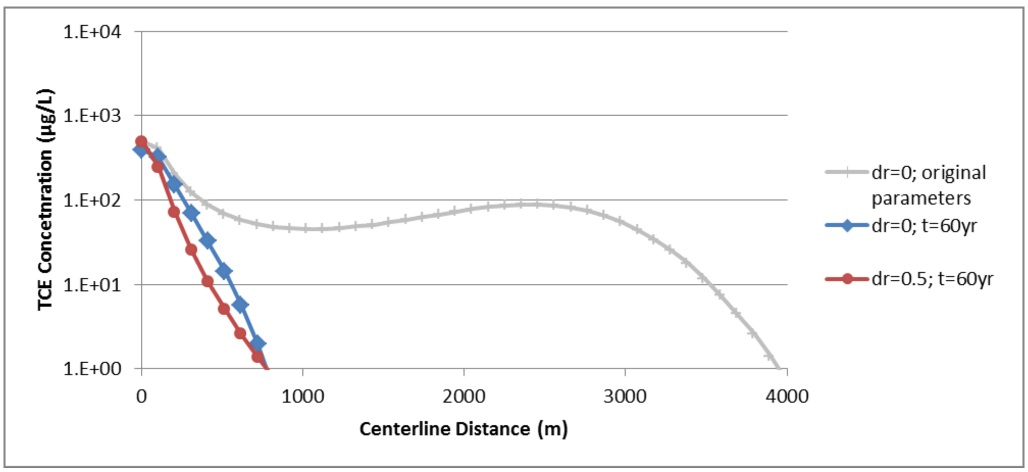
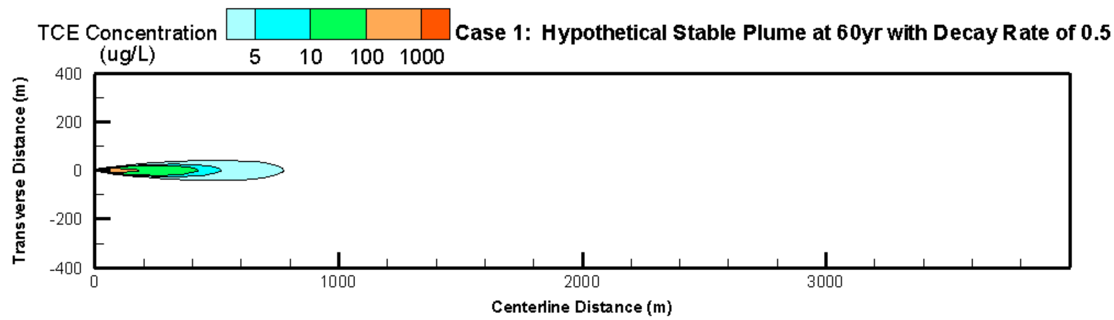


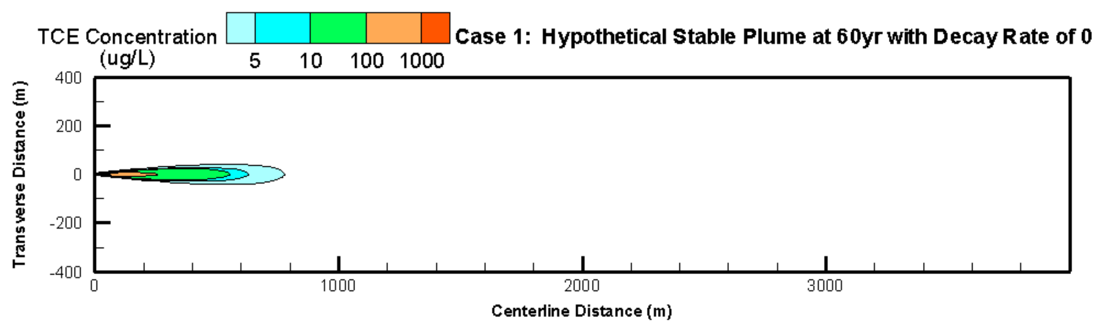
Figure 4.1.26: Centerline plot for base-case (dr=0.5) and match-case (dr=0) at 60yr

manipulations was to stretch the match-case curve in the X-direction and to move it down the chart along the concentration axis to force it to match the base-case curve between the X values of 0 and approximately 800 meters.

The transverse plot was created by adjusting the value of α_T, as previously stated, to cause the plumes to match in the X-Y spatial plane, and was given a rank of #12 of 13. Figures 4.1.27a & b show the comparison of the contour plots at 60 years. This match, like the centerline plot, is close in shape and size. Differences exist in the concentration contour placement within the two plumes.



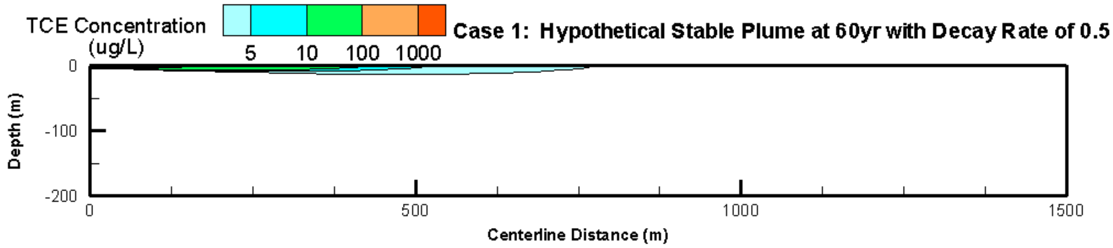
(a) base-case



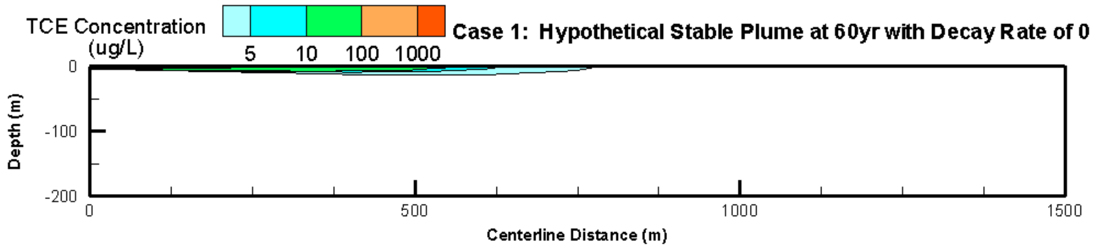
(b) match-case

Figures 4.1.27a & b: Transverse plot pair at 60yr with base-case decay rate of 0.5 and match-case decay rate of 0

The vertical plume plots, ranked #7 of 13, are similar despite the lack of effort to match them, though there are differences in concentration contour placement as is shown in Figures 4.1.27a & b. The relative similarity in both the centerline and X-Y plots show that it is possible to match, though not perfectly, the base-case (λ=0) to the match-case (λ=0.5 yr^{-1} and $t_{1/2}$=1.39 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above.



(a) base-case



(b) match-case

Figures 4.1.28a & b: Vertical plot pair at 60yr with base-case decay rate of 0.5 and match-case decay rate of 0

The centerline, transverse, and vertical plots were made again without further parameter manipulations at 40 years from the time of the initial contaminant release. The centerline plot, Figure 4.1.29 (ranked #10 of 13), shows that the overall TCE concentration for the base-case curve at 40 years is higher than that of the match-case curve at 40 years. The geometry of the curves is not similar and a distinct divergence of the curves occurs at approximately 500 meters along the X-axis.

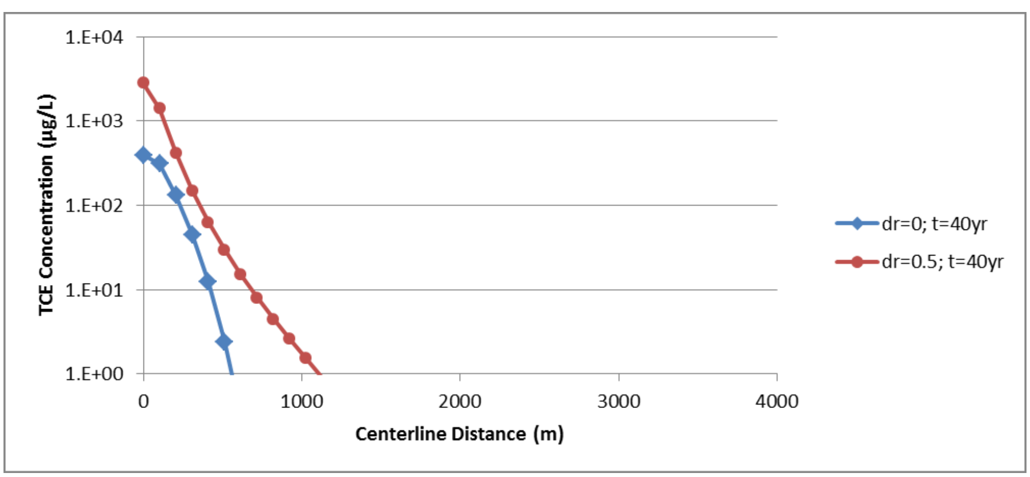
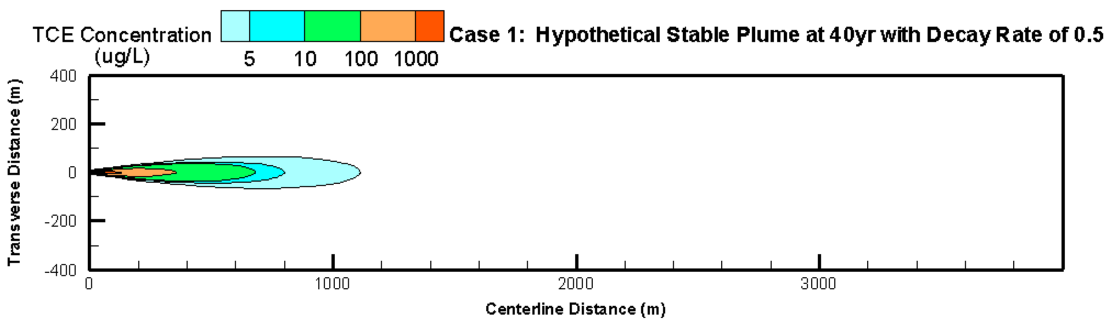
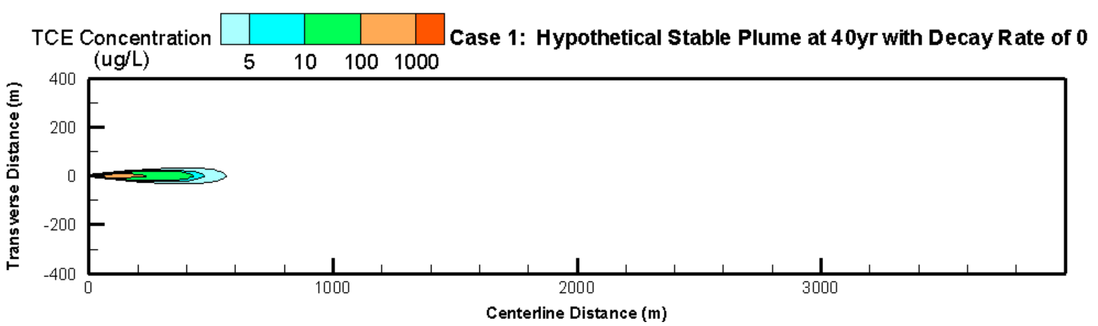


Figure 4.1.29: Centerline plot for base-case (dr=0.5) and match-case (dr=0) at 40yr

Transverse and vertical plots at 40 years are shown in Figures 4.1.30a & b and Figures 4.1.31a & b respectively. The transverse plots, ranked #11 of 13, show that the 40-year base-case plume has a much greater expanse and set of TCE concentrations than does the 40-year match-case plume. The vertical plots show that the base-case plume has a much greater expanse and higher TCE concentrations over its vertical extent than does the match-case plume, and was ranked #12 of 13 at 40 years. These comparisons show that the centerline, transverse, and vertical models at 40 years do not match and that time is an important variable in the match-making process.

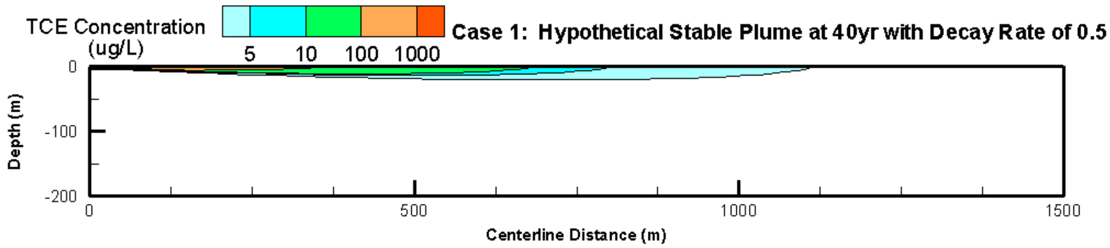


(a) base-case

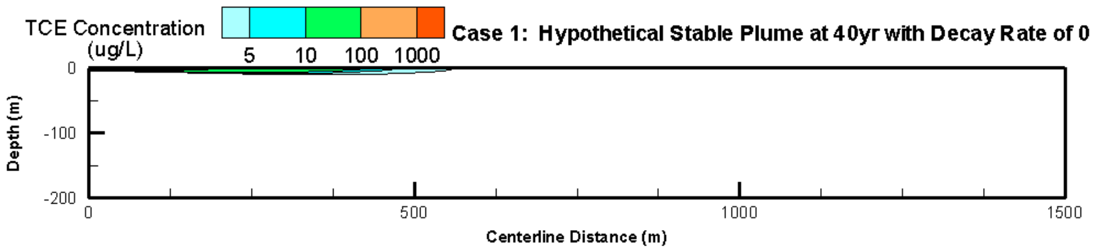


(b) match-case

Figures 4.1.30a & b: Transverse plot pair at 40yr with base-case decay rate of 0.5 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.31a & b: Vertical plot pair at 40yr with base-case decay rate of 0.5 and match-case decay rate of 0

Plume decay rate = 1.0 yr^{-1}

corresponding half-life of 0.69 years

This centerline chart shown in Figure 4.1.32 describes the manipulated pairing of curves along the centerline between base-case and match-case at 60 years where the decay rate is set at 1.0 for the base-case and 0 for the match-case. This pairing also requires a stretch of the imagination to call a "match" since the two curves have opposing geometries. This model pair required a total of 7 trials to produce the centerline match along with its corresponding transverse match. Table 4.1.6 shows the beginning and final

Case 1: Stable plume with hypothetical parameter values (model pair 6)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	1.0	0
C_0 (g/L)	0.1	0.0004
M_0 (kg)	1000	1000
V_D (m/yr)	30	4.3
R	2	3.8
α_L (m)	x/100	x/10
α_T (m)	x/1,000	x/2,500
α_V (m)	x/10,000	x/25,000
φ	0.3	0.3
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.6: Comparison of base-case and final match-case parameter values (model pair 6)

values of the parameters for this set of trials. It was possible to move the curve down the chart slightly along the concentration axis by lowering the value of C_0 from 0.1 to 0.0004 g/L, while maintaining the base-case value for M_0. V_D was decreased from 30 to 4.3 m/yr and R was increased from 2 to 3.8 to change the length of the match-case curve in the X-direction to more closely match that of the base-case curve. The Darcy velocity and Retardation factor were adjusted similarly in the previous sets of trials at lower decay rates, but the change applied to V_D and R in this set of trials in order to try to match the much faster decay rate of 1.0 (yr^{-1}) was greater than the previous scenarios. It was necessary to increase the value of α_L from x/100 to x/10 to force the match-case curve into a much more steeply declining pattern, one of quicker decay, like that of the base-case curve. The change in value for α_T from x/1,000 to x/2,500 and in α_V from x/10,000 to x/25,000 was necessary to force the match-case plume width in the Y-direction to match that of the slightly narrower base-case plume as plotted in Figures 4.1.33a & b. The decrease in value of α_V seemed to have a negligible effect on the vertical extent of the plume as is shown in Figures 4.1.34a & b.

It was not possible to create a perfect match with this model pair at the decay rate of 1.0 as shown in Figure 4.1.32, and this chart was ranked #9 of 13. The overall effect

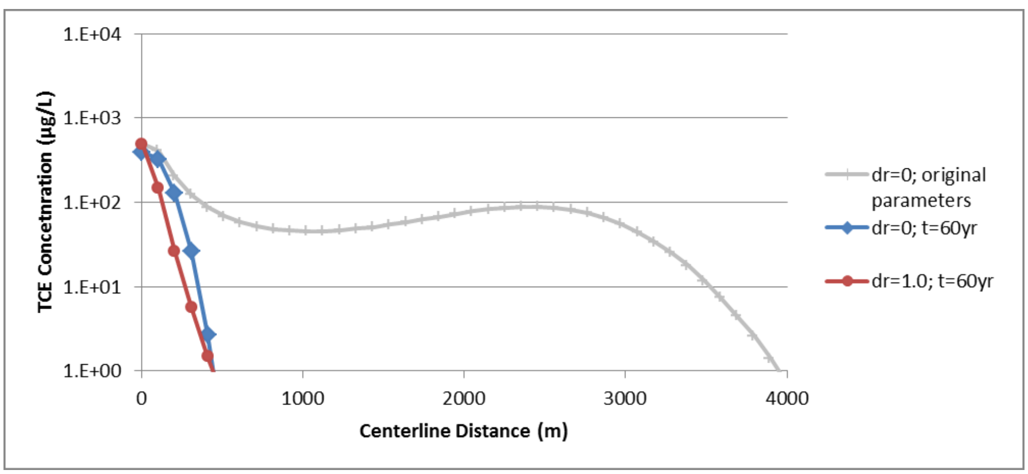
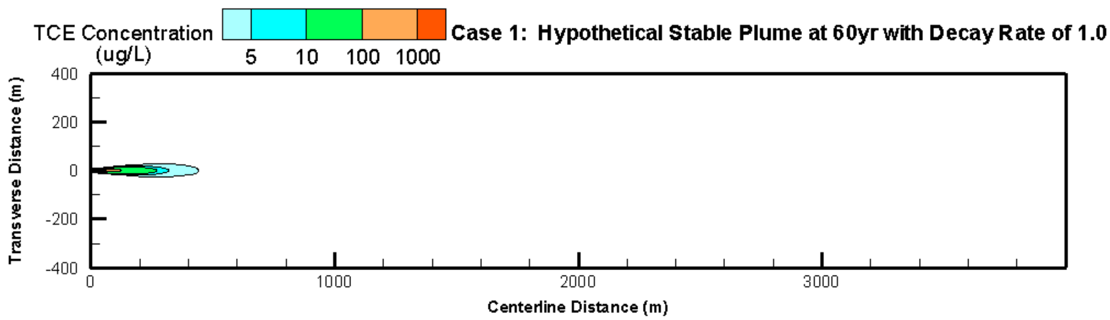


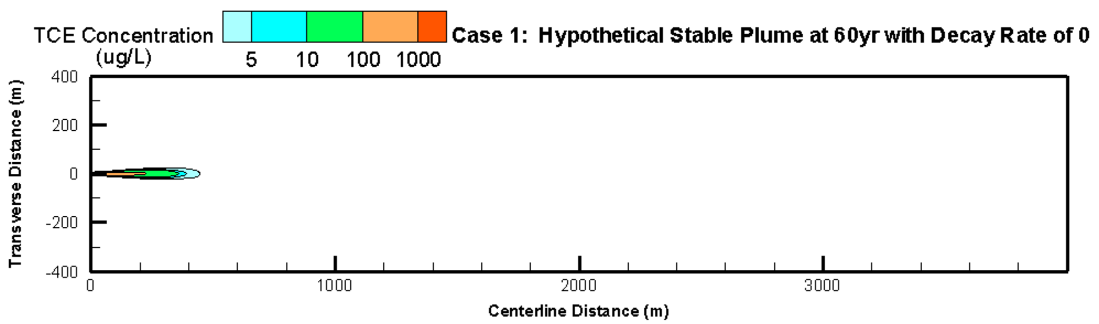
Figure 4.1.32: Centerline plot for base-case (dr=1.0) and match-case (dr=0) at 60yr

of the parameter manipulations was to stretch the match-case curve in the X-direction and to move it down the chart along the concentration axis to force it to match the base-case curve between the X values of 0 and approximately 500 meters.

The transverse, X-Y spatial plane, plume plots at 60 years are shown in Figures 4.1.33a & b. This match, ranked #9 of 13, is relatively close in shape and size, but differences exist in the plumes' concentration contour placements.



(a) base-case

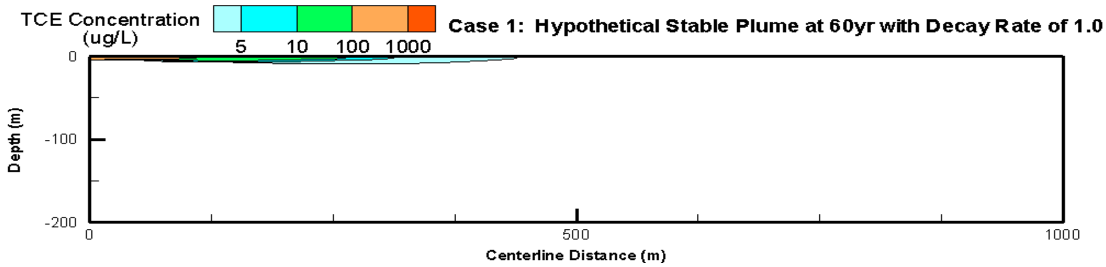


(b) match-case

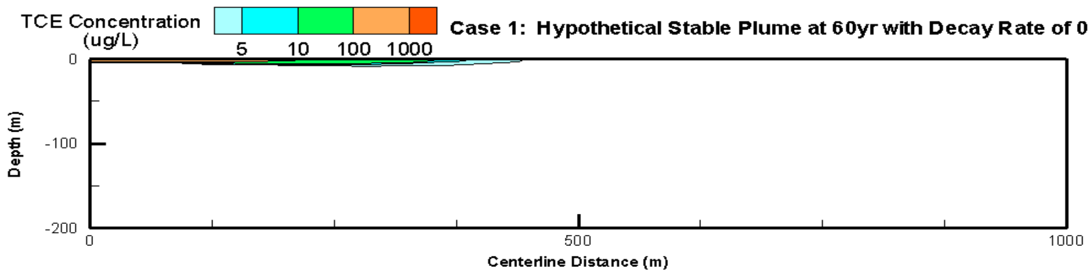
Figures 4.1.33a & b: Transverse plot pair at 60yr with base-case decay rate of 1.0 and match-case decay rate of 0

Vertical contour plots were made along the centerlines with no attempt at match-making and are shown in Figures 4.1.34a & b, which were ranked #8 of 13 at 40 years. The main difference between the base- and match-case vertical plume plots is in their concentration contour placement.

The centerline and X-Y plots serve to show that it is possible to match the base-case (λ=0) to the match-case (λ=1.0 yr^{-1} and $t_{1/2}$=0.69 yr) at 60 years from the time of the original TCE release by manipulation of the other parameters as explained above, though not perfectly.



(a) base-case



(b) match-case

Figures 4.1.34a & b: Vertical plot pair at 60yr with base-case decay rate of 1.0 and match-case decay rate of 0

Using the same parameter values, the centerline, transverse, and vertical plots were made for each of the plumes at 40 years from the time of the initial contaminant release. The centerline plot, Figure 4.1.35, shows that the overall TCE concentration for the base-case curve at 40 years is higher than that of the match-case curve at 40 years. The geometry of the curves is not similar and a distinct divergence of the curves occurs at approximately 300 meters along the X-axis. This comparison was ranked #9 of 13 at 40 years.

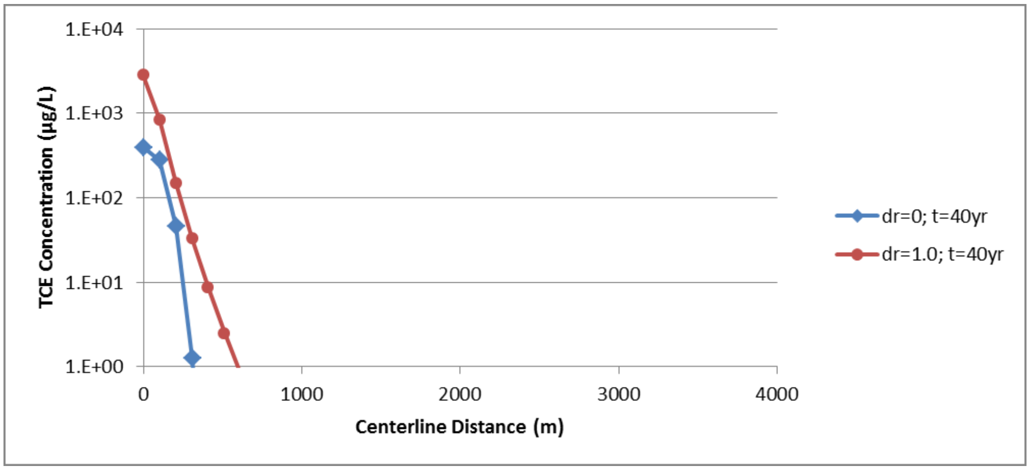
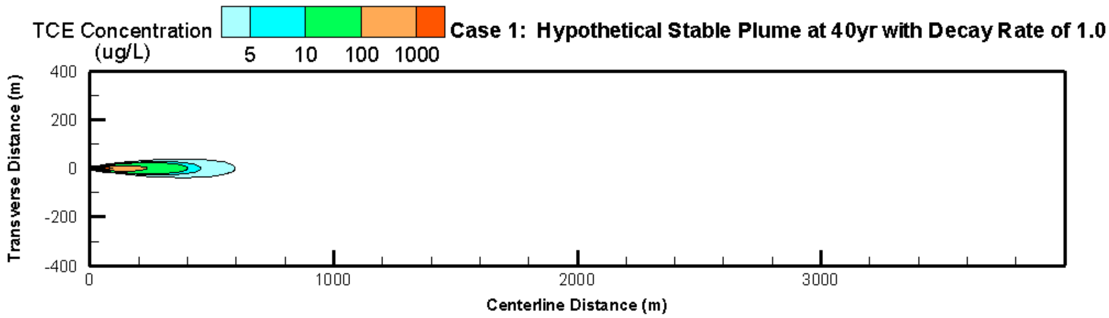


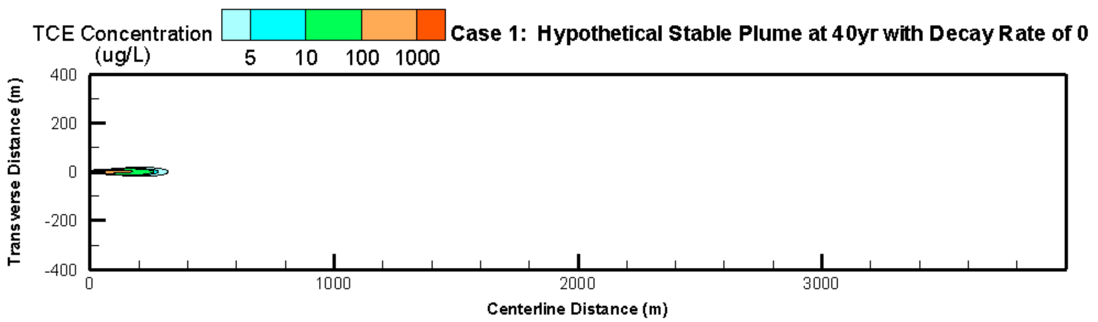
Figure 4.1.35: Centerline plot for base-case (dr=1.0) and match-case (dr=0) at 40yr

Transverse and vertical plots are shown in Figures 4.1.36a & b and Figures 4.1.37a & b respectively. The transverse plots show that the 40-year base-case plume has a much greater expanse and set of TCE concentrations than does the 40-year match-case plume, and were ranked #12 of 13 for goodness of fit. The vertical plots show that the base-case plume has a much greater expanse and higher TCE concentrations over its vertical extent than does the match-case plume, which led to a ranking of #13 of 13 at 40 years. Additional parameter manipulation would be necessary in order to force the 40-year plots to match, but this would upset the 60-year match, which reaffirms the importance of the time variable.

Overall, the results for Case 1 show that it is increasingly difficult to create model matches as the plume decay rates increase, and indicate that time is an important variable.

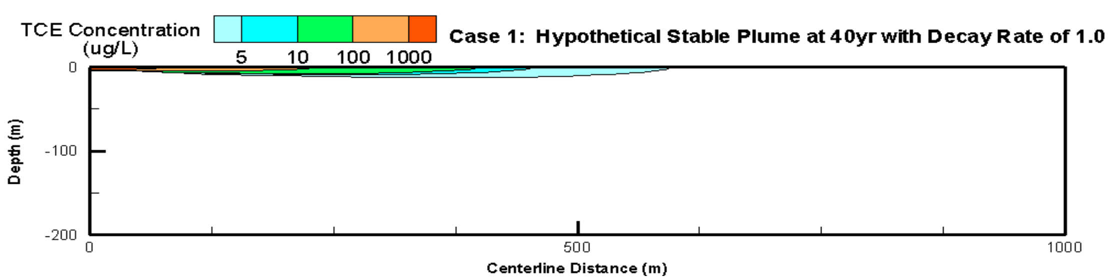


(a) base-case

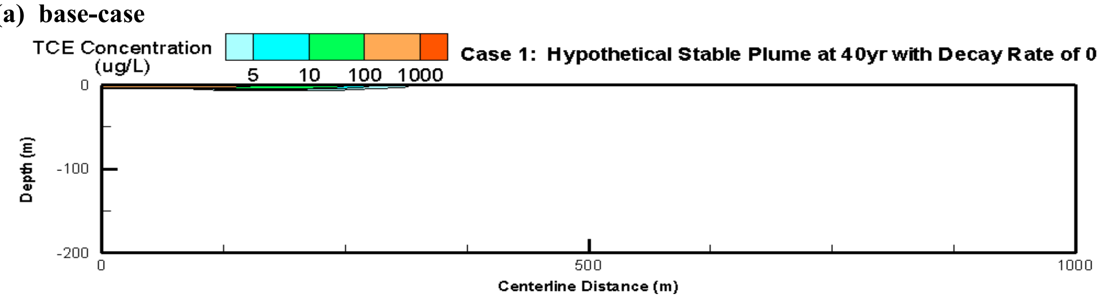


(b) match-case

Figures 4.1.36a & b: Transverse plot pair at 40yr with base-case decay rate of 1.0 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.37a & b: Vertical plot pair at 40yr with base-case decay rate of 1.0 and match-case decay rate of 0

Case 1b: Stable plume with parameter values from Liang [2009]

This set of scenarios is a secondary version of Case 1, in which a stable, non-expanding plume was modeled with a different set of base-case parameter values than those used in Case 1. As in the previous scenario, the plume for this scenario is a "stable" plume which remains at approximately the same spatial extent, not expanding, and has a slowly declining TCE concentration over time with the contaminant mass partially in the source zone and partially in the plume [Pate, 2010; Liang, 2009]. In this scenario, Case 1b, two different plume decay rate values (0.1 and 0.2 yr^{-1}) were chosen for the match-cases to determine if their resultant plots could be matched to plots made with plume decay rates of zero by manipulation of certain other parameter values. These rates correspond to half-lives of 6.93 and 3.47 years respectively, which are quite fast when compared with the half-lives from the literature review that are shown in Table 1.1.1. The model pairs were matched at 60 years from the initial time of TCE release. The data at 40-years with no further parameter manipulation were then plotted for comparison. A total of four each of centerline plots, transverse plots, and vertical plots were compared for visual similarity.

The parameters for the base-case were taken from a case study in Liang [2009] and are shown in Tables 4.1.7 and 4.1.8 as they are discussed in order in this section. For each model pair in this Case, the original TCE concentration (C_0) is 0.006 g/L (less than the 0.1 g/L used in the previous scenario), the original TCE mass (M_0) is 136 kg (less than the 1000 kg used in the previous scenario), the Darcy velocity (V_D) is 8 m/yr (less than the 30 m/yr used in the previous scenario), the retardation factor (R) is 2.0 (the same as in the previous scenario), the longitudinal dispersivity (α_L) is approximated as x/20 (greater than the x/100 used in the previous scenario), the transverse dispersivity (α_T) is approximated as x/1,000 (the same as in the previous scenario), the vertical dispersivity (α_V) is approximated as x/10,000 (the same as in the previous scenario), porosity of the matrix (φ) is assigned a value of 0.33 (slightly greater than the 0.3 used in the previous scenario), the source width (W) is 8 m (less than the 10 m used in the previous scenario), and the source depth (D) is 3.5 m (slightly greater than the 3 m used in the previous scenario) [Liang, 2009].

Plume decay rate = 0.1 yr^{-1}

corresponding half-life of 6.93 years

Figure 4.1.38 shows the centerline match between base-case and match-case at 60 years where the decay rate is set at 0.1 for the base-case and 0 for the match-case. This relatively close match, ranked #5 of 13, was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.7. Parameter adjustments were made in a total of 57 trials to produce the centerline match and transverse matches for this model pair. C_0 was reduced from 0.006 to 0.004 g/L and M_0 was increased from 136 to 200 kg in a balancing act that forced the match-case curve down the chart along the concentration axis. V_D was increased from 8 to 10.9 m/yr and R was increased from 2 to 3.7 to force the match-case curve to the same X-axis-length as the base-case curve. The geometry of the two curves was similar to begin with, but increasing the value of α_L from x/20 to x/10 caused the match-case curve to better approximate the more steeply declining form of the base-case curve. The transverse

Case 1b: Stable Plume with base-case values from Liang [2009] (model pair 7)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.1	0
C_0 (g/L)	0.006	0.004
M_0 (kg)	136	200
V_D (m/yr)	8	10.9
R	2	3.7
α_L (m)	x/20	x/10
α_T (m)	x/1,000	x/1,111
α_V (m)	x/10,000	x/1,428
φ	0.33	0.33
W (m)	8	8
D (m)	3.5	3.5
evaluation at t=60yrs		

Table 4.1.7: Comparison of base-case and final match-case parameter values (model pair 7)

dispersivity value, α_T, was decreased from x/1,000 to x/1,111 in order to decrease the width of the plume in the Y-direction to force a match between the base- and match-case plumes as they were plotted in the X-Y spatial plane as shown in Figures 4.1.39a & b. Usually the vertical dispersivity value is an order of magnitude smaller than the transverse dispersivity value, but in this match α_V had to be adjusted up (from x/10,000 to x/1,428) to nearly equal the value of α_T in order to force the centerline plot and transverse plume plot matches. This increase in α_V caused the match-case plume in the vertical plots to be significantly greater in vertical expanse than was the base-case plume, as is shown below in Figures 4.1.40a & b.

This model pair has a high amount of similarity, though it is not a perfect match as shown in Figure 4.1.38. The effect of the parameter manipulations was to move the match-case curve down the chart along the concentration axis, to control its length along the X-axis, and to steepen it enough to match the quicker decline of the base-case curve.

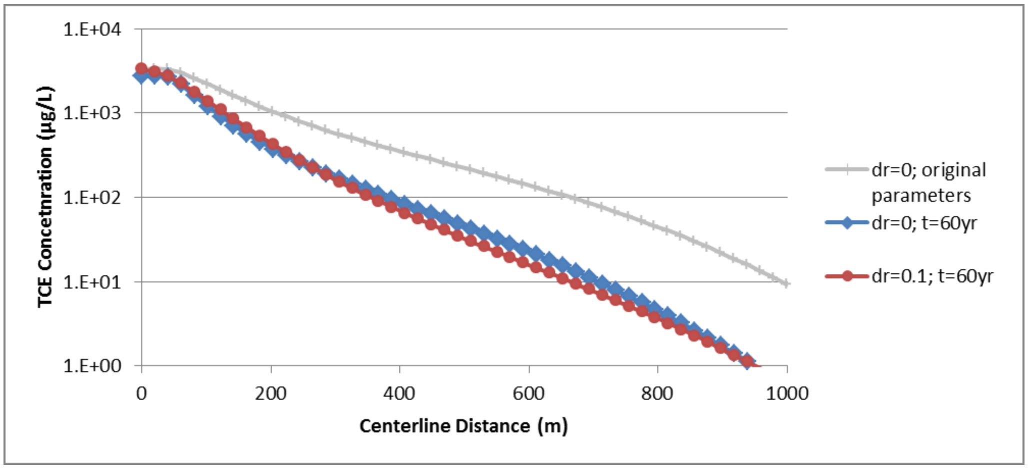
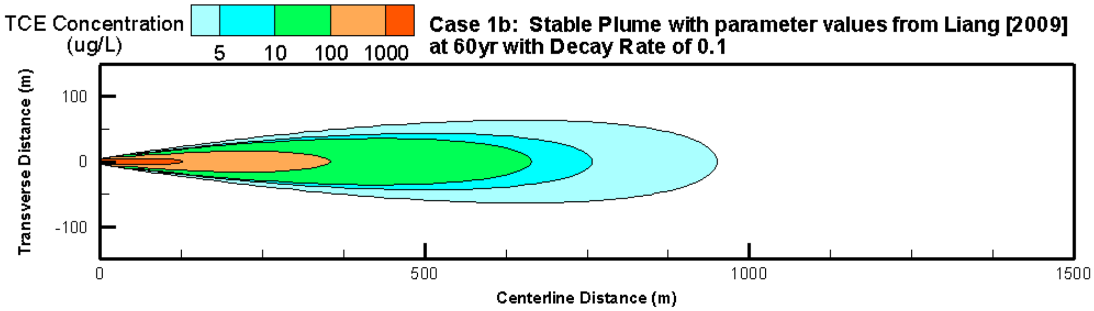


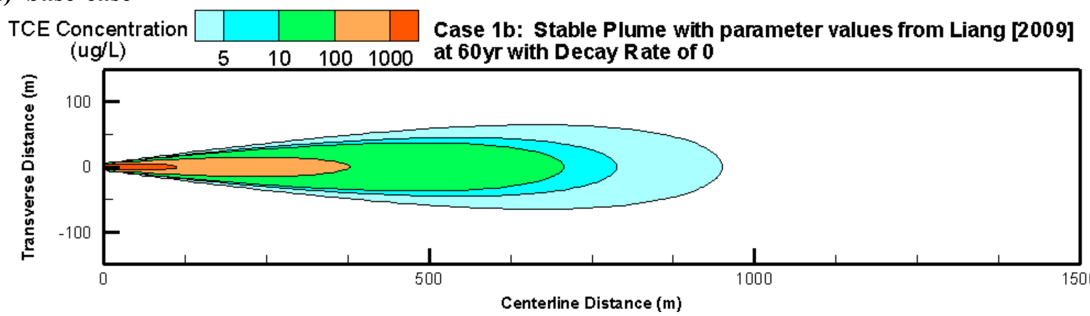
Figure 4.1.38: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 60yr

The transverse plot comparison was created by adjusting the value of α_T, as stated above, and plotting the resulting data in the X-Y spatial plane. Figures 4.1.39a & b, ranked #5 of 13, show the contour plot depiction of the base- and match-case plumes at 60 years. This match, much like the centerline match for this particular pair, was fairly close. Contour plots of vertical slices of the plumes along their centerlines were made with no attempt at matching them. Increasing the value of α_V caused a higher degree of variance in the vertical plots of the plumes as shown in Figures 4.1.40a & b, which resulted in a ranking of #10 of 13.

The high degree of similarity in both the centerline and X-Y plots show that it is possible to match the base-case (λ=0) to the match-case (λ=0.1 yr^{-1} and $t_{1/2}$=6.93 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above. The X-Z plots, though, show a high degree of dissimilarity because of the high value assigned to the vertical dispersion parameter (α_V), an order of magnitude greater than is normally assigned, in order to force the centerline and transverse matches.

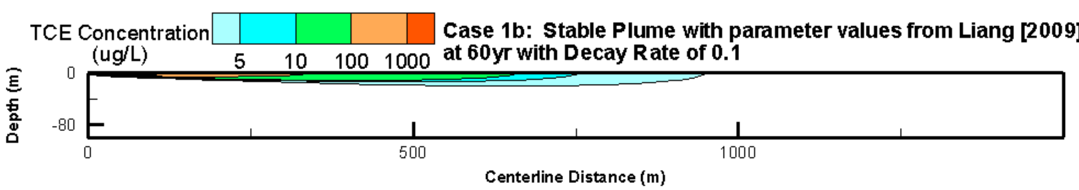


(a) base-case

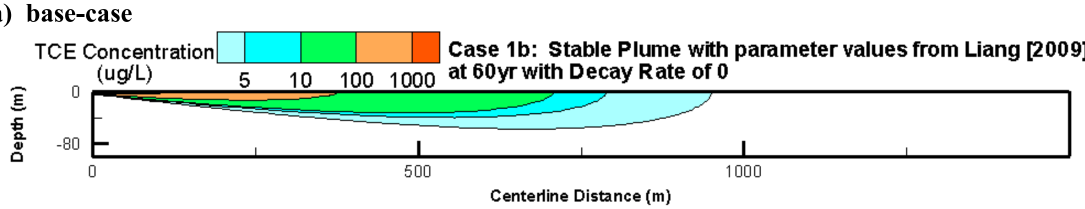


(b) match-case

Figures 4.1.39a & b: Transverse plot pair at 60yr with base-case decay rate of 0.1 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.40a & b: Vertical plot pair at 60yr with base-case decay rate of 0.1 and match-case decay rate of 0

The centerline, transverse and vertical plots were made again using the data at 40 years with no additional parameter manipulation. The centerline plot, Figure 4.1.41,

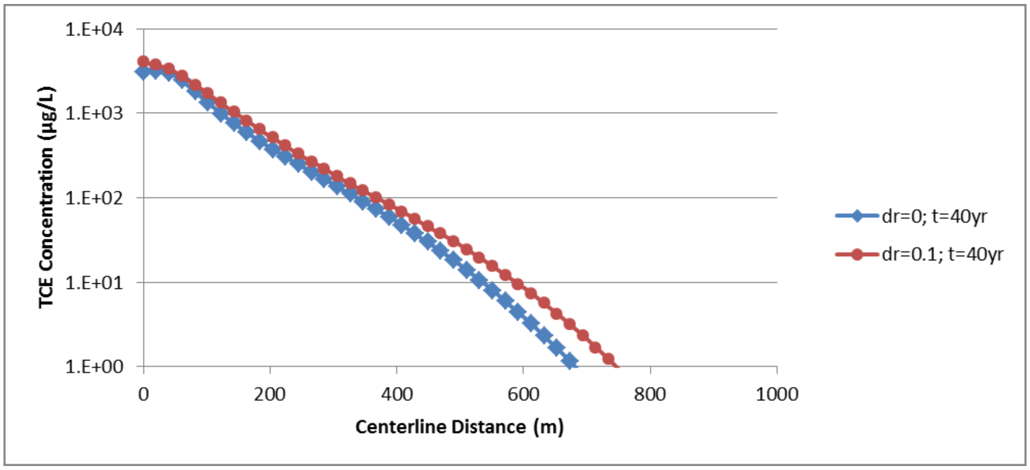
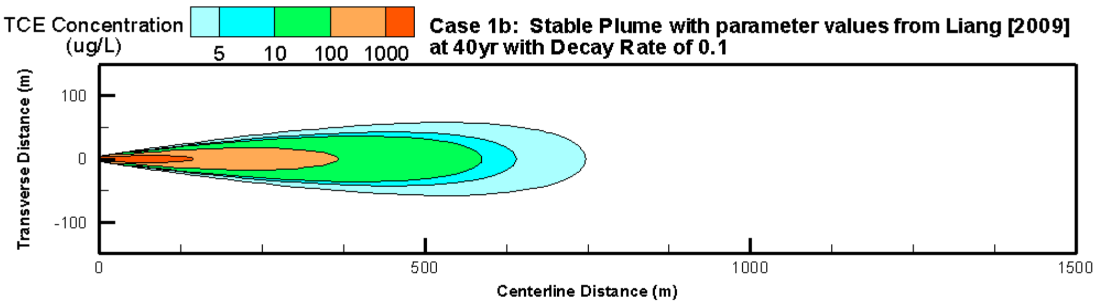


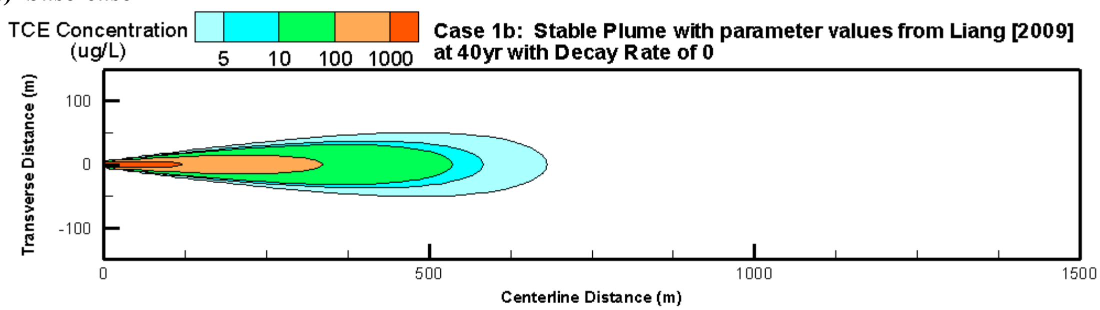
Figure 4.1.41: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 40yr

shows that the overall TCE concentration for the base-case curve at 40 years is a bit higher than that of the match-case curve at 40 years, and was ranked #1 of 13 in the 40-year centerline plots.

Transverse and vertical plots are shown in Figures 4.1.42a & b and Figures 4.1.43a & b respectively. The transverse plots, ranked #6 of 13, show that the 40-year base-case plume has a slightly greater expanse than the 40-year match-case plume, but that the TCE concentration contours between the pair are similar for their respective sizes. Ranked at #6 of 13, the vertical plots show that the match-case plume is more vertically extensive than the base-case plume.

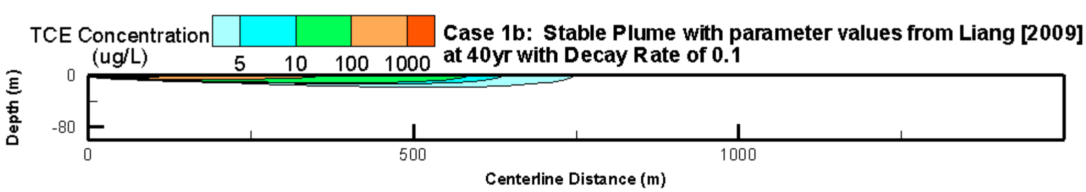


(a) base-case

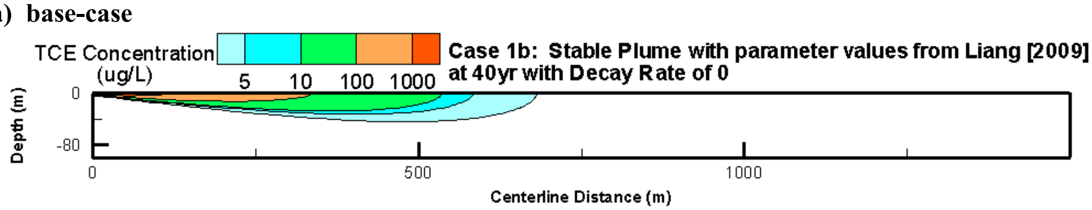


(b) match-case

Figures 4.1.42a & b: Transverse plot pair at 40yr with base-case decay rate of 0.1 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.43a & b: Vertical plot pair at 40yr with base-case decay rate of 0.1 and match-case decay rate of 0

Plume decay rate = 0.2 yr^{-1}

corresponding half-life of 3.47 years

The chart in Figure 4.1.44 shows the manipulated match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.2 for the base-case and 0 for the match-case. The match is closer at TCE concentrations greater than 500 μg/L and at the assumed detection limit concentration of 1 μg/L. This match was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.8, and required a total of 9 trials to produce centerline and

Case 1b: Stable Plume with base-case values from Liang [2009] (model pair 8)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.2	0
C_0 (g/L)	0.006	0.003
M_0 (kg)	136	200
V_D (m/yr)	8	7.5
R	2	3.7
α_L (m)	x/20	x/10
α_T (m)	x/1,000	x/1,428
α_V (m)	x/10,000	x/1,000
φ	0.33	0.33
W (m)	8	8
D (m)	3.5	3.5
evaluation at t=60yrs		

Table 4.1.8: Comparison of base-case and final match-case parameter values (model pair 8)

transverse matches. C_0 was decreased from 0.006 to 0.003 g/L and M_0 was increased from 136 to 200 kg to force the match-case curve down the chart along the concentration axis. V_D was decreased from 8 to 7.5 m/yr and R was increased from 2 to 3.7 in order to force the match-case curve to the same X-axis-length as the base-case curve. The geometry of the curves was similar to begin with, but increasing the value of α_L from x/20 to x/10 caused the match-case curve to better approximate the more steeply declining form of the base-case curve. The transverse dispersivity value, α_T, was decreased from x/1,000 to x/1,428 in order to decrease the width of the match-case plume in the Y-direction to force a match between the base- and match-case plumes as they were plotted in the X-Y spatial plane (Figures 4.1.45a & b). This match required that α_V be adjusted from x/10,000 to x/1,000, a value greater than that of α_T , which is not usually done, in order to force the centerline plot and transverse plume plot matches. The increase in α_V caused the match-case plume to be significantly greater in vertical expanse than was the base-case plume, as shown in Figures 4.1.46a & b.

This matched model pair has less similarity than did the previous match in this Case at the decay rate of 0.1 as shown in Figure 4.1.44, which was ranked #12 of 13. The

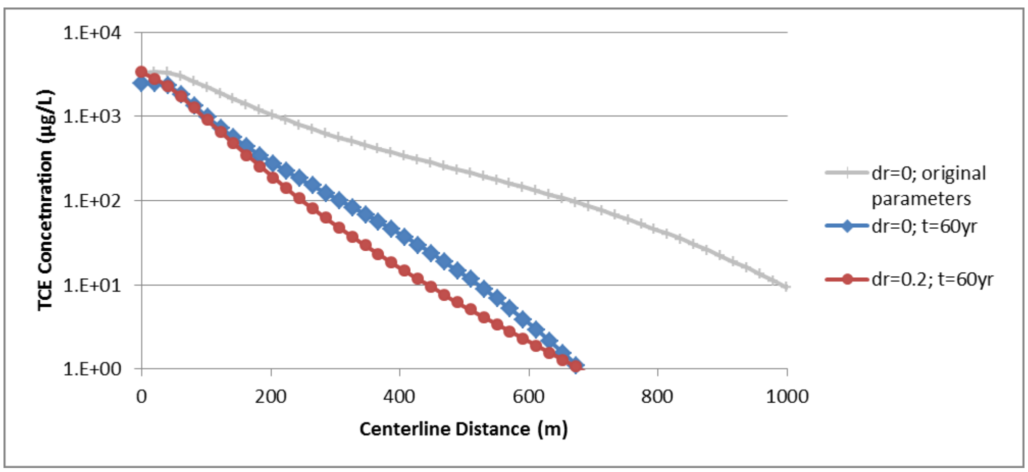
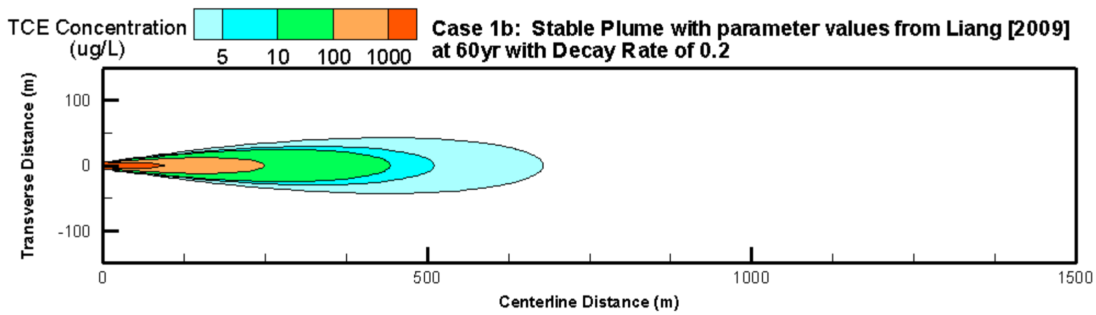


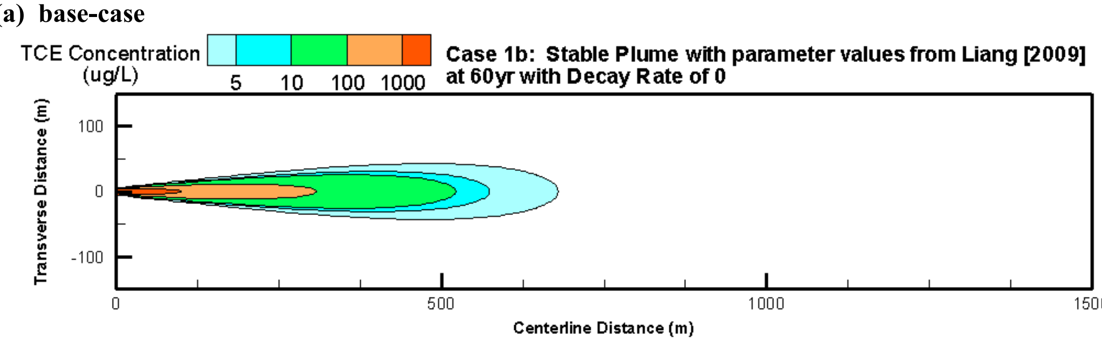
Figure 4.1.44: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 60yr

overall effect of the parameter manipulations was to move the match-case curve down the chart along the concentration axis, to control its length along the X-axis, and to steepen it enough to match the quicker decline of the base-case curve.

Figures 4.1.45a & b, ranked #4 of 13, show the transverse contour plot comparison between the base- and match-case at 60 years. This match, like the centerline match for this particular pair, was fairly close with the main difference being in the placement of concentration contour lines within the plumes.



(a) base-case

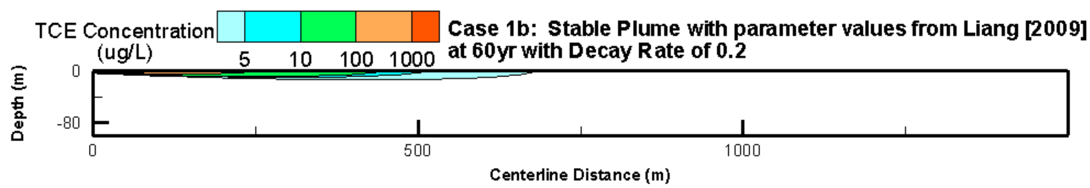


(b) match-case

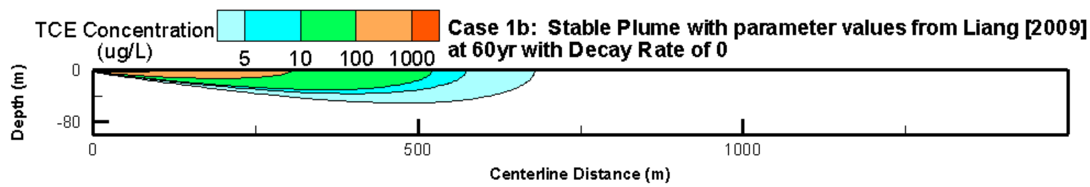
Figures 4.1.45a & b: Transverse plot pair at 60yr with base-case decay rate of 0.2 and match-case decay rate of 0

Contour plots of vertical slices of the plumes were made along their centerlines with no attempt to force them to match. Increasing value of α_V caused the vertical plots for this model pair to lack similarity, as shown in Figures 4.1.46a & b (ranked #9 of 13).

The centerline and X-Y plots show that it is possible to match the base-case (λ=0) to the match-case (λ=0.2 yr^{-1} and $t_{1/2}$=3.47 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above. The X-Z plots, though, show a high degree of dissimilarity because of the high value assigned to the vertical dispersion parameter (α_V), a value greater than the value of the transverse dispersivity parameter (α_T), in order to force the centerline and transverse matches.



(a) base-case



(b) match-case

Figures 4.1.46a & b: Vertical plot pair at 60yr with base-case decay rate of 0.2 and match-case decay rate of 0

The centerline, transverse, and vertical plots were made again with the 40-year data with no further parameter manipulation. The centerline plot, Figure 4.1.47, shows that the match is quite good from 0 to approximately 300 meters along the X-axis, but the match-case curve then declines much more rapidly than does the base-case curve. This centerline comparison was ranked #2 of 13 at 40 years.

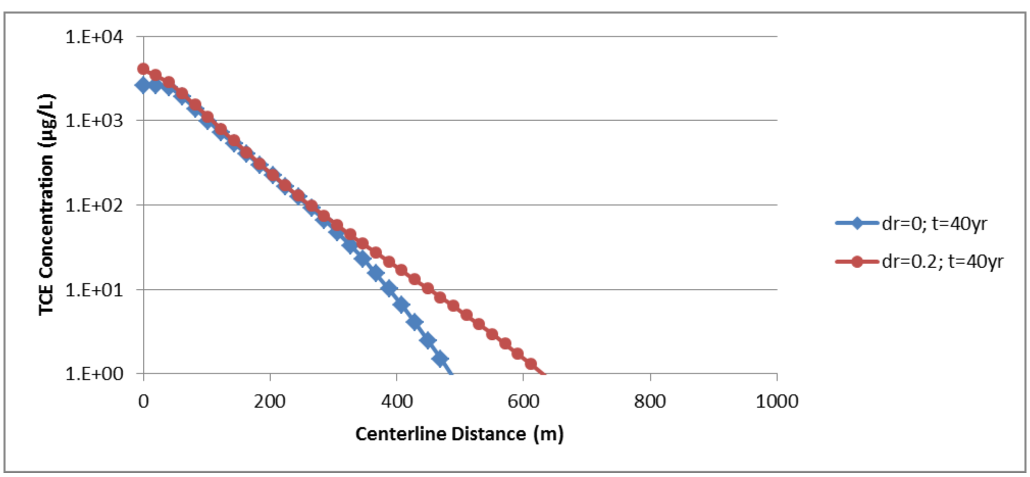
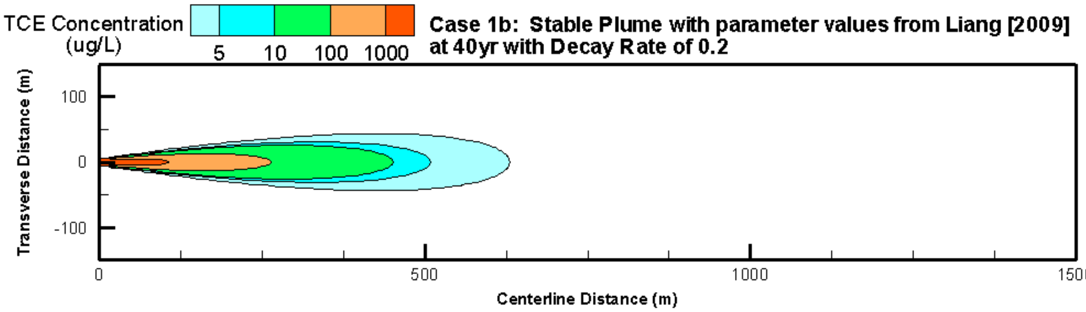


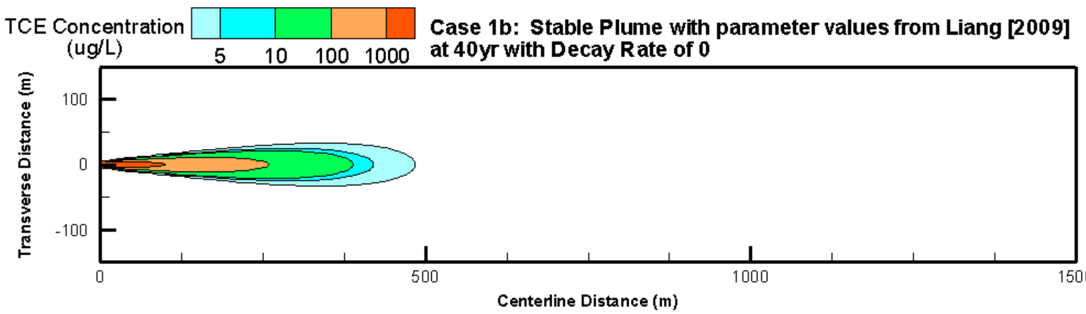
Figure 4.1.47: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 40yr

Transverse and vertical plots were produced with the 40-year data as shown in Figures 4.1.48a & b and Figures 4.1.49a & b respectively. The transverse plots (ranked #7 of 13) show that the 40-year base-case plume has a greater expanse than the 40-year match-case plume, but that the TCE concentration contours between the pair are similar for their respective sizes. The vertical plots show that the match-case plume has a much greater expanse over its vertical extent than does the base-case plume, and were assigned a rank of #8 of 13 at 40 years.

Though this Case presents a stable plume as in Case 1, the matches were not as close and were more difficult to create, possibly because of the different values in the parameter set used in this Case. As in Case 1, though, the models of the lower of the two plume decay rates were more easily matched than were those of the higher plume decay rates. The lack of similarity in the 40-year comparisons reinforced the earlier finding that time acts as a controlling variable in the similarity of base- and match-case plumes at multiple points in the plumes' histories.

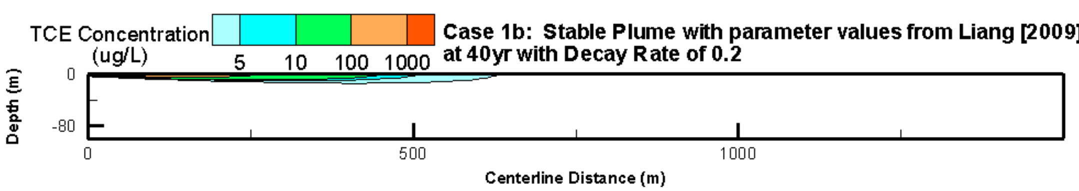


(a) base-case

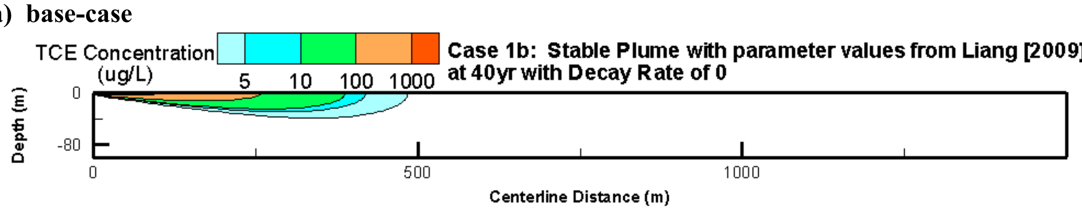


(b) match-case

Figures 4.1.48a & b: Transverse plot pair at 40yr with base-case decay rate of 0.2 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.49a & b: Vertical plot pair at 40yr with base-case decay rate of 0.2 and match-case decay rate of 0

Case 2: Growing-disconnected plume with parameter values from Liang [2009]

In this Case a different type of plume behavior is studied: the growing plume, disconnected from its TCE source with all of its contaminant mass present in the plume [Liang, 2009]. Due to the very quick washing-out behavior of the models in this Case, the years at which the models were run are 54 and 34 (years since initial release of TCE) instead of 60 and 40 years as in the previous Cases. Two decay rates (0.1 and 0.2 yr^{-1}) were studied in the trials for this scenario. These rates correspond to half-lives of 6.93 and 3.47, which are quite fast when compared with the half-lives from the literature review that are shown in Table 1.1.1. The models were matched at 54 years from time of initial release of TCE, and in order to determine whether the plumes would match as well at an earlier point in each of their histories they were run and plotted again at 34 years after the initial TCE release with all the parameters held the same as for the 54-year matches. A total of four each of centerline plots, transverse plots, and vertical plots were compared for visual similarity.

The parameters for the base-case for this scenario were taken from a case study in Liang [2009] and are shown in Tables 4.1.9 and 4.1.10 in this section as they are discussed. For each model pair in this Case, the original TCE concentration (C_0) is 0.1 g/L, the original TCE mass (M_0) is 324 kg, the Darcy velocity (V_D) is 20 m/yr, the retardation factor (R) is 2.0, the longitudinal dispersivity (α_L) is approximated as x/100, the transverse dispersivity (α_T) is approximated as x/1,000, the vertical dispersivity (α_V) is approximated as x/10,000, porosity of the matrix (φ) is assigned a value of 0.33, the source width (W) is 10 m, and the source depth (D) is 3 m [Liang, 2009]. Comparatively, this set of base-case parameters is similar to that utilized in Case 1 since the only parameters that vary from the Case 1 set are M_0 (1000 kg in Case 1), V_D (30 m/yr in Case 1), and φ (0.3 in Case 1).

Plume decay rate = 0.1 yr^{-1}

Figure 4.1.50 shows the manipulated match along the centerline between base-case and match-case at 54 years where the decay rate is set at 0.1 for the base-case and 0 for the match-case. The match for this pair is quite good both in proximity and geometry of the curves, as is shown in the following figures. This match was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.9,

Case 2: Growing-Disconnected plume with base-case values from Liang [2009] (model pair 9)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.1	0
C_0 (g/L)	0.1	0.007
M_0 (kg)	324	35
V_D (m/yr)	20	22
R	2	2.2
α_L (m)	x/100	x/100
α_T (m)	x/1,000	x/1,000
α_V (m)	x/10,000	x/10,000
φ	0.33	0.33
W (m)	10	10
D (m)	3	3
evaluation at t=54yrs		

Table 4.1.9: Comparison of base-case and final match-case parameter values (model pair 9)

and required a total of 45 trials to produce the centerline match and its corresponding transverse match. As explained earlier in Figure 4.1.7 and Equation 4.1, the proportional relationship of the source concentration to the mass and original concentration terms described by the source equation allows for the significant lowering of C_0 (from 0.1 to 0.007 g/L) and of M_0 (from 324 to 35 kg) in order to create the model pair matches. V_D

was increased from 20 to 22 m/yr and R was increased from 2 to 2.2 to adjust the length of the match-case curve along the X-axis and to force it to better fit that of the base-case curve. The geometry of the curves was already very similar, with neither at a rate of decline that outpaced the other, so the α_L value was kept the same for the match-case curve as it was for the base-case curve (x/100). The transverse and vertical dispersivity values, α_T (x/1,000) and α_V (x/10,000) respectively, were kept the same because the width of the match-case plume in the Y-direction on the transverse plume plot was the same as that of the base-case plume as shown in Figures 4.1.51a & b. By keeping the three dispersivity values the same in the match-case as they were for the base case, it was necessary to very significantly reduce the values of the concentration (from 0.1 to 0.007 g/L) and mass (from 324 to 35 kg) parameters in order to force the centerline and transverse plot matches.

This matched model pair has almost perfect similarity between the match- and base-case curves (ranked #2 of 13) as shown in Figure 4.1.50. The overall effect of the

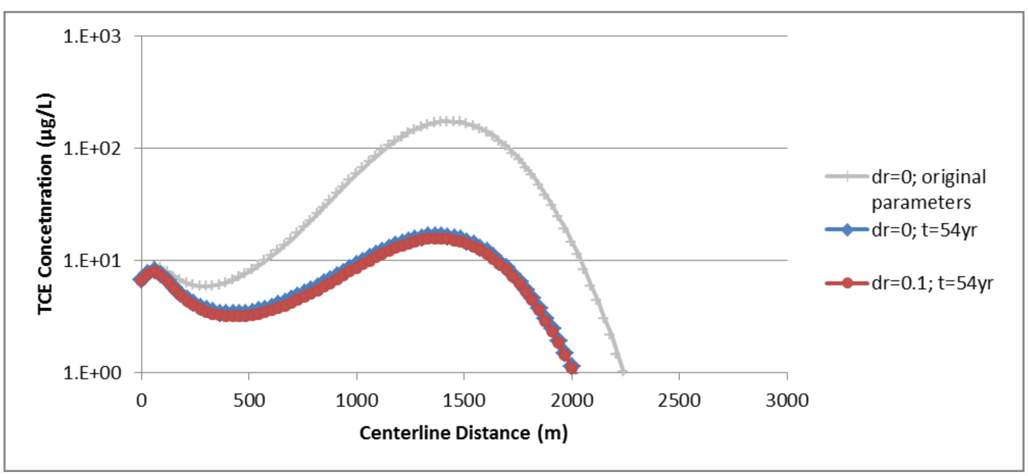
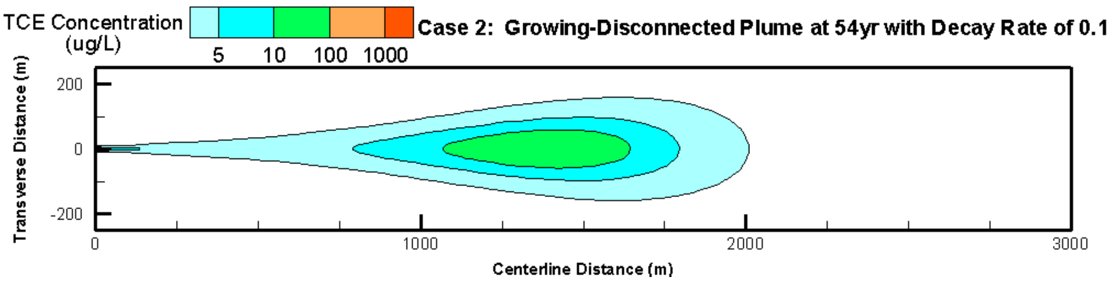


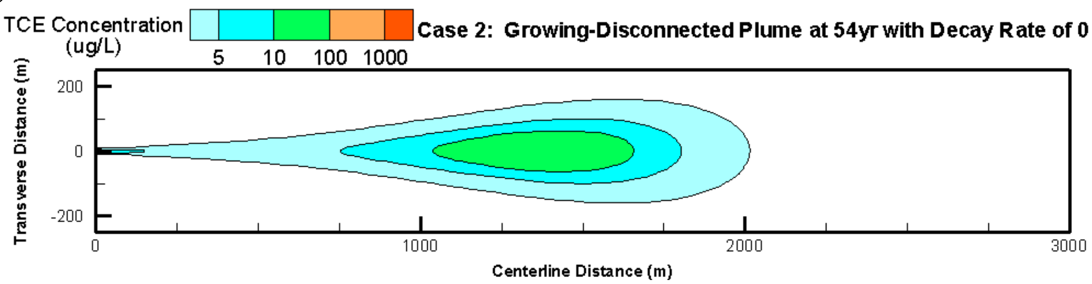
Figure 4.1.50: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 54yr

parameter manipulations was to move the match-case curve down the chart along the concentration axis and to shorten it in the X-direction to fit the length of the base-case curve.

Figures 4.1.51a & b, ranked #2 of 13, show the transverse contour plot depiction of the base- and match-case plumes at 54 years. This match, much like the centerline match for this particular pair, was nearly perfect.



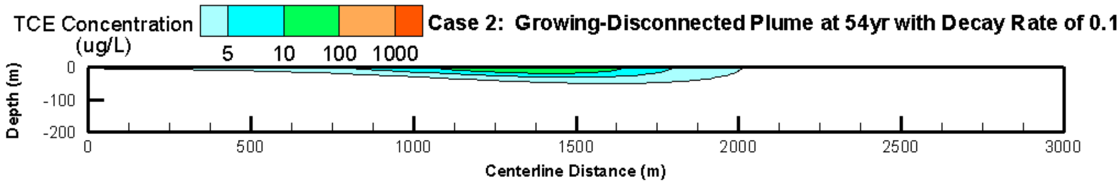
(a) base-case



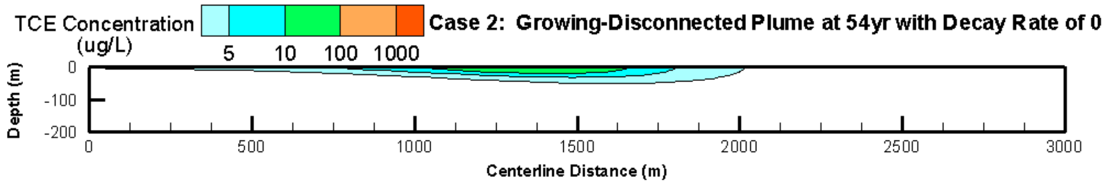
(b) match-case

Figures 4.1.51a & b: Transverse plot pair at 54yr with base-case decay rate of 0.1 and match-case decay rate of 0

The vertical plots, with no further parameter manipulation applied, show a high degree of similarity between the base- and match-case plume expanses and concentration contours as shown in Figures 4.1.52a & b, which resulted in their rank of #2 of 13.



(a) base-case



(b) match-case

Figures 4.1.52a & b: Vertical plot pair at 54yr with base-case decay rate of 0.1 and match-case decay rate of 0

The almost perfect match in both the centerline and X-Y plots and the serendipitous match in the X-Z plot show that it is possible to match the base-case (λ=0) to the match-case (λ=0.1 yr^{-1} and $t_{1/2}$=6.93 yr) at 54 years from the time of the initial TCE release by manipulation of the other parameters as explained above.

The centerline, transverse, and vertical plots were made again using the data at 34 years without further parameter adjustments. The centerline plot, Figure 4.1.53, shows

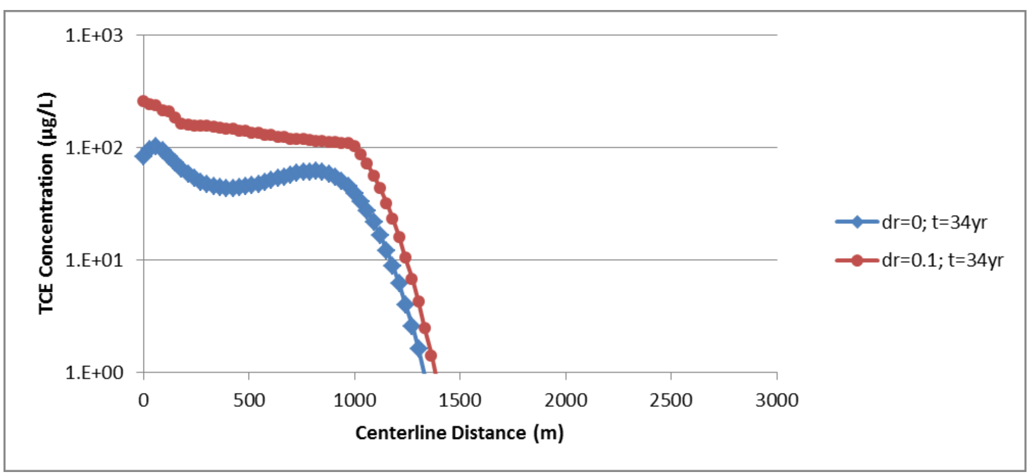
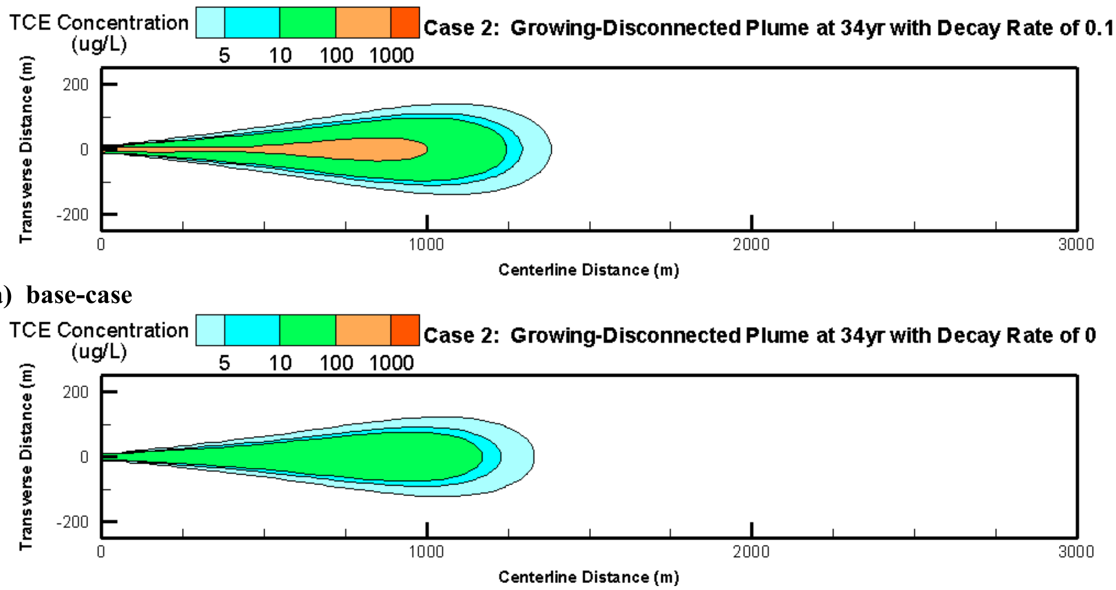


Figure 4.1.53: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 34yr

that the overall TCE concentration for the base-case curve at 34 years is higher than that of the match-case curve. This centerline plot was ranked #13 of 13, most likely due to the great difference in the curves' geometries. Lowering M_0 and C_0 in the 34-year comparison could result in increased similarity for the 34-year pair. Certainly some changes in α_L would be necessary to smooth the jagged turns of the base-case curve to more closely resemble the sinuous line of the match-case curve. These changes in parameter value, though, would upset the 54-year match.

Transverse and vertical plots were created for the 34-year as shown in Figures 4.1.54a & b and Figures 4.1.55a & b respectively. The transverse plots (ranked #5 of 13) show that the 34-year base-case plume is slightly more expansive than the 34-year match-case plume and has a higher set of TCE concentration contours within it. The vertical plots were ranked #1 of 13 in the 34/40-year vertical plot chart and show that the base-case plume is slightly more vertically expansive than the match-case plume with a higher set of TCE concentration contours throughout.

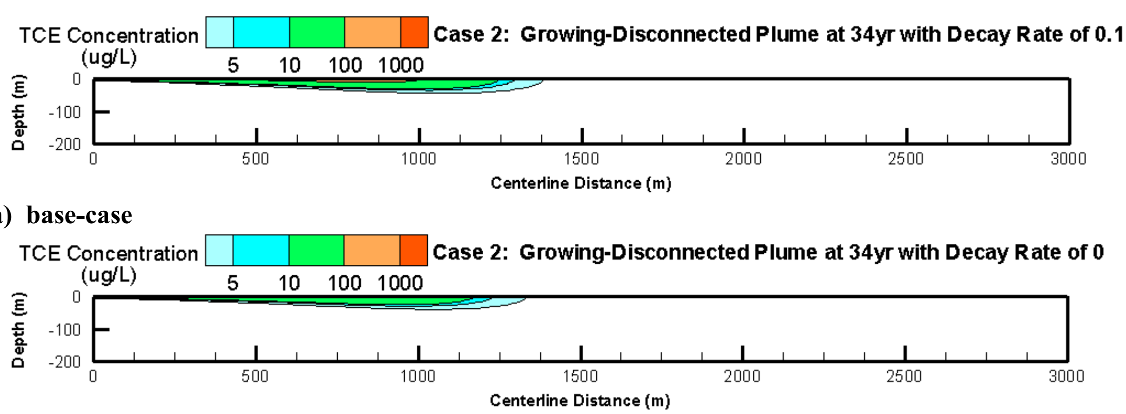
The comparisons of the base-case to match-case plots at 34 years show again that time is the controlling variable in matching the plumes at multiple points in a plume's history.



(a) base-case

(b) match-case

Figures 4.1.54a & b: Transverse plot pair at 34yr with base-case decay rate of 0.1 and match-case decay rate of 0



(a) base-case

(b) match-case

Figures 4.1.55a & b: Vertical plot pair at 34yr with base-case decay rate of 0.1 and match-case decay rate of 0

Plume decay rate = 0.2 yr^{-1}

corresponding half-life of 3.47 years

Figure 4.1.56 shows the manipulated match along the centerline between base-case and match-case at 54 years where the decay rate is set at 0.2 for the base-case and 0 for the match-case. The match is very good, as shown in the following figures, but not as close as it was for the previous decay rate of 0.1 in this Case. This match was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.10, and required a total of 34 trials to produce the centerline match and its

Case 2: Growing-Disconnected plume with base-case values from Liang [2009] (model pair 10)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.2	0
C_0 (g/L)	0.1	0.00032
M_0 (kg)	324	2.7
V_D (m/yr)	20	22
R	2	2.2
α_L (m)	x/100	x/100
α_T (m)	x/1,000	x/1,428
α_V (m)	x/10,000	x/14,280
φ	0.33	0.33
W (m)	10	10
D (m)	3	3
evaluation at t=54yrs		

Table 4.1.10: Comparison of base-case and final match-case parameter values (model pair 10)

corresponding transverse match. C_0 was reduced from 0.1 to 0.00032 g/L and M_0 was reduced from 324 to 2.7 kg in order to move the match-case curve to an overall lower concentration. The proportionality in the source concentration equation, Equation 4.1, allows for C_0 to be lowered in this manner in order to create the model matches. This was explained earlier with the example shown in Figure 4.1.7. V_D was increased from 20 to 22 m/yr and R was increased from 2 to 2.2 in order to control the length of the match-case curve along the X-axis and to force it to better fit that of the base-case curve. The geometry of the curves was already very similar, so the α_L value was kept the same (x/100) for the match-case curve as it was for the base-case curve.

This matched model pair has decent similarity (ranked #4 of 13) between the match-case and base-case curves as shown in Figure 4.1.56. The overall effect of the

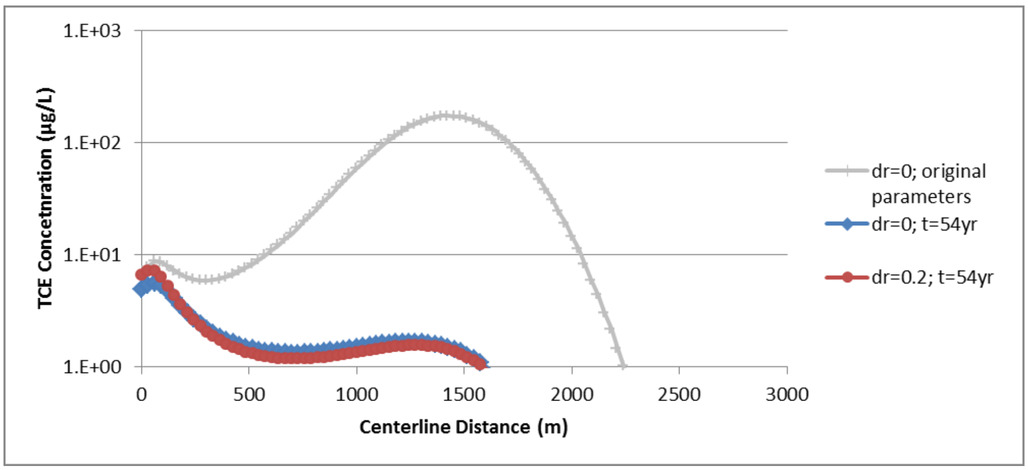
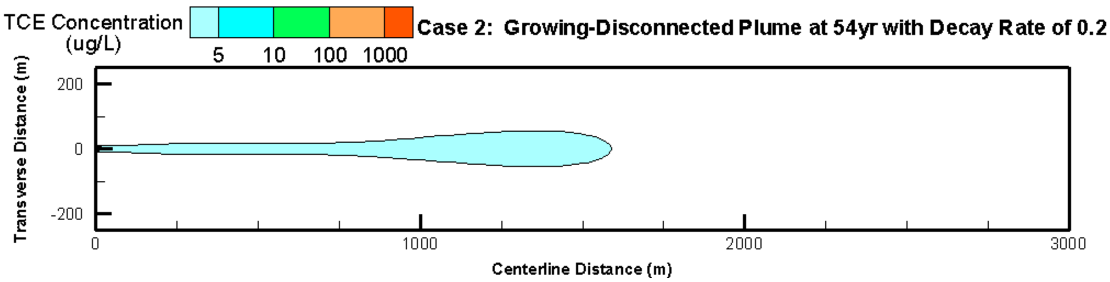


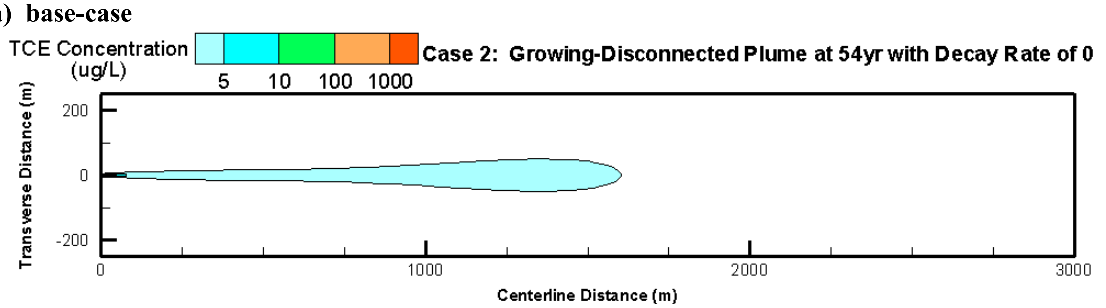
Figure 4.1.56: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 54yr

parameter manipulations was to move the match-case curve down the chart along the concentration axis and to shorten it in the X-direction to fit the length of the base-case curve.

The transverse plot comparison was created by decreasing the value of α_T from x/1,000 to x/1,428 and plotting the resulting data in the X-Y spatial plane. The value of α_V was decreased in proportion with α_T from x/10,000 to x/14,280. Figures 4.1.57a & b shows the transverse contour plot depiction of the base- and match-case at 54 years, which was ranked #7 of 13. This match, much like the centerline match for this model pair, was only a little off in similarity.



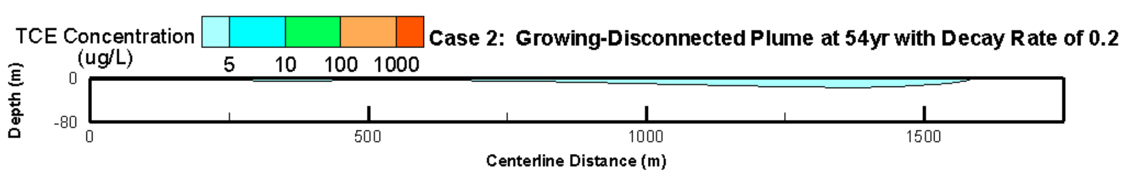
(a) base-case



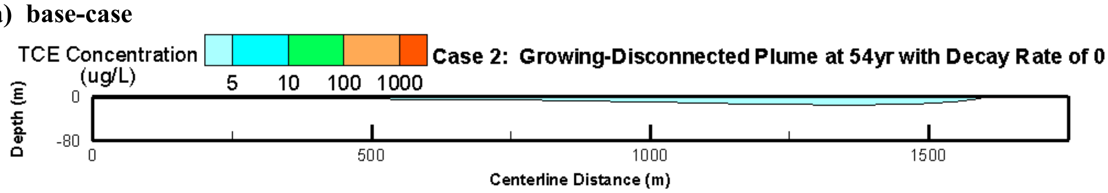
(b) match-case

Figures 4.1.57a & b: Transverse plot pair at 54yr with base-case decay rate of 0.2 and match-case decay rate of 0

The vertical contour plots show a good deal of similarity in their plumes' expanses and concentration, as is shown in Figures 4.1.58a & b (ranked #4 of 13). The similarity in the centerline and X-Y plots and the serendipitous match in the X-Z plot show that it is possible to match the base-case (λ=0) to the match-case (λ=0.2 yr^{-1} and $t_{1/2}$=3.47 yr) at 54 years from the time of the initial TCE release by manipulation of the other parameters as explained above. Of course, there is no way to know the actual mass



(a) base-case



(b) match-case

Figures 4.1.58a & b: Vertical plot pair at 54yr with base-case decay rate of 0.2 and match-case decay rate of 0

and concentration of the initial TCE release, and using this matching method there are many combinations of these values that could produce the desired model matches.

The centerline, transverse, and vertical plots were made again using the 34-year data with no additional manipulations. The centerline plot, Figure 4.1.59, shows that the

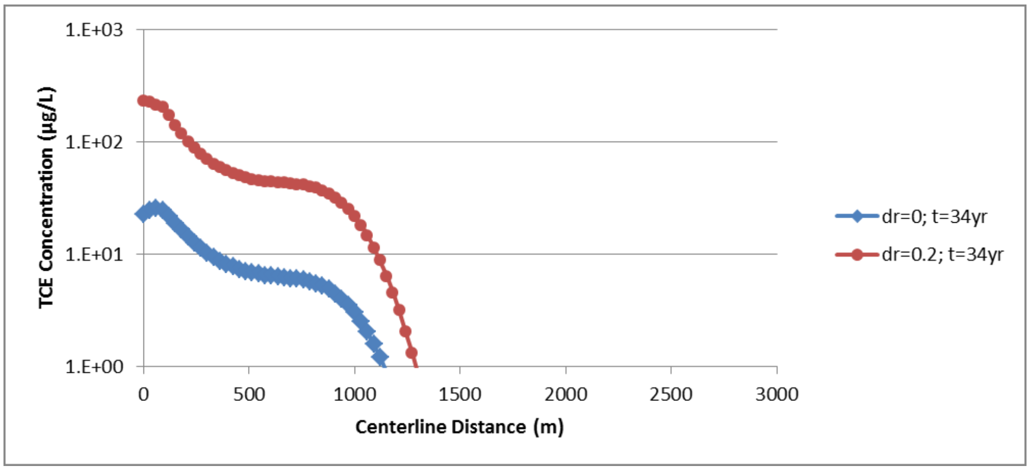
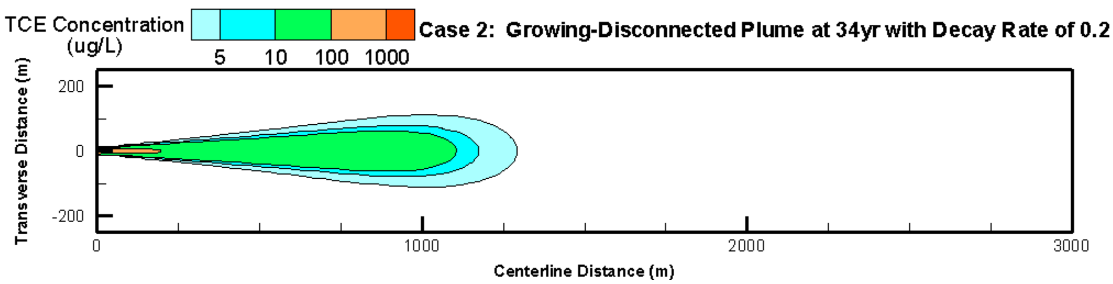


Figure 4.1.59: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 34yr

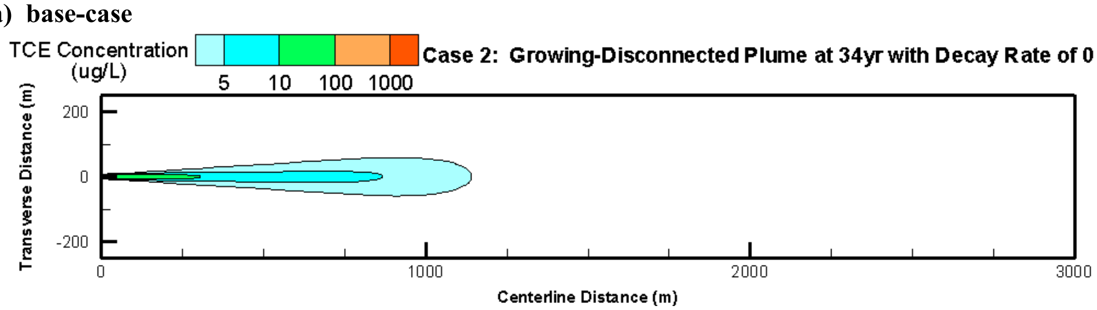
overall TCE concentration for the base-case curve at 34 years is higher than that of the match-case curve at 34 years and resulted in a ranking of #8 of 13. The geometry and length of the two curves at 34 years is similar, but if a match for this model pair were desired at 34 years, additional manipulation of parameters would be necessary.

Transverse and vertical plots are shown in Figures 4.1.60a & b and Figures 4.1.61a & b respectively. The transverse plots, ranked at #10 of 13, show that the 34-year base-case plume is a good deal more expansive than that of the match-case and has a higher set of TCE concentrations. The vertical plots show that the base-case plume is a good deal more vertically expansive than is the match-case plume and has a higher set of TCE concentration contours and was assigned a rank of #3 of 13 at 34/40 years.

While this Case does not result in perfect matches between model pairs, it reiterates the findings of the previous Cases that it is possible to create a match between a base-case with a greater than zero decay rate and a match-case with a plume decay rate of zero. The matches were more difficult to make for the greater of the two decay rates, and time played a major role in the lack of similarity between the plumes at different points in their histories.

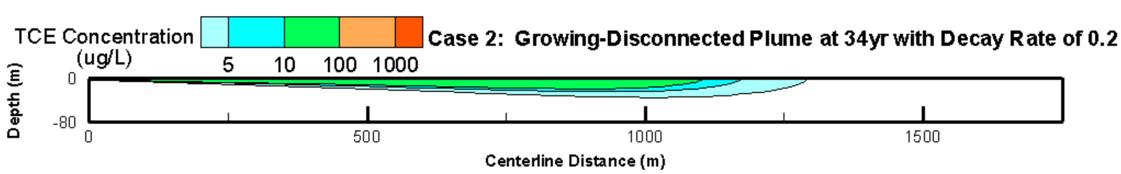


(a) base-case

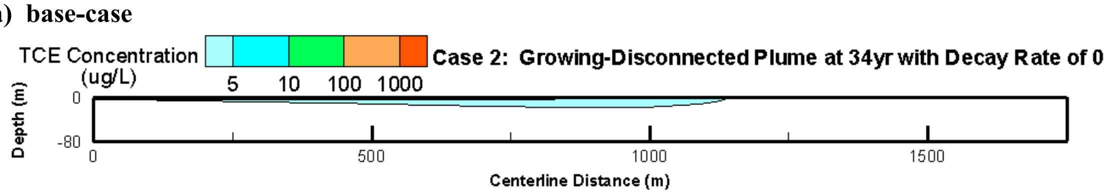


(b) match-case

Figures 4.1.60a & b: Transverse plot pair at 34yr with base-case decay rate of 0.2 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.61a & b: Vertical plot pair at 34yr with base-case decay rate of 0.2 and match-case decay rate of 0

Case 3: Growing-connected plume with parameter values from Liang [2009]

In this Case another type of plume behavior is studied: a growing plume, connected to its TCE source with the contaminant mass partially in the source zone and partially in the plume [Liang, 2009]. Three different plume decay rates were studied in the trials for this Case to determine if their resultant plots could be matched to plots made with plume decay rates of zero by manipulation of certain other parameter values. The parameters for this scenario were taken from a case study in Liang [2009] and are shown in Table 4.1.11 through 4.1.13 in this section. For each of the three model pairs in this Case, the original TCE concentration (C_0) is 0.1 g/L, the original TCE mass (M_0) is 1,620 kg, the Darcy velocity (V_D) is 10 m/yr, the retardation factor (R) is 2.0, the longitudinal dispersivity (α_L) is approximated as x/200, the transverse dispersivity (α_T) is approximated as x/1,000, the vertical dispersivity (α_V) is approximated as x/10,000, porosity of the matrix (φ) is assigned a value of 0.33, the source width (W) is 10 m, and the source depth (D) is 3 m [Liang, 2009]. Comparatively, this set of base-case parameters is also similar to that utilized in Case 1 since the only parameters that vary from the Case 1 set are M_0 (1000 kg in Case 1), V_D (30 m/yr in Case 1), α_L (x/100 in Case 1), and φ (0.3 in Case 1).

The plume decay rates used for the model pairs in this Case are respectively 0.1, 0.2, and 0.3 (in units of yr^{-1}), with half-lives of 6.93, 3.47, and 2.31 years respectively, and cause a significant amount of degradation of the TCE in the plume when compared with the rates from the literature review shown in Table 1.1.1. The models were matched at 60 years from time of initial contaminant release. The 40-year data were then plotted to create corresponding plots of the plumes at 40 years from initial TCE release. A total of six each of centerline plots, transverse plots and vertical plots were compared for visual similarity.

Plume decay rate = 0.1 yr^{-1}

corresponding half-life of 6.93 years

The chart shown in Figure 4.1.62 describes the match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.1 for the base-case and 0 for the match-case. The match for this pair was close but not perfect, as shown in the following figures, since the match-case curve is more sinuous than the base-case curve. This match was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.11, and required a total of 25 trials to

Case 3: Growing-Connected plume with base-case values from Liang [2009] (model pair 11)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.1	0
C_0 (g/L)	0.1	0.03
M_0 (kg)	1620	5000
V_D (m/yr)	10	11.3
R	2	2.5
α_L (m)	x/200	x/100
α_T (m)	x/1,000	x/1,000
α_V (m)	x/10,000	x/2,500
φ	0.33	0.33
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.11: Comparison of base-case and final match-case parameter values (model pair 11)

produce the centerline and corresponding transverse matches. The value of C_0 was lowered from 0.1 to 0.03 g/L and the value of M_0 was raised from 1620 to 5000 kg in the match-case to force the match-case curve to emulate the overall TCE concentration of the base-case curve. The model seemed to be rather insensitive to the value of the mass parameter, though, with the match-case centerline curve only creeping up to meet that of the base-case; even when increased to five times its value in the base-case set of parameters. V_D was increased from 10 to 11.3 m/yr and R was increased from 2 to 2.5 in order to force the match-case curve to have the same length in the X-direction as the base-case curve. The geometry of the curves was fairly similar to begin with, but the value of α_L had to be increased from x/200 to x/100 in order to force the match-case curve into the steeper pattern of decline of the base-case curve. This had the added effect of increasing the sinuosity of the match-case curve. The transverse dispersivity value, α_T, for the match-case was kept at the same value (x/1,000) as it was in the base-case since the width of the plume in the Y-direction when plotted in the X-Y plane was the same as that of the base-case (Figures 4.1.63a & b). Usually the vertical dispersivity value is an order of magnitude smaller than that of the transverse dispersivity, but in this match α_V had to be adjusted up from x/10,000 to x/2,500 in order to force the centerline plot and transverse plume plot matches. This increase in α_V caused the match-case plume in the vertical plots to be significantly greater in vertical expanse than was the base-case plume, as is shown in Figures 4.1.64a & b.

This matched model pair has a decent amount of similarity between the base- and match-case curves as shown in Figure 4.1.62, which was ranked #6 of 13. The overall effect of the parameter manipulations was to move the match-case curve down the chart along the concentration axis and to shorten it in the X-direction to fit the length of the base-case curve.

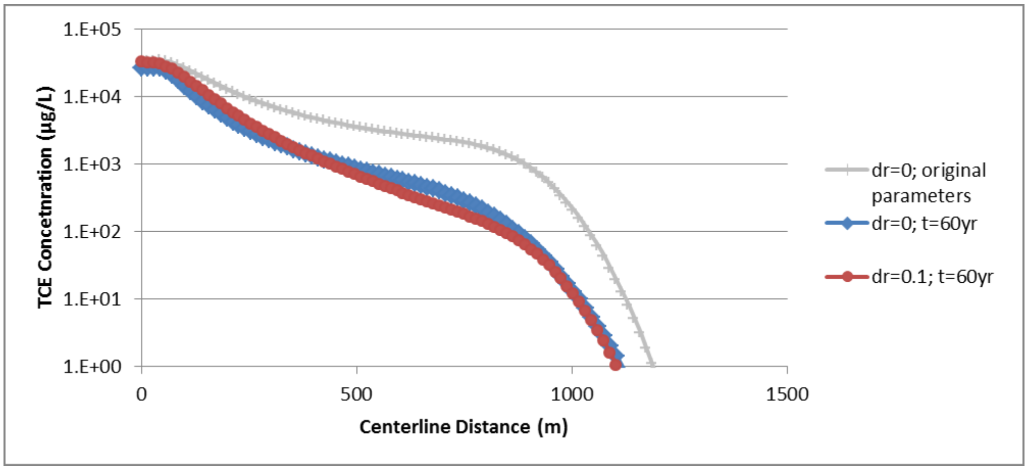
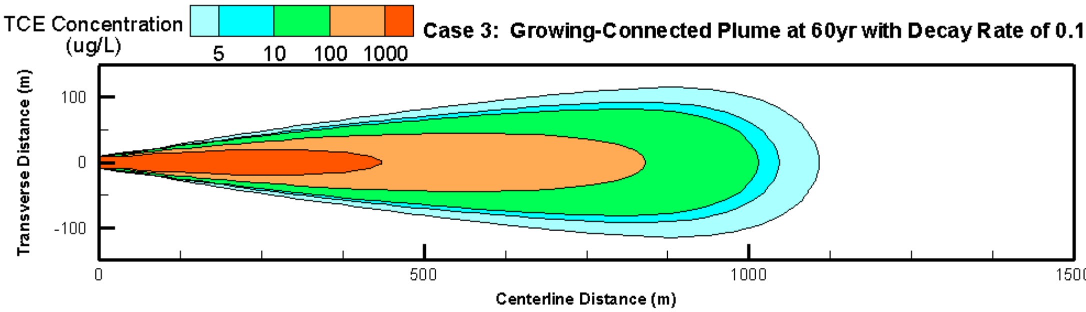


Figure 4.1.62: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 60yr

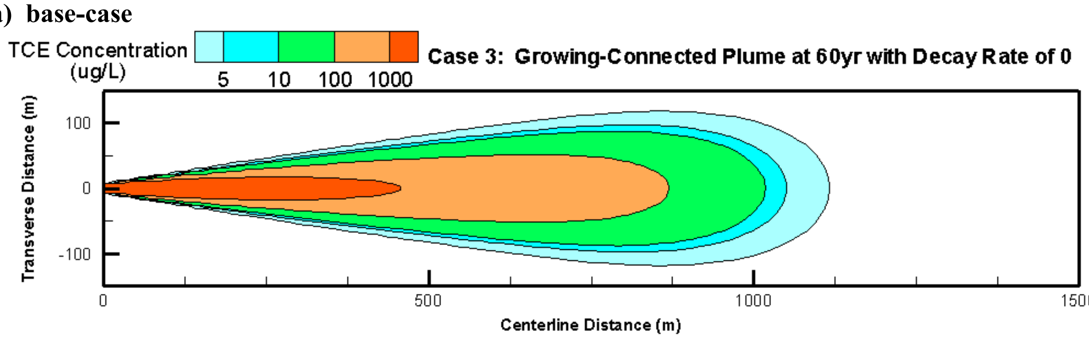
Figures 4.1.63 shows the transverse contour plot depiction of the base- and match-case plumes at 60 years. This match, much like the centerline match for this particular pair, was very close with only very minimal differences in contour line placement and was ranked #3 of 13.

Contour plots were made of vertical slices of the plumes along their centerlines with no attempt to force matches in the vertical direction. The previously explained manipulation of the value of α_V ensured that the base- and match-case plumes in the vertical plots did not match as shown in Figures 4.1.64a & b (ranked #12 of 13).

The reasonably good match in both the centerline and X-Y plots shows that it is possible to match the base-case (λ=0) to the match-case (λ=0.1 yr^{-1} and $t_{1/2}$=6.93 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above. The X-Z plots, though, display a marked difference in vertical extent due to the large increase in α_V, as explained above, that was necessary to force the centerline and transverse plot matches.

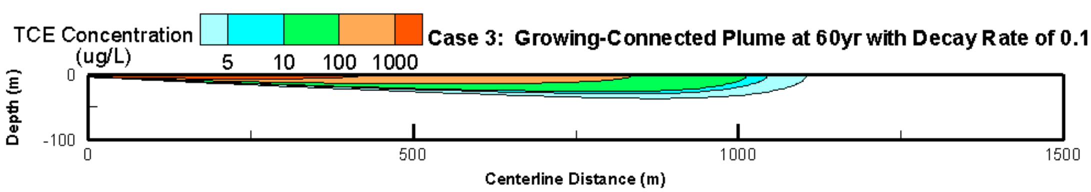


(a) base-case

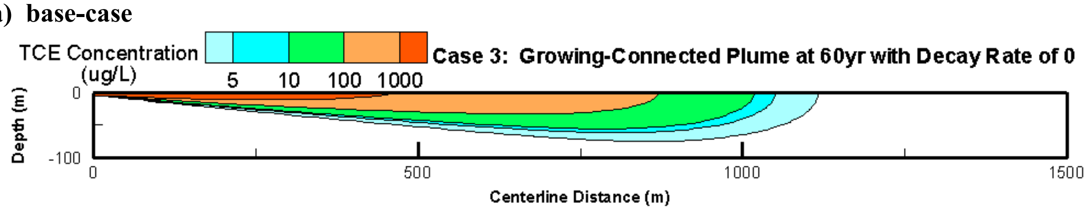


(b) match-case

Figures 4.1.63a & b: Transverse plot pair at 60yr with base-case decay rate of 0.1 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.64a & b: Vertical plot pair at 60yr with base-case decay rate of 0.1 and match-case decay rate of 0

The centerline, transverse, and vertical plots were made again with 40-year data to check for a match. The centerline plot, Figure 4.1.65, shows that the overall TCE

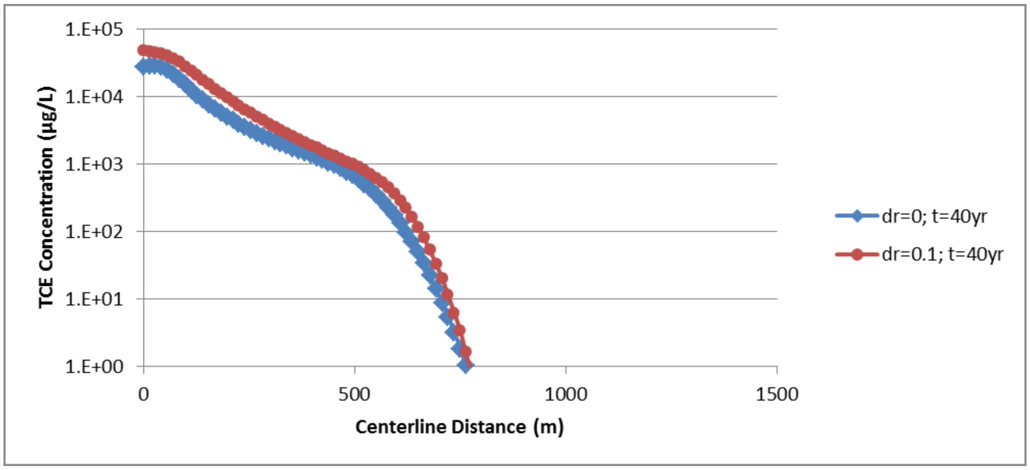
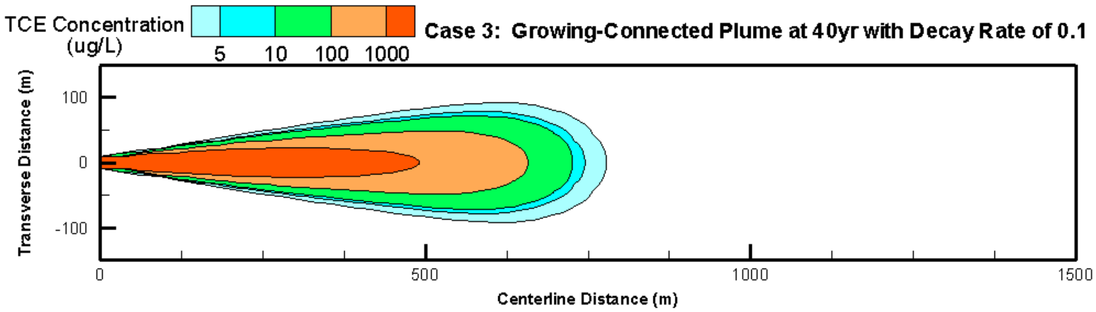


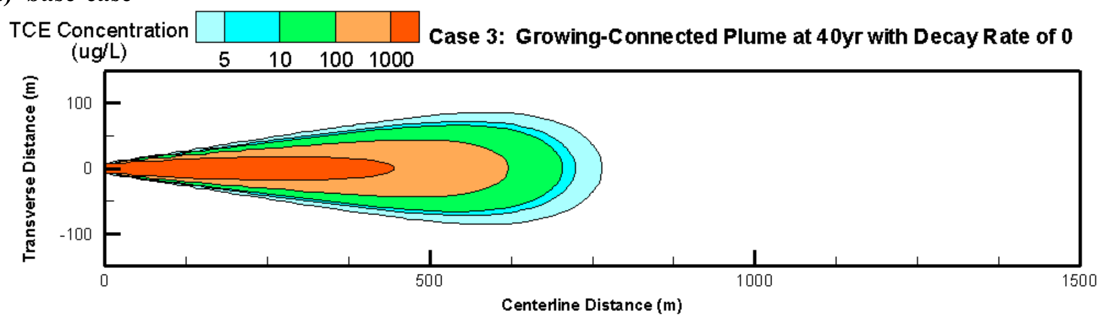
Figure 4.1.65: Centerline plot for base-case (dr=0.1) and match-case (dr=0) at 40yr

concentration for the base-case curve at 40 years is only a little higher than that of the match-case curve at 40 years, and was ranked #4 of 13. The geometry of the curves is quite similar, though, and this might represent the best similarity between base- and match-case curves at 40 years in the whole project.

Transverse and vertical plots are shown in Figures 4.1.66a & b and Figures 4.1.67a & b respectively. The transverse plots (ranked #1 of 13) show that the 40-year base-case plume is only very slightly greater in expanse than the 40-year match-case plume and the concentration contour lines for the base-case plume at 40 years is only slightly different from those of the match-case plume at 40 years. The vertical plots show that the match-case plume is more expansive than the base-case plume, which resulted in a rank of #4 of 13 for this comparison. The comparisons of the base-case to match case in the 40-year plots show that time is an important variable that effects how well the models match.

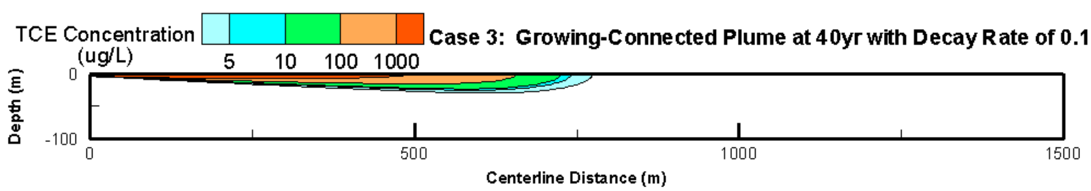


(a) base-case

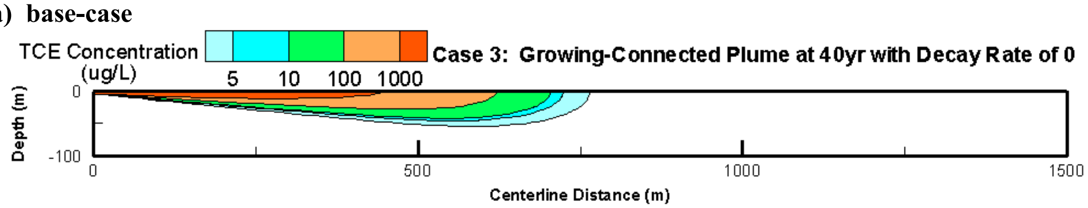


(b) match-case

Figures 4.1.66a & b: Transverse plot pair at 40yr with base-case decay rate of 0.1 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.67a & b: Vertical plot pair at 40yr with base-case decay rate of 0.1 and match-case decay rate of 0

Plume decay rate = 0.2 yr^{-1}

corresponding half-life of 3.47 years

Figure 4.1.68 shows the match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.2 for the base-case and 0 for the match-case. The match was not as close for this model pair as it was in the previous pair at the decay rate of 0.1, and its goodness of fit decreases as the curves diverge between TCE concentrations of 10 and 1,000 μg/L. This match was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.12, and required

Case 3: Growing-Connected plume with base-case values from Liang [2009] (model pair 12)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.2	0
C_0 (g/L)	0.1	0.03
M_0 (kg)	1620	5000
V_D (m/yr)	10	10.1
R	2	3.8
α_L (m)	x/200	x/10
α_T (m)	x/1,000	x/1,000
α_V (m)	x/10,000	x/1,000
φ	0.33	0.33
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.12: Comparison of base-case and final match-case parameter values (model pair 12)

a total of 20 trials to produce the centerline match and its corresponding transverse match. The value of C_0 was lowered from 0.1 to 0.03 g/L and the value of M_0 was raised from 1,620 to 5,000 kg in the match-case to force the match-case curve to fit the overall lower TCE concentration of the base-case curve. V_D was increased from 10 to 10.1 m/yr and R was increased from 2 to 3.8 in order to force the match-case curve to have the same length in the X-direction as the base-case curve. The geometry of the curves was not similar at the outset and the value of α_L had to be increased from x/200 to x/10 in order to force the match-case curve into the same steeply declining behavior as the base-case curve. This change in α_L could not cause the coincidence of the two curves' patterns of sinuosity. The transverse dispersivity value, α_T, for the match-case was kept at the same value (x/1,000) as it was in the base-case since the width of the plume in the Y-direction when plotted in the X-Y spatial plane was the same as that of the base-case (Figures 4.1.69a & b). Usually the vertical dispersivity value is an order of magnitude smaller than that of the transverse dispersivity, but in this match α_V had to be adjusted up from x/10,000 to x/1,000 (the same value as α_T) in order to force the centerline plot and transverse plume plot matches. This increase in α_V caused the match-case plume in the vertical plots to be significantly greater in vertical expanse than the base-case plume, as is shown in Figures 4.1.70a & b.

This matched model pair, ranked #7 of 13, has a fair degree of similarity between the base- and match-case curves as shown in Figure 4.1.68. The overall effect of the

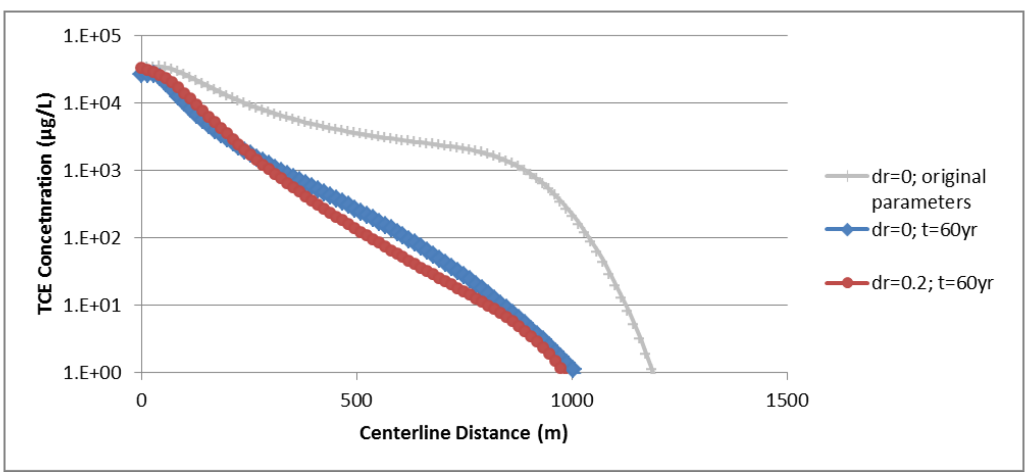
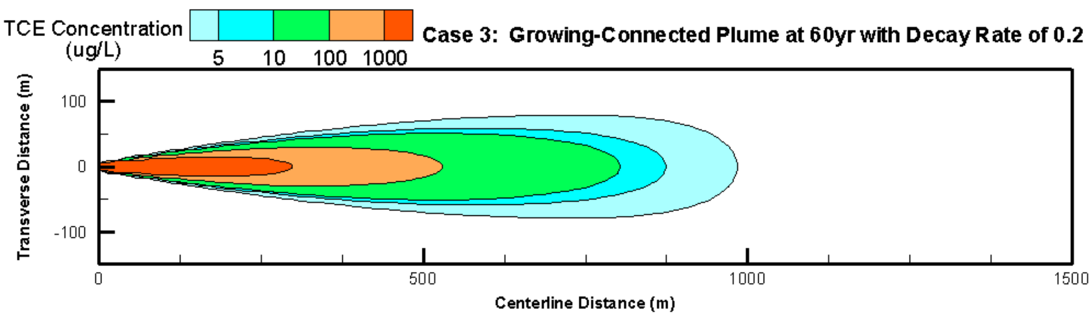


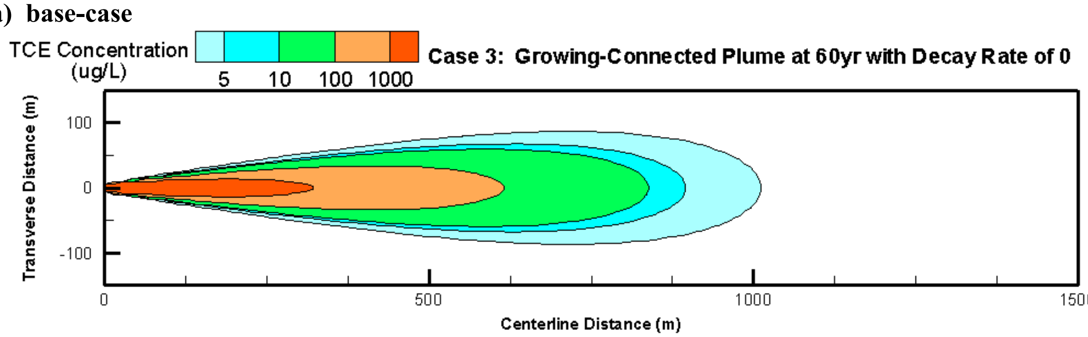
Figure 4.1.68: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 60yr

parameter manipulations was to move the match-case curve down the chart along the concentration axis, to shorten it to the same length in the X-direction as the base-case curve, and to steepen it to match the faster rate of decline of the base-case curve.

Figures 4.1.69a & b (ranked #8 of 13) show the transverse contour plot depiction of the base- and match-case plume at 60 years. This match, much like the centerline match for this particular pair, is close overall with slight differences in shape and size.



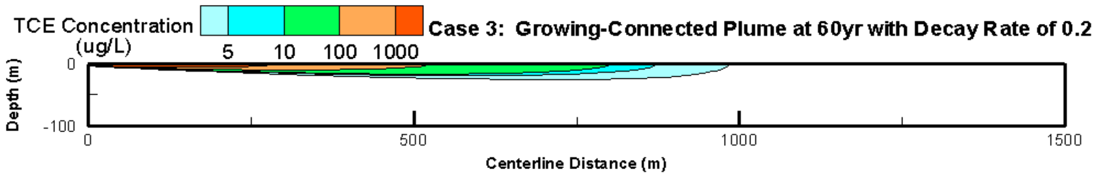
(a) base-case



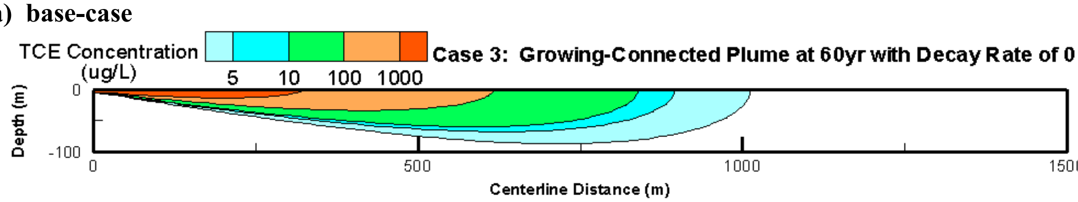
(b) match-case

Figures 4.1.69a & b: Transverse plot pair at 60yr with base-case decay rate of 0.2 and match-case decay rate of 0

Contour plots were made of vertical slices of the plumes along their centerlines with no attempt made to force them to match. The previously explained manipulation of the value of α_V ensures that the base- and match-case plumes in the vertical plots do not match as shown in Figures 4.1.70a & b, and this comparison was ranked #11 of 13.



(a) base-case



(b) match-case

Figures 4.1.70a & b: Vertical plot pair at 60yr with base-case decay rate of 0.2 and match-case decay rate of 0

The centerline and X-Y plots show that it is possible, though challenging, to match the base-case (λ=0) to the match-case (λ=0.2 yr^{-1} and $t_{1/2}$=3.47 yr) at 60 years from the time of the initial TCE release by manipulation of the other parameters as explained above. The X-Z plots emphasize the difficulty encountered in forcing this match by displaying a definite difference in vertical extent due to the atypically high value of α_V that was necessary to force the centerline and transverse plot matches.

All the plots were made again using the 40-year data for each of the plumes. The centerline plot, Figure 4.1.71, shows that the overall TCE concentration for the base-case curve at 40 years is a little higher than that of the match-case curve at 40 years, which resulted in a rank of #5 of 13. The geometry of the curves is similar between the X-axis values of 0 and approximately 500 meters, but after that the base-case curve turns away from the match-case curve for a bit.

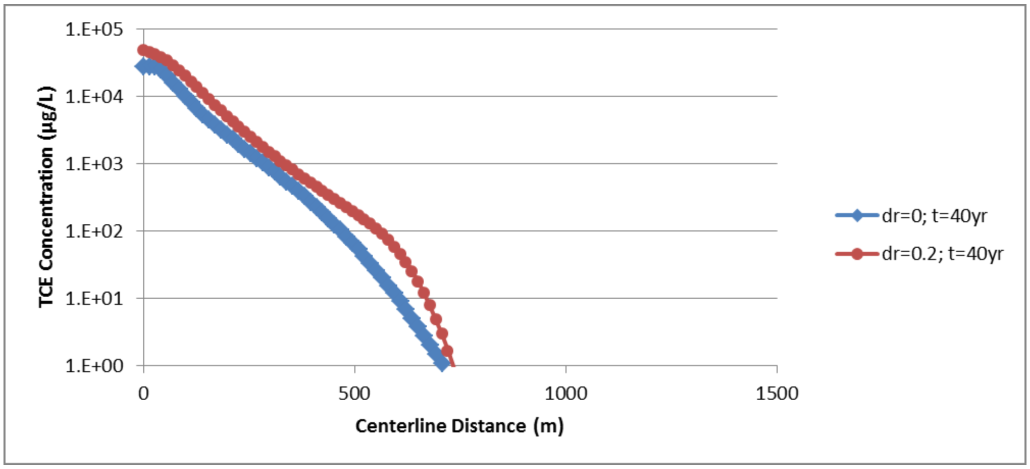
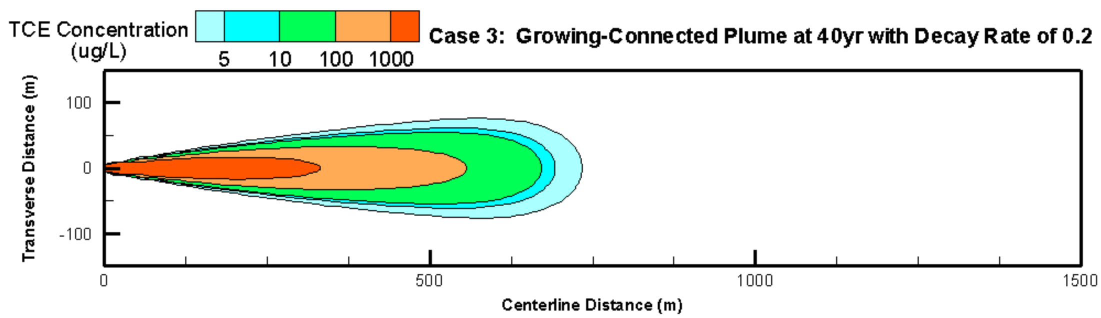


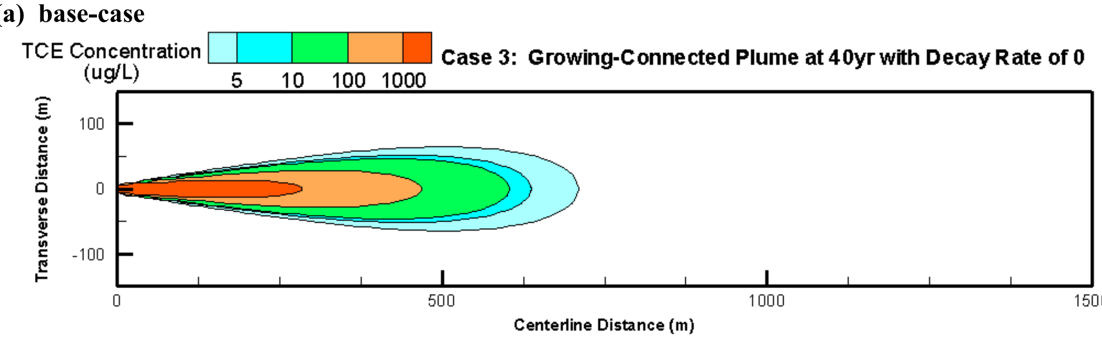
Figure 4.1.71: Centerline plot for base-case (dr=0.2) and match-case (dr=0) at 40yr

Transverse and vertical plots are shown in Figures 4.1.72a & b and Figures 4.1.73a & b respectively. The transverse plots show that the 40-year base-case plume is only slightly greater in expanse than the 40-year match-case plume and the concentration contour lines for the base-case plume at 40 years is only slightly different from those of the match-case plume at 40 years. This plot comparison was ranked #2 of 13 at 40 years. The main difference between the pair of plumes as plotted in Figures 4.1.72a & b is that the base-case plume's shape is more oblate than the match-case plume's narrower shape. The vertical plots show that the match-case plume is much greater in expanse than the base-case plume, and there are differences in the placement of the TCE concentration contour lines between the pair at 40 years as well.

The comparisons of the base-case to match-case centerline and X-Y plots at 40 years show that a match does not exist between the base- and match-case at 40 years without performing additional parameter manipulations. It should be noted, though, that the centerline match and transverse plots for this model pair at 40 years show more similarity between the base- and match-case than have any of the previous trials in any of the previous scenarios. The X-Z plots at 40 years (ranked #5 of 13) suffer from the same disparity caused by the high α_V value as the X-Z plots at 60 years. Time again prevents the 40-year match without further manipulation of the parameters.

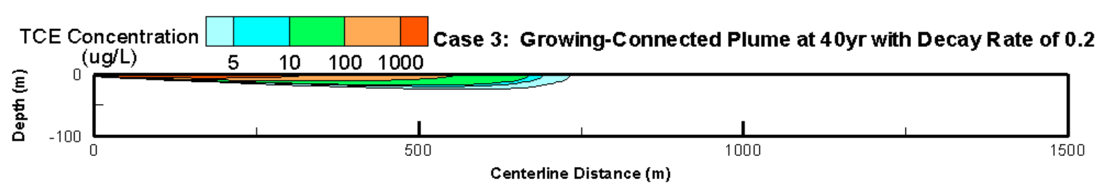


(a) base-case

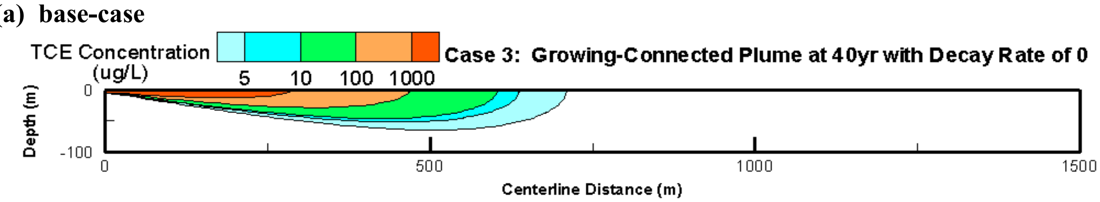


(b) match-case

Figures 4.1.72a & b: Transverse plot pair at 40yr with base-case decay rate of 0.2 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.73a & b: Vertical plot pair at 40yr with base-case decay rate of 0.2 and match-case decay rate of 0

Plume decay rate = 0.3 yr^{-1}

corresponding half-life of 2.31 years

The chart shown in Figure 4.1.74 displays the match along the centerline between base-case and match-case at 60 years where the decay rate is set at 0.3 for the base-case and 0 for the match-case. This pairing did not match well beyond 100 meters along the X-axis, after which the curves are geometric opposites. This match was developed by a series of parameter adjustments in the match-case, the result of which is shown in Table 4.1.13, and required a total of 16 trials to produce the centerline match and its

Case 3: Growing-Connected plume with base-case values from Liang [2009] (model pair 13)		
Parameter	**Base-case**	**Match-case**
λ (1/yr)	0.3	0
C_0 (g/L)	0.1	0.03
M_0 (kg)	1620	5000
V_D (m/yr)	10	8.2
R	2	3.8
α_L (m)	x/200	x/10
α_T (m)	x/1,000	x/1,515
α_V (m)	x/10,000	x/1,250
φ	0.33	0.33
W (m)	10	10
D (m)	3	3
evaluation at t=60yrs		

Table 4.1.13: Comparison of base-case and final match-case parameter values (model pair 13)

corresponding transverse match. The value of C_0 was decreased from 0.1 to 0.03 g/L and the value of M_0 was raised from 1620 to 5000 kg in the match-case to force the match-case curve to fit the overall lower TCE concentration of the base-case curve. V_D was decreased from 10 to 8.2 m/yr and R was increased from 2 to 3.8 in order to force the match-case curve to have the same length in the X-direction as the base-case curve. The geometry of the curves was not similar to begin with and the value of α_L had to be increased from x/200 to x/10 in an attempt to force the match-case curve into the same steeply declining behavior as the base-case curve. This change in α_L could not cause the coincidence of the two curves' geometries. The transverse dispersivity value, α_T, for the match-case was decreased from x/1,000 to x/1,515 in order to decrease the Y-direction-width of the match-case plume to coincide with that of the narrower base-case plume as shown in Figures 4.1.75a & b. Usually the vertical dispersivity value is an order of magnitude smaller than that of the transverse dispersivity, but in this match α_V had to be increased beyond the usual range of values from x/10,000 to x/1,250, which is greater than that of α_T in order to force the centerline plot and transverse plume plot matches. This increase in α_V caused the match-case plume in the vertical plots to be much greater in vertical expanse than was the base-case plume, as is shown in Figures 4.1.76a & b.

This matched model pair does not have a great degree of similarity between the base-case and match-case curves as shown in Figure 4.1.74 and was ranked #13 of 13.

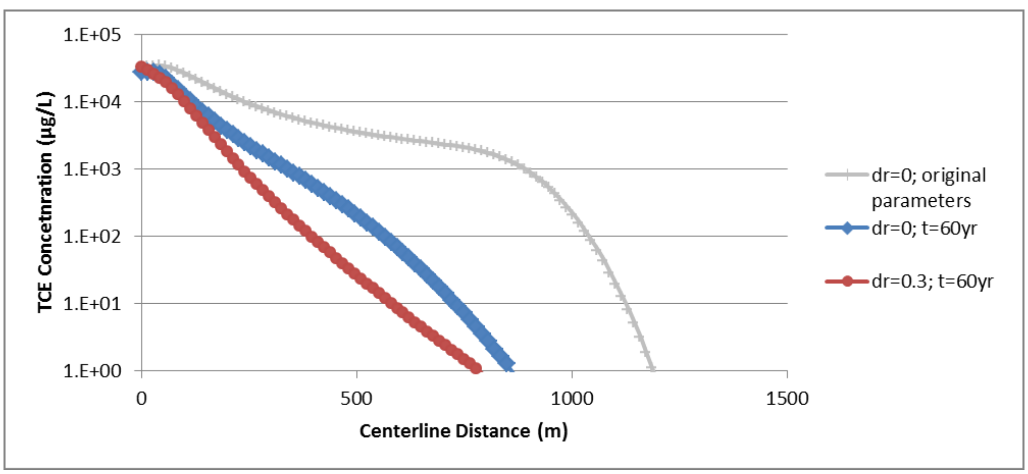
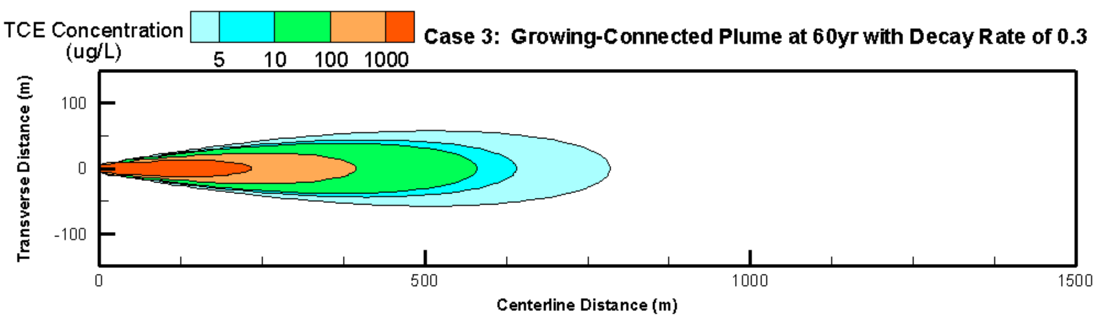


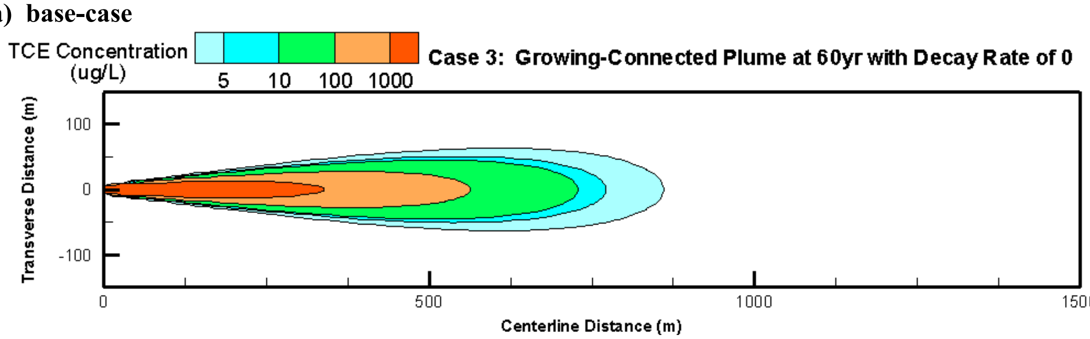
Figure 4.1.74: Centerline plot for base-case (dr=0.3) and match-case (dr=0) at 60yr

The overall effect of the parameter manipulations was to move the match-case curve down the chart along the concentration axis, to shorten it in the X-direction to try to match the base-case curve's length, and to steepen it to try to match the faster rate of decline of the base-case curve. Even after applying these parameter manipulations, a good match could not be accomplished for the centerline comparison for this model pair.

The transverse plume plot was created by adjusting the value of α_T and plotting the resulting data in the X-Y spatial plane. Figures 4.1.75a & b show the transverse contour plot comparison of the base- and match-case plumes at 60 years, which was also ranked #13 of 13. This match, like the centerline pairing, is off a bit and the match-case plume is more expansive than the base-case plume with contour lines that might match if only the match-case plume were not so long in the X-direction. As in the last scenario, a really good match could not be accomplished for the transverse plots for this model pair at the plume decay rate of 0.3 (yr^{-1}).



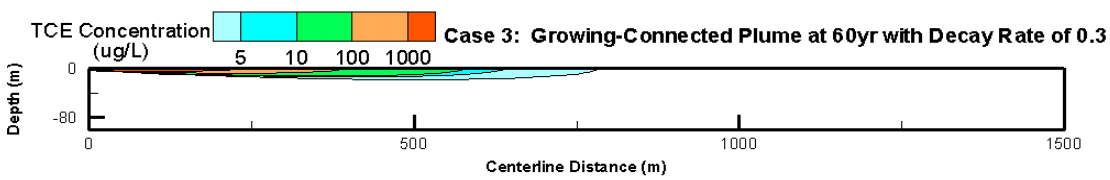
(a) base-case



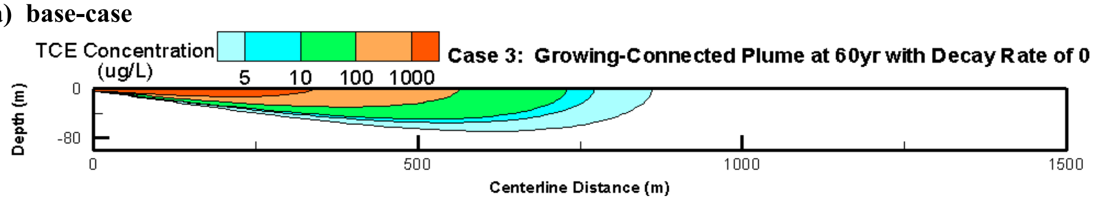
(b) match-case

Figures 4.1.75a & b: Transverse plot pair at 60yr with base-case decay rate of 0.3 and match-case decay rate at 0

Contour plots were made of vertical slices of the plumes along their centerlines with no intention of forcing a match. The previously explained high value of α_V caused the extreme variance between the vertical expanses of the base-case and match-case plumes as shown in Figures 4.1.76a & b, and this comparison was ranked #13 of 13. Logic suggests that for such high vertical dispersion to occur in a plume, such as in the match-case plume shown in Figure 4.1.76b, there would have to exist at the site some geological structure or anthropological disturbance that would allow for such extreme vertical migration of the contaminant.



(a) base-case



(b) match-case

Figures 4.1.76a & b: Vertical plot pair at 60yr with base-case decay rate of 0.3 and match-case decay rate of 0

The relatively poor match in the centerline and X-Y plots serves to show that it is difficult to create a perfect match for this scenario by parameter manipulation. The X-Z plots emphasize the difficulty encountered in forcing this match by displaying a definite variance in vertical extent between the base- and match-case plumes due to the high value of α_V that was necessary to force the centerline and transverse plot matches.

The centerline, transverse, and vertical plots were made again using 40-year data. The centerline plot, Figure 4.1.77, which was ranked #3 of 13, shows that the unassisted match at 40 years is actually closer than the manipulated match at 60 years.

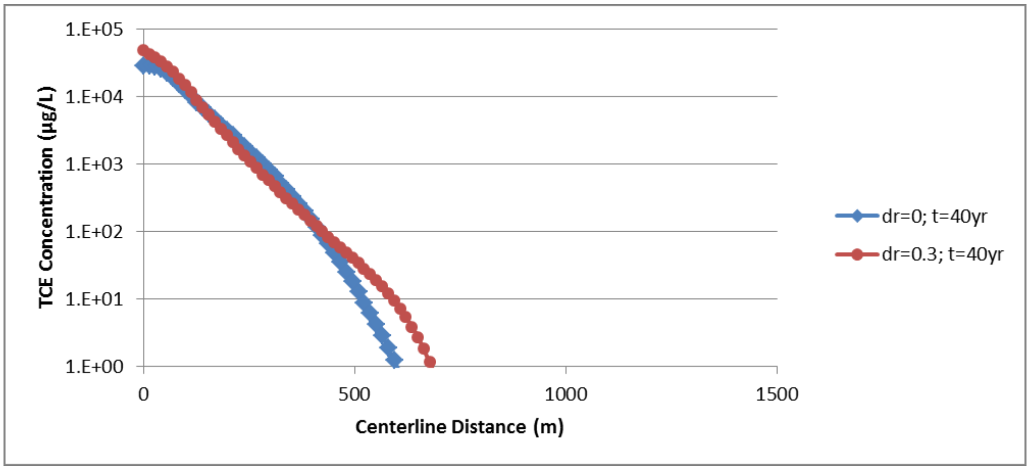
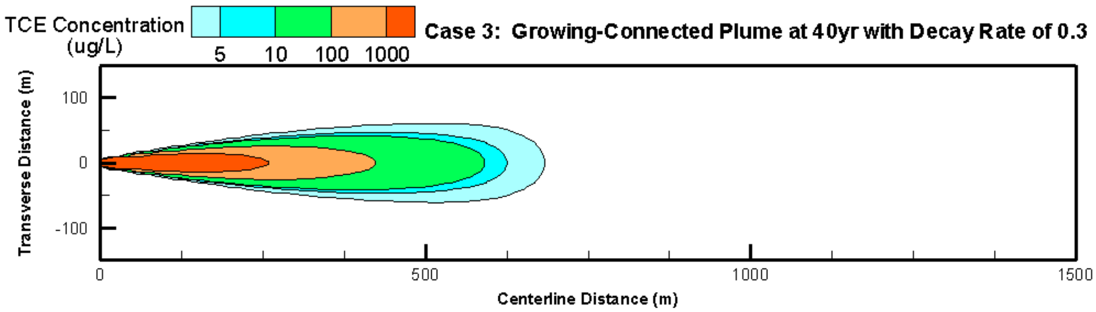
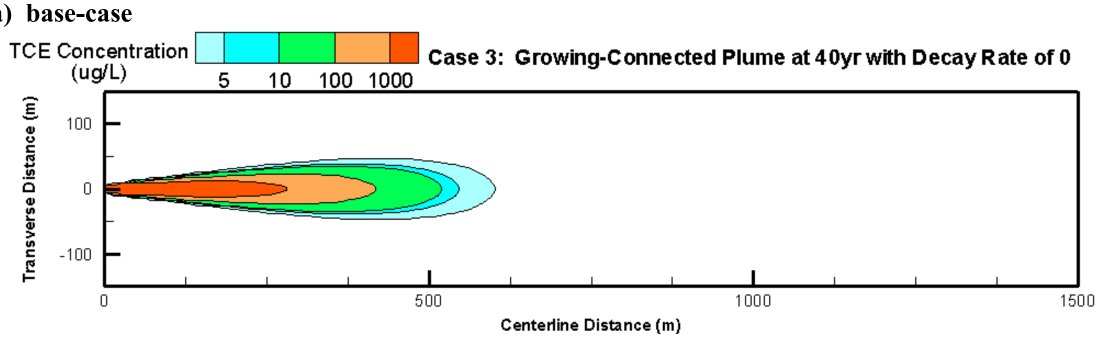


Figure 4.1.77: Centerline plot for base-case (dr=0.3) and match-case (dr=0) at 40yr

Transverse and vertical plots were produced to show the 40-year plumes in the X-Y and X-Z spatial planes, Figures 4.1.78a & b and Figures 4.1.79a & b respectively. The transverse plots were ranked #3 of 13 and show that the 40-year base-case plume is greater in expanse than the 40-year match-case plume with slightly longer TCE concentration contours. The main difference between the pair of plumes at 40 years as plotted in Figures 4.1.79a & b is that the base-case plume's shape is more oblate than the match-case plume's more tapered shape. The vertical plots (ranked #7 of 13) show that the match-case plume is much greater in expanse vertically than the base-case plume and there are differences in the placement of the TCE concentration contour lines between the pair at 40 years as well.

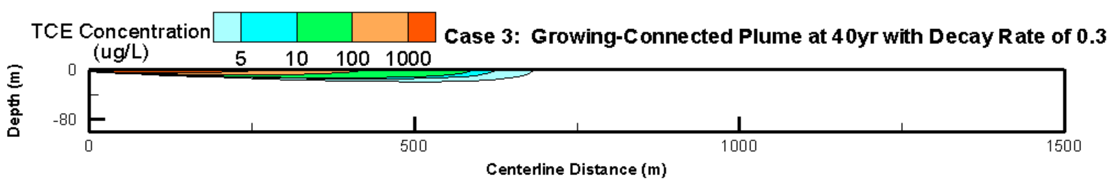


(a) base-case

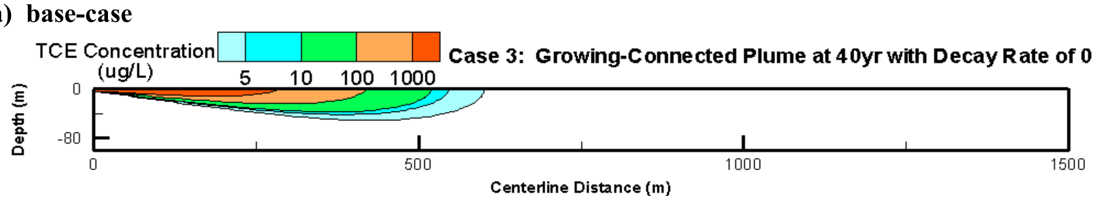


(b) match-case

Figures 4.1.78a & b: Transverse plot pair at 40yr with base-case decay rate of 0.3 and match-case decay rate of 0



(a) base-case



(b) match-case

Figures 4.1.79a & b: Vertical plot pair at 40yr with base-case decay rate of 0.3 and match-case decay rate of 0

The comparisons of the base-case to match-case centerline and X-Y plots at 40 years show that there is no match between the base- and match-case at 40 years without performing additional parameter manipulations. It should be noted, though, that the centerline match for this model pair at 40 years shows more similarity between the base-and match-case than did the match at 60 years. The X-Z plots at 40 years suffer from the same disparity caused by the high α_V value as the X-Z plots at 60 years.

Overall, this Case is in agreement with the previous Cases in that the matches were more difficult to make as the plume decay rates were increased. Time is once again shown to have control over the plume matches at multiple points in the plumes' histories.

4.2 Statistical analysis results

As explained in the Methodology section, the Root Mean Squared error (RMS) method was chosen for its simplicity and for the fact that it only describes average error in the data sets [Anderson & Woessner 1992]. The formula for calculating the root mean squared error (RMS) was reformatted from Anderson & Woessner [1992], was introduced as Equation 3.5, and was modified to work with the log of concentration values. Equation 3.5 was applied to the data sets in multiple steps within the Excel™ worksheets for each matched-model pair. These calculations were performed for all three dimensions (X, Y, and Z) for all of the matched model pairs. The RMS values were divided by the mean of the base-case log of concentration values (per Equation 3.6).

The value resulting from the NRMS is a value between zero and infinity where zero indicates a perfect fit and higher values represent increasing randomness [van Ruijven et al., 2009]. The calculated NRMS value can then be multiplied by 100 to produce a value that expresses the percentage of variance (or deviation) between the base- and match-case for the data set in question [van Ruijven et al., 2009].

The statistical analysis has been broken down in this section by each of the four Cases (1, 1b, 2 and 3) for convenience and clarity. The complete, tabulated results of the statistical analysis are compiled in Tables 4.2.2, 4.2.3, and 4.2.4 in Appendix B. Three sets of ranking charts were created for the centerline, transverse, and vertical plots at each study time (at 60/54 years and at 40/34 years) to help with the visual comparisons of the graphical analysis results. These charts, Tables 4.1.14-16, are located in Appendix C for ease of reference.

Case 1: Stable plume

The statistical analysis for this Case was completed in a series of three sets of calculations for each model pair; X-direction for centerline plots, X-Y spatial plane for transverse plots, and X-Z spatial plane for vertical plots. This analysis is designed to mathematically describe the degree of variance between the base- and match-case in each of the comparison plots for both of the times modeled (60 years and 40 years from initial TCE release).

This scenario is one of a “stable” TCE groundwater plume that is not migrating and that has its contaminant mass partially in the source zone and partially in the plume [Pate, 2010; Liang, 2009]. Six different plume decay rates were chosen for study in this Case: 0.1, 0.2, 0.3, 0.4, 0.5, and 1.0 in units of yr^{-1} with corresponding half-lives of 6.93, 3.47, 2.31, 1.73, 1.39, and 0.69 years respectively. These plume decay rates each were assigned to a base-case to be modeled and compared with a match-case with a plume decay rate of 0 through multiple series of parameter manipulations. The parameters used in each of the base- and match-cases in this scenario can be found in Tables 4.1.1 through 4.1.6 in the Graphical analysis section.

Centerline plot matches (X-direction)

Table 4.2.5, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the centerline comparison plots for the six model pairs that were examined in Case 1.

NRMS Analysis Table (Centerline: X-direction) Case 1: Stable plume with hypothetical base-case parameter values								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
1	0.1	6.93yr	60yr 40yr	0.01 0.42	2.19	0.003 0.19	0.35 19.40	4.1.1 4.1.4
2	0.2	3.47yr	60yr 40yr	0.47 1.21	2.10	0.22 0.58	22.29 57.79	4.1.8 4.1.11
3	0.3	2.31yr	60yr 40yr	1.39 1.91	2.04	0.68 0.94	68.30 93.57	4.1.14 4.1.17
4	0.4	1.73yr	60yr 40yr	1.26 1.68	2.00	0.63 0.84	62.97 84.02	4.1.20 4.1.23
5	0.5	1.39yr	60yr 40yr	0.89 1.71	1.96	0.45 0.87	45.35 87.17	4.1.26 4.1.29
6	1.0	0.69yr	60yr 40yr	0.90 1.77	1.86	0.48 0.95	48.30 95.23	4.1.32 4.1.35

Table 4.2.5: Centerline (X-direction) NRMS results for Case 1

The Model Pair 1 match was created between a match-case with a plume decay rate of 0 and a base-case with a plume decay rate of 0.1 (yr^{-1}) and a half-life of 6.93 years. The match for this model pair along the centerline in the X-direction at 60 years from initial TCE release was visually almost perfect, as shown previously in Figure 4.1.1, which was ranked #1 of 13. When this model pair was plotted without further manipulation of parameter values at 40 years from initial TCE release, the curves no longer matched on the centerline plot because the match-case curve plotted at an overall greater TCE concentration than did the base-case curve, as shown in Figure 4.1.4 (ranked #6 of 13 at 40 years). The results of the statistical analysis for this model pair (that a higher degree of variance exists for the 40-year match than the 60-year match) is in agreement with the findings of the graphical comparison. The final calculated percent of deviation for the Model Pair 1 match at 60 years after initial TCE release is 0.35%

deviation between the base- and match-case centerline curves. The final calculated percent of deviation for the Model Pair 1 match at 40 years after initial TCE release is 19.40% deviation between base- and match-case centerline curves.

The Model Pair 2 match was created between a match-case with a plume decay rate of 0 (yr^{-1}) and a base-case with a plume decay rate of 0.2 (yr^{-1}) and a half-life of 3.47 years. The centerline match for this model pair at 60 years from initial TCE release was not as perfect as was the 60-year match in Model Pair 1, as shown in Figure 4.1.8 (ranked #3 of 13). The centerline plot for Model Pair 2 at 40 years from initial TCE release showed the match-case curve at an overall higher TCE concentration than the base-case curve, as shown in Figure 4.1.11 (ranked #7 of 13 at 40 years), and with the Model Pair 2 curves having less similar geometries between them than had the curves in the centerline plot for Model Pair 1. The statistical analysis results for Model Pair 2 are in agreement with the findings of the graphical analysis. The final calculated percent of deviation between the base- and match-case curves for Model Pair 2 at 60 years after initial TCE release was 22.29%, while the final calculated percent of deviation between the base- and match-case curves for Model Pair 2 at 40 years from initial TCE release was 57.79%. When these values are compared to those calculated for Model Pair 1, it is found that there is a greater percent of deviation between the base- and match-case centerline curves for Model Pair 2 at 60 years (22.29%) than there was for the base- and match-case curves for Model Pair 1 at 60 years (0.35%). The comparison at 40 years after initial TCE release shows the same result with the Model Pair 2 centerline curves having a higher percent of deviation (57.79%) than did the Model Pair 1 centerline curves (19.40%).

The Model Pair 3 match was created between a match-case with plume decay rate of 0 (yr^{-1}) and base-case with a plume decay rate of 0.3 (yr^{-1}) and a half-life of 2.31 years. The centerline match for this model pair at 60 years was not as close as for the previous two model pairs, as shown in Figure 4.1.14 (ranked #11 of 13). The centerline match for Model Pair 3 at 40 years was not close at all, with the match-case curve being at an overall greater TCE concentration than the base-case curve and with both curves having different geometries, as shown in Figure 4.1.17 (ranked #12 of 13 at 40 years). The statistical analysis results for Model Pair 3 are in agreement with the findings of the graphical analysis. The final calculated percent of deviation for the Model Pair 3 centerline curves at 60 years was 68.30% while the percent of deviation for the Model Pair 3 centerline curves at 40 years was 93.57%. Model Pair 3 has a greater amount of variation between its base- and match-cases for both the 60- and 40-year centerline comparisons than did Model Pair 2 or Model Pair 1, which is again in agreement with the graphical analysis.

Model Pair 4 was created with a match-case with a plume decay rate of 0 (yr^{-1}) and a base-case with plume decay rate of 0.4 (yr^{-1}) and a half-life of 1.73 years. The centerline match for Model Pair 4 at 60 years after initial TCE release showed relative similarity between the base- and match-case curves, as shown in Figure 4.1.20 (ranked #10 of 13), but was not as close a match visually as the 60-year centerline plots of Model Pairs 1 and 2. Visually, the centerline match for Model Pair 4 seemed to resemble that of Model Pair 3, but with an overall greater rate of decline in the curves. The centerline match for Model Pair 4 at 40 years after initial TCE release showed that the base- and match-case curves were not similar in concentration or geometry, as shown in Figure 4.1.23 (ranked #11 of 13 at 40 years). The statistical analysis of Model Pair 4 is in agreement with its graphical analysis. The percent of deviation between the Model Pair 4 centerline curves at 60 years was 62.97% while the percent of deviation between the curves at 40 years was 84.02%. These degrees of variation between the base- and match-case curves are greater than those of the Model Pair 1 and 2 comparisons, but not the Model Pair 3 comparison. The percentages of deviation for Model Pair 4 for both 60- and 40-year comparisons are fractionally less than those of Model Pair 3. This deviation in the pattern (i.e. higher plume decay rates leading to greater variation between the matched curves) could be due to error in visually judging the similarity between the curves as they were being matched.

Model Pair 5 was created with a match-case with a plume decay rate of 0 (yr^{-1}) and a base-case with plume decay rate of 0.5 (yr^{-1}) and a half-life of 1.39 years. The centerline match for Model Pair 5 at 60 years after initial TCE release showed relative similarity between the base- and match-case centerline curves, as shown in Figure 4.1.26 (ranked #8 of 13), but was not as good a visual match as those of Model Pairs 1 and 2. The centerline comparison for Model Pair 5 at 40 years after TCE release failed to match because of the differences between the base- and match-case curves' concentrations and geometries, as shown in Figure 4.1.29 (ranked #10 of 13 at 40 years). The statistical analysis of the two centerline comparisons for Model Pair 5 is in agreement with its graphical analysis. The final calculated percent of deviation for Model Pair 5 at 60 years was 45.35%, while the percent of deviation for Model Pair 5 at 40 years was 87.17%.

The degree of variation in the base- and match-case centerline plot for Model Pair 5 at 60 years is greater than those of Model Pairs 1 and 2 (as expected), but less than those of Model Pairs 3 and 4. This could be caused by error in judging the visual similarity of the base- and match-case curves when forcing the matches.

Model Pair 6 was created with a match-case with plume decay rate of 0 (yr^{-1}) and base-case with a plume decay rate of 1.0 (yr^{-1}) and a half-life of 0.693 years. The centerline match for Model Pair 6 at 60 years after TCE release showed relative similarity between base- and match-case curves, as shown in Figure 4.1.32 (ranked #9 of 13), but clearly was not as good a visual match as those of Model Pairs 1 and 2. The centerline comparison for Model Pair 6 at 40 years after initial TCE release was an obvious mismatch because of the differences in concentration and geometry of the base- and match-case curves, as shown in Figure 4.1.35 (ranked #9 of 13 at 40 years). The statistical analysis of Model Pair 6 is very much in agreement with its graphical analysis. The final calculated percent of deviation for Model Pair 6 at 60 years was 48.30% while the percent of deviation for Model Pair 6 at 40 years was 95.23%. The degree of variation between the base- and match-case centerline curves for Model Pair 6 at 60 years after TCE release is greater than those of Model Pairs 1, 2, and 5 (as expected), but is less than those of Model Pairs 3 and 4. This could be caused by error in judging the visual similarity of the base- and match-case curves when forcing the matches. The percent of deviation between the base- and match-case curves for Model Pair 6 at 40 years is greater than that of the other five model pairs, making this statistically the least similar of all the Case 1 centerline plots.

Transverse plot matches (X-Y spatial plane)

Table 4.2.6, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the transverse comparison plots for the six model pairs that were examined in Case 1. To perform these calculations, the concentration data for each model at the appropriate year (60, 40, 54, or 34 yr) was exported from REMChlor into Excel™ where the NRMS formula was applied.

NRMS Analysis Table (Transverse: X-Y spatial plane) Case 1: Stable plume with hypothetical base-case parameter values								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
1	0.1	6.93yr	60yr 40yr	0.03 0.41	0.94	0.03 0.44	3.16 44.00	4.1.2a & b 4.1.5a & b
2	0.2	3.47yr	60yr 40yr	1.83 2.10	0.89	2.06 2.37	205.65 236.99	4.1.9a & b 4.1.12a & b
3	0.3	2.31yr	60yr 40yr	2.32 2.62	0.73	3.19 3.60	319.13 360.42	4.1.15a & b 4.1.18a & b
4	0.4	1.73yr	60yr 40yr	1.76 3.31	0.51	3.47 6.52	347.16 652.07	4.1.21a & b 4.1.24a & b
5	0.5	1.39yr	60yr 40yr	1.60 3.01	0.76	2.11 3.95	210.65 395.08	4.1.27a & b 4.1.30a & b
6	1.0	0.69yr	60yr 40yr	2.18 3.75	0.80	2.74 4.70	273.73 469.69	3.1.33a & b 4.1.36a & b

Table 4.2.6: Transverse (X-Y spatial plane; Z=0) NRMS results for Case 1

The match between the transverse plume plots for Model Pair 1 at 60 years from initial TCE release was visually almost perfect, as shown in Figures 4.1.2a & b, which was ranked #1 of 13. The match between the transverse plume plots for Model Pair 1 at 40 years from initial TCE release was less than perfect, as shown in Figures 4.1.5a & b (ranked #4 of 13 at 40 years), with the base-case plume having a slightly larger expanse than the match-case plume. The statistical analysis results are in agreement with the graphical analysis results (that a higher degree of variance exists for the 40-year match than the 60-year match) for Model Pair 1. The final calculated percent of deviation for the transverse base-case to match-case plume comparison at 60 years for Model Pair 1 was 3.16%, while the percent of deviation for the base-case to match-case transverse plume match at 40 years for Model Pair 1 was 44.00%.

The match between the transverse plume plots for Model Pair 2 at 60years was fairly close, as shown in Figures 4.1.9a & b (ranked #6 of 13), with the match-case plume being only slightly more expansive than the base-case plume. The match between the transverse plume plots for Model Pair 2 at 40 years from initial TCE release was not very close, as shown in Figures 4.1.12a & b (ranked #8 of 13 at 40 years), with the base-case plume being much more expansive than the match-case plume. The statistical analysis results are in agreement with the graphical analysis results (that a higher degree of variance exists for the 40-year match than the 60-year match) for Model Pair 2. The final calculated percent of deviation between the base- and match-case transverse plume plots for Model Pair 2 at 60 years was 205.65% while that at 40 years was 236.99%. The degree of variance for both the 60- and 40-year transverse plume plots for Model Pair 2 is much greater than that of either of the transverse plume plots for Model Pair 1.

The match between the transverse plume plots for the base- and match-case for Model Pair 3 at 60 years is shown in Figures 4.1.15a & b (ranked #10 of 13), with the match-case plume having a greater expanse of higher TCE concentrations within its 1 μg/L (assumed detection limit) contour. The match between the base- and match-case transverse plume plots for Model Pair 3 at 40 years is shown in Figures 4.1.18a & b (ranked #9 of 13 at 40 years), and shows that the base-case plume is much more expansive than the match-case plume. The statistical analysis results for Model Pair 3 are in agreement with its graphical analysis in that a higher degree of variance exists between the 40-year transverse plume plots than does between the 60-year transverse plume plots. The final calculated percent of deviation between the base- and match-case transverse plume plots for Model Pair 3 at 60 years is 319.13% while that of the 40-year transverse plume plots is 360.42%. The degree of variance for both the 60- and 40-year transverse plume plots for Model Pair 3 is greater than those of Model Pairs 1 and 2.

The match between the base- and match-case transverse plume plots for Model Pair 4 at 60 years is shown in Figures 4.1.21a & b (ranked #11 of 13), with the match-case plume having a greater areal extent of higher TCE concentrations than did the base-case plume. The comparison between the base- and match-case transverse plume plots at 40 years showed that there was no match at all, as in Figure 4.1.24a &b (ranked #13 of 13 at 40 years), with the base-case plume being more expansive than the match-case plume. The statistical analysis results for Model Pair 4 agree with the findings of the graphical analysis. The final calculated percent of deviation for the transverse plots for Model Pair 4 at 60 years is 347.16%, while that of the 40-year plots was 652.07%. The degree of variance for both the 60- and 40-year transverse plume plots for Model Pair 4 is greater than those of Model Pairs 1, 2, and 3.

The match between the base- and match-case for Model Pair 5 at 60 years is shown in Figures 4.1.27a & b (ranked #12 of 13), with the match-case plume having a greater expanse of higher TCE concentrations within its 1 μg/L perimeter. The comparison between the base- and match-case transverse plume plots for Model Pair 5 at 40 years, as shown in Figures 4.1.30a & b (ranked #11 of 13), is not a good match because the base-case plume is much larger than the match-case plume. The statistical analysis results of the transverse plume plots for Model Pair 5 agree with the graphical analysis results of the same in that there is more variance between base- and match-case plume plots at 40 years than there is at 60 years. The percentage of deviation for the transverse plume plots for Model Pair 5 at 60 years is 210.65% and at 40 years it is 395.08%. The degree of variation for Model Pair 5 is greater than that of Model Pairs 1 and 2, but less than that of Model Pairs 3 and 4 (much like the Model Pair 5 results for the centerline plots). This could be due to error in visually determining the matches.

The comparison between base- and match-case transverse plume plots for Model Pair 6, in Figures 4.1.33a & b (ranked #9 of 13), shows the match-case plume being a bit narrower than the base-case plume and having a greater expanse of higher TCE concentrations than the base-case plume. The comparison between the transverse plume plots for Model Pair 6 at 40 years, shown in Figures 4.1.36a & b (ranked #12 of 13 at 40 years), shows almost no similarity between the base- and match-cases. The results of the statistical analysis for Model Pair 6 agree with the results of its graphical analysis in that the 40-year comparison has a greater degree of variance between base- and match-case plume plots than does the 60-year comparison. The percent of deviation for the transverse plume plot pair for Model 6 at 60 years is 273.73% and for Model Pair 6 at 40 years is 469.69%. The degree of variation for Model Pair 6 is greater than that of Model

Pairs 1, 2, and 5, but is less than that of Model Pairs 3 and 4 (at 60 years). This could be due to some error in performing the visual match-making of the pairs.

Vertical plot matches (X-Z spatial plane)

Table 4.2.7, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the vertical comparison plots for the six model pairs that were examined in Case 1.

NRMS Analysis Table (Vertical: X-Z spatial plane) Case 1: Stable plume with hypothetical base-case parameter values								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
1	0.1	6.93yr	60yr 40yr	0.03 0.41	1.04	0.03 0.39	3.00 39.31	4.1.3a & b 4.1.6a & b
2	0.2	3.47yr	60yr 40yr	0.58 1.50	0.79	0.74 1.90	74.16 189.99	4.1.10a & b 4.1.13a & b
3	0.3	2.31yr	60yr 40yr	2.78 2.97	0.65	4.29 4.58	428.96 458.03	4.1.16a & b 4.1.19a & b
4	0.4	1.73yr	60yr 40yr	2.30 4.01	0.56	4.13 7.20	412.66 719.93	4.1.22a & b 4.1.25a & b
5	0.5	1.39yr	60yr 40yr	3.22 4.53	0.49	6.55 9.22	654.51 922.06	4.1.28a & b 4.1.31a & b
6	1.0	0.69yr	60yr 40yr	4.37 5.38	0.29	14.85 18.26	1485.37 1825.78	4.1.34a & b 4.1.37a & b

Table 4.2.7: Vertical (X-Z spatial plane; Y=0) NRMS results for Case 1

The vertical plume plots for Model Pair 1 at 60 years, shown in Figures 4.1.3a & b, make for an almost perfect match, and were ranked #1 of 13 in the visual evaluation. The vertical plume plots for Model Pair 1 at 40 years, shown in Figures 4.1.6a & b (ranked #2 of 13 at 40 years), are one of the closer matches for the 40 year comparisons. The results of the statistical analysis of the vertical plume plots for Model Pair 1 agree with the graphical analysis in that there is more variation between the base- and match-case plumes in the 40-year comparison than there is in the 60-year match. The percent of deviation for the vertical plume plots for Model Pair 1 at 60 years is 3.00% and for the 40-year plots is 39.31%.

The vertical plume plot comparison for Model Pair 2 at 60 years, shown in Figures 4.1.10a & b (ranked #6 of 13), shows that the base- and match-case plumes are a fair match. The vertical plume plot comparison for Model Pair 2 at 40 years, shown in Figures 4.1.13a & b (ranked #9 of 13 at 40 years), shows that the base- and match-case are not a good match. The statistical analysis of the vertical plume plot pairs for Model Pair 2 is consistent with the findings of the graphical analysis in that there is a greater amount of variation between the plumes in the 40-year comparison than in the 60 year comparison. The final calculated percent of deviation for the vertical plume plots for Model Pair 2 at 60 years is 74.16% while that of the pair at 40 years is 189.99%. The degree of variation of the vertical plume plots for Model Pair 2 is greater than that of the vertical plume plots of Model Pair 1.

The vertical plume plots for Model Pair 3 at 60 years, shown in Figures 4.1.16a & b (ranked #5 of 13), are quite a good match. The vertical plume plots for Model Pair 3 at 40 years, shown in Figures 4.1.19a &b (ranked #10 of 13 at 40 years), are not a match because the base- case plume is much more expansive than that of the match-case. The statistical analysis of the vertical plume plots for Model Pair 3 are in agreement with the findings of the graphical analysis that there is a greater degree of variation in the base- and match-case at 40 years than there is at 60 years. The percent of deviation for the base- and match-case vertical plume plots for Model Pair 3 at 60 years is 428.96% and that of the plots at 40 years is 458.03%. Model Pair 3 has a greater amount of variation between the base- and match-case vertical plume plots than do Model Pairs 1 and 2.

The vertical plume plots for Model Pair 4 at 60 years, shown in Figures 4.1.22a & b (ranked #3 of 13), are relatively similar with the match-case plume having a greater expanse of higher TCE concentrations within its perimeter than does the base-case plume. The vertical plume plots for Model Pair 4 at 40 years, shown in Figures 4.1.25a & b (ranked #11 of 13 at 40 years), show that a match does not exist between the base- and match case. The statistical analysis of the vertical plume plots for Model Pair 4 is in agreement with the results of the graphical analysis in that there is more variation between base- and match-cases at 40 years than there is at 60 years. The percent of deviation for the vertical plume plots for Model Pair 4 at 60 years is 412.66% and for the vertical plume plots at 40 years is 719.93%. Model Pair 4 has a higher degree of variation for the 40-year vertical plume plots than do Model Pairs 1, 2, and 3. In the 60-year plume plots, Model Pair 4 has a higher degree of variation than do Model Pairs 1 and two, but has slightly less (only 16 percentage points) variance than did Model Pair 3.

The vertical plume plots for Model Pair 5 at 60 years, shown in Figures 4.1.28a & b (ranked #7 of 13), are fairly similar with the match-case plume having a greater expanse of higher concentrations of TCE within it that does the base-case plume. The vertical plume plots for Model Pair 5 at 40 years, shown in Figures 4.1.31a & b (ranked #12 of 13 at 40 years), are not a match because the base-case plume is much greater in expanse than the match-case plume. The statistical analysis agrees with the findings of the graphical analysis in that there is a greater degree of variation between the base- and match-cases at 40 years than there is at 60 years. The percent of deviation for the vertical plume plots for Model Pair 5 at 60 years is 654.51% and at 40 years is 922.06%. Model Pair 5 has an overall higher degree of variation than any of the previous four model pairs.

The vertical plume plots for Model Pair 6 at 60 years, in Figures 4.1.34a & b (ranked #8 of 13), show that the match-case plume has a greater expanse of higher levels of TCE within its perimeter than does the base-case plume. The vertical plume plots for Model Pair 6 at 40 years, shown in Figures 4.1.37a & b (ranked #13 of 13 at 40 years), are not similar due to the much greater expanse of the base-case plume. The statistical analysis performed for Model Pair 6 agrees with the findings of its graphical analysis in that there is a greater amount of variation in the vertical plot pair at 40 years than there is at 60 years. The percent of deviation for the vertical plume plots for Model Pair 6 at 60 years is 1485% and that of the 40-year plots is 1825%. Model Pair 6 has a higher degree of variation for both the 60- and 40-year plots than any of the previous five model pairs.

Case 1b: Stable plume with parameter values from Liang [2009]

The statistical analysis for this Case was completed in a series of three sets of calculations for each model pair; X-direction for centerline plots, X-Y spatial plane for transverse plots, and X-Z spatial plane for vertical plots. This analysis is designed to mathematically describe the degree of variance between the base- and match-case in each of the comparison plots for both of the times modeled (60 years and 40 years from initial TCE release).

This scenario is one of a "stable" TCE groundwater plume that is not migrating and that has its contaminant mass partially in the source zone and partially in the plume [Pate, 2010; Liang, 2009]. Two plume decay rates were chosen for study in this Case: 0.1 and 0.2 in units of yr^{-1} with corresponding half-lives of 6.93 and 3.47 years respectively. These plume decay rates each were assigned to a base-case to be modeled and compared with a match-case with a plume decay rate of 0 through multiple series of parameter manipulations. The parameters used in each of the base- and match-cases in this scenario can be found in Tables 4.1.7 and 4.1.8 in the Graphical analysis section.

Centerline plot matches (X-direction)

Table 4.2.8, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the centerline comparison plots for the two model pairs that were examined in Case 1b.

NRMS Analysis Table (Centerline: X-direction) Case 1b: Stable plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**$\log(C_m)$**	**NRMS**	**%Deviation**	**Figure Ref.**
7	0.1	6.93yr	60yr 40yr	0.11 0.28	2.74	0.04 0.10	3.84 10.38	4.1.38 4.1.41
8	0.2	3.47yr	60yr 40yr	0.27 0.99	2.61	0.10 0.38	10.18 38.03	4.1.44 4.1.47

Table 4.2.8: Centerline (X-direction) NRMS results for Case 1b

Model Pair 7 was created with a match-case with plume decay rate of 0 and a base-case with a plume decay rate of 0.1 (yr^{-1}) with a half-life of 6.93 years. The centerline plot for Model Pair 7 at 60 years, shown in Figure 4.1.38 (ranked #5 of 13), shows a close match between the base- and match-case curves. The centerline plot for Model Pair 7 at 40 years, shown in Figure 4.1.41 (ranked #1 of 13 at 40 years), shows fair similarity between the base- and match-case curves, but they are not quite a match. The statistical analysis of the centerline plots for Model Pair 7 is in agreement with the results of the graphical analysis in that there is a slightly higher degree of variation in the 40-year comparison than there is in the 60-year match. The percent of deviation for the centerline comparison for Model Pair 7 at 60 years is 3.84% and at 40 years is 10.38%.

Model Pair 8 was created with a match-case with a plume decay rate of 0 and a base-case with plume decay rate of 0.2 (yr^{-1}) with a half-life of 3.47 years. The centerline plot for Model Pair 8 at 60 years, Figure 4.1.44 (ranked #12 of 13), shows that the base- and match-case curves are not a good match visually. The centerline plot for Model Pair 8 at 40 years, shown in Figure 4.1.47 (ranked #2 of 13 at 40 years), shows that the base- and match-case comparison at 40 years has less similarity between the curves than did the 60-year match. The statistical analysis of the centerline plots for Model Pair 8 agrees with the findings of the graphical analysis in that there is more variation between the base- and match-case curves at 40 years than there is at 60 years. The percent of deviation for the centerline plot for Model Pair 8 at 60 years is 10.18% and that of the plot at 40 years is 38.03%. Model Pair 8 has overall greater variation between the base- and match-case curves at both 60- and 40-years than does Model Pair 7.

Transverse plot matches (X-Y spatial plane)

Table 4.2.9, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the transverse comparison plots for the two model pairs that were examined in Case 1b.

NRMS Analysis Table (Transverse: X-Y spatial plane) Case 1b: Stable plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
7	0.1	6.93yr	60yr	3.16	1.47	2.15	214.68	4.1.39a & b
			40yr	3.44		2.34	233.72	4.1.42a & b
8	0.2	3.47yr	60yr	1.90	1.50	1.26	126.41	4.1.45a & b
			40yr	2.50		1.67	166.62	4.1.48a & b

Table 4.2.9: Transverse (X-Y spatial plane; Z=0) NRMS results for Case 1b

The transverse plume plots for Model Pair 7 at 60 years, shown in Figure 4.1.39a &b, show that the two plumes are visually similar and were ranked #5 of 13. The transverse plume plots for Model Pair 7 at 40 years, shown in Figures 4.1.42a & b (ranked #6 of 13 at 40 years), show that the base-case plume has a greater expanse than does the match-case plume. The statistical analysis for Model Pair 7 is in agreement with the graphical similarity assessment in that there is more variation between the base- and match-case plumes at 40 years than there is at 60 years. The percent of deviation for the transverse plume plots for Model Pair 7 at 60 years is 214.68% and for the plots at 40 years is 233.72%.

The transverse plume plots for Model Pair 8 at 60 years, shown in Figures 4.1.45a & b (ranked #4 of 13), show the relative similarity between the base- and match-case plumes with the match-case plume having slightly more elongated concentration contours than the base-case plume. The transverse plume plots for Model Pair 8 at 40 years, shown in Figures 4.1.48a & b (ranked #7 of 13 at 40 years), show that there is no match between the base- and match-case plumes at 40 years due to the greater expanse of the base-case plume. The statistical analysis of the transverse plume plots for Model Pair 8 are in agreement with the graphical analysis in that there is more variation between the base- and match-cases in the 40-year plot than there is in the 60-year plot. The percent of deviation for the transverse plume plots for Model Pair 8 at 60 years is 126.41% and for the pair at 40 years is 166.62%. Model Pair 8 has overall less variation between the base- and match-cases for both the 60- and 40-year plots than has Model Pair 7. This unexpected result could be due to errors in visual matching of the model pairs.

Vertical plot matches (X-Z spatial plane)

Table 4.2.10, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the vertical comparison plots for the two model pairs that were examined in Case 1b.

NRMS Analysis Table (Vertical: X-Z spatial plane) Case 1b: Stable plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
7	0.1	6.93yr	60yr	3.04	1.66	1.83	182.91	4.1.40a & b
			40yr	3.27		1.96	196.31	4.1.43a & b
8	0.2	3.47yr	60yr	1.85	1.61	1.15	115.13	4.1.46a & b
			40yr	2.18		1.35	135.31	4.1.49a & b

Table 4.2.10: Vertical (X-Z spatial plane; Y=0) NRMS results for Case 1b

The vertical plume plots for Model Pair 7 at 60 years, shown in Figures 4.1.40a & b (ranked #10 of 13), do not match well due to the much greater vertical dispersion in the match-case plume. The vertical plume plots for Model Pair 7 at 40 years, shown in Figures 4.1.43a & b (ranked #6 of 13 at 40 years), do not match due to the much greater expanse of the match-case plume. The percent of deviation for the vertical plume plots for Model Pair 7 at 60 years is 182.91% and at 40 years is 196.31%, showing that there is statistically more variation between the base- and match-case vertical plume plots at 40 years than there is at 60 years. It is difficult to tell, visually, which of the plots had the greater degree of variation because they both are such poor matches.

The vertical plume plots for Model Pair 8 at 60 years, shown in Figures 4.1.46a & b (ranked #9 of 13), show that there much greater vertical expanse in the match-case plume than in the base-case plume. The vertical plume plots for Model Pair 8 at 40 years, shown in Figures 4.1.49a & b (ranked #8 of 13 at 40 years), show that the match-case plume has a greater vertical expanse than does the base-case plume. The percent of deviation for the vertical plume plots for Model Pair 8 at 60 years is 115.13% and for the pair at 40 years is 135.31%. The overall degree of variation for Model Pair 8 is lower than that of Model Pair 7. This could be due to errors in the visual match-making or it could stem from the changes made to the dispersion parameters.

Case 2: Growing-disconnected plume with parameter values from Liang [2009]

The statistical analysis for this Case was completed in a series of three sets of calculations for each model pair; X-direction for centerline plots, X-Y spatial plane for transverse plots, and X-Z spatial plane for vertical plots. This analysis is designed to mathematically describe the degree of variance between the base- and match-case in each of the comparison plots for both of the times modeled (54 years and 34 years from initial TCE release).

This scenario is one of a "growing" TCE groundwater plume that is migrating and that has its contaminant mass in the plume [Pate, 2010; Liang, 2009]. Two plume decay rates were chosen for study in this Case: 0.1 and 0.2 in units of yr^{-1} with corresponding half-lives of 6.93 and 3.47 years respectively. These plume decay rates each were assigned to a base-case to be modeled and compared with a match-case with a plume decay rate of 0 through multiple series of parameter manipulations. The parameters used in each of the base- and match-cases in this scenario can be found in Tables 4.1.9 and 4.1.10 in the Graphical analysis section.

Centerline plot matches (X-direction)

Table 4.2.11, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the centerline comparison plots for the two model pairs that were examined in Case 2.

NRMS Analysis Table (Centerline: X-direction) Case 2: Growing-disconnected plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
9	0.1	6.93yr	54yr 34yr	0.02 119.36	1.71	0.01 69.78	1.43 6977.57	4.1.50 4.1.53
10	0.2	3.47yr	54yr 34yr	0.04 0.86	1.40	0.03 0.61	2.72 61.40	4.1.56 4.1.59

Table 4.2.11: Centerline (X-direction) NRMS results for Case 2

Model Pair 9 was created with a match-case with plume decay rate of 0 and a base-case with a plume decay rate of 0.1 (yr^{-1}) with a half-life of 6.93 years. The centerline curve plot for Model Pair 9 at 54 years, shown in Figure 4.1.50 (ranked #2 of 13), shows an almost perfect match between the base- and match-case curves. The centerline curve plot for Model Pair 9 at 34 years, shown in Figure 4.1.53 (ranked #13 of 13 at 40/34 years), shows that there is no match between the curves at 34 years. The statistical analysis for Model Pair 9 is in agreement with the findings of the graphical analysis in that there is more variation between the base- and match-case curves at 34 years than there is at 54 years. The percent of deviation for the centerline plot for Model Pair 9 at 54 years is 1.43% and that of the comparison at 34 years is 6978%, which accurately describes just how far off the match is in the 34-year plot.

Model Pair 10 was created with a match-case with plume decay rate of 0 and a base-case with a plume decay rate of 0.2 (yr^{-1}) with a half-life of 3.47 years. The centerline curve plot for Model Pair 10 at 54 years, shown in Figure 4.1.56 and ranked #4 of 13, shows the very close match between the base- and match-case centerline curves. The centerline curve plot for Model Pair 10 at 34 years, shown in Figure 4.1.59 (ranked #8 of 13 at 40/34 years), shows that the curves do not match, but do have similar geometry with the match-case curve having an overall higher TCE concentration. The statistical analysis of the centerline plots for Model Pair 10 agrees with the graphical analysis that the 34-year comparison has a greater degree of variance than does the 54-year match. The percent of deviation for the centerline plot for Model Pair 10 at 54 years is 2.72% and that of the comparison at 34 years is 61.40%. The Model Pair 10 match at 54 years had a greater degree of variation than did the Model Pair 9 match at 54 years. The Model Pair 9 comparison at 34 years had a greater degree of variation than did the Model Pair 10 comparison at 34 years; possibly due to the fact that the Model Pair 9 centerline curves' geometries were so dissimilar, while those of the Model Pair 10 centerline curves were more similar to each other.

Transverse plot matches (X-Y spatial plane)

Table 4.2.12, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the transverse comparison plots for the two model pairs that were examined in Case 2.

NRMS Analysis Table (Transverse: X-Y spatial plane) Case 2: Growing-disconnected plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
9	0.1	6.93yr	54yr 34yr	0.03 0.41	0.97	0.03 0.42	2.61 42.45	4.1.51a & b 4.1.54a & b
10	0.2	3.47yr	54yr 34yr	2.02 2.20	0.47	4.29 4.68	429.20 467.68	4.1.57a & b 4.1.60a & b

Table 4.2.12: Transverse (X-Y spatial plane; Z=0) NRMS results for Case 2

The transverse plume plots for Model Pair 9 at 54 years, shown in Figures 4.1.51a & b (ranked #2 of 13), show that the match between the base- and match-case plumes was nearly perfect. The transverse plume plots for Model Pair 9 at 34 years, shown in Figures 4.1.54a & b (ranked #5 of 13 at 40/34 years), show that there is greater expansiveness and higher TCE concentrations of the base-case plume than in the match-case plume. The statistical analysis of the transverse plume plots for Model Pair 9 is in agreement with the graphical analysis in that there is a greater degree of variance between the base- and match-case plots at 34 years than there is at 54 years. The percent of deviation for the transverse plume plots for Model Pair 9 at 54 years is 2.61% and at 34 years is 42.45%.

The transverse plume plots for Model Pair 10 at 54 years, shown in Figures 4.1.57a & b (ranked #7 of 13), shows a good match between the base- and match-case plume plots. The transverse plume plots for Model Pair 10 at 34 years, shown in Figures 4.1.60a & b (ranked #10 of 13 at 40/34 years), show that the base- and match-case plumes do not match at 34 years with the base-case plume having a much greater expanse and higher TCE concentrations than the match-case plume. The statistical analysis of the transverse plume plots for Model Pair 10 is in agreement with the graphical analysis that there is a higher degree of variation between the base- and match-case plumes at 34 years than there is at 54 years. The percent of deviation for the transverse plume plots for Model Pair 10 at 54 years is 429% and at 34 years is 468%. The overall degree of variation for the transverse plume plots for Model Pair 10 is higher than that of Model Pair 9, as was expected.

Vertical plot matches (X-Z spatial plane)

Table 4.2.13, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the vertical comparison plots for the two model pairs that were examined in Case 2.

NRMS Analysis Table (Vertical: X-Z spatial plane) Case 2: Growing-disconnected plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
9	0.1	6.93yr	54yr 34yr	0.03 0.41	0.83	0.03 0.49	3.00 49.21	4.1.52a & b 4.1.55a & b
10	0.2	3.47yr	54yr 34yr	1.28 2.38	0.36	3.56 6.61	356.19 661.18	4.1.58a & b 4.1.61a & b

Table 4.2.13: Vertical (X-Z spatial plane; Y=0) NRMS results for Case 2

The vertical plume plots for Model Pair 9 at 54 years, shown in Figures 4.1.52a & b and ranked #2 of 13, show a high degree of similarity between the base- and match-case plumes. The vertical plume plots for Model Pair 9 at 34 years, in Figures 4.1.55a & b and ranked #1 of 13 at 40/34 years, show that the base- and match-case plumes are very similar. The statistical analysis of the vertical plume plots agrees with the findings of the graphical analysis that the plume plots at 54 years are more similar to each other than those at 34 years. The percent of deviation for the vertical plume plots for Model Pair 9 at 54 years is 3.00% and at 34 years is 49.21%.

The vertical plume plots for Model Pair 10 at 54 years, shown in Figures 4.1.58a

& b (ranked #4 of 13), show that the base- and match-case plumes are fairly similar to each other at 54 years. The vertical plume plots for Model Pair 10 at 34 years, shown in Figures 4.1.61a & b (ranked #3 of 13 at 40/34 years), show that the base-case plume is more vertically expansive than the match-case plume. The statistical analysis of the vertical plume plots for Model Pair 10 agrees with the graphical analysis that there is a higher degree of variation in the 34-year comparison than in the 54-year comparison. The percent of deviation for the vertical plume plots for Model Pair 10 at 54 years is 356% and at 34 years is 661%. The overall degree of variation for Model Pair 10 is greater than that of Model Pair 9, as expected.

Case 3: Growing-connected plume with parameter values from Liang [2009]

The statistical analysis for this Case was completed in a series of three sets of calculations for each model pair; X-direction for centerline plots, X-Y spatial plane for transverse plots, and X-Z spatial plane for vertical plots. This analysis is designed to mathematically describe the degree of variance between the base- and match-case in each of the comparison plots for both of the times modeled (60 years and 40 years from initial TCE release).

This scenario is one of a "growing" TCE groundwater plume that is migrating and that has its contaminant mass partially in the source zone and partially in the plume [Pate, 2010; Liang, 2009]. Three different plume decay rates were chosen for study in this Case: 0.1, 0.2, and 0.3 in units of yr^{-1} with corresponding half-lives of 6.93, 3.47, and 2.31 years respectively. These plume decay rates each were assigned to a base-case to be modeled and compared with a match-case with a plume decay rate of 0 through multiple series of parameter manipulations. The parameters used in each of the base- and match-cases in this scenario can be found in Tables 4.1.11 through 4.1.13 in the Graphical analysis section.

Centerline plot matches (X-direction)

Table 4.2.14, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the centerline comparison plots for the three model pairs that were examined in Case 3.

NRMS Analysis Table (Centerline: X-direction) Case 3: Growing-connected plume with base-case parameter values from Liang [2009]								
Model Pair	λ	$t_{1/2}$	Time	RMS	$\log(C_m)$	NRMS	%Deviation	Figure Ref.
11	0.1	6.93yr	60yr 40yr	0.20 0.25	3.79	0.05 0.07	5.30 6.62	4.1.62 4.1.65
12	0.2	3.47yr	60yr 40yr	0.54 0.44	3.65	0.15 0.12	14.69 12.01	4.1.68 4.1.71
13	0.3	2.31yr	60yr 40yr	0.58 0.59	3.55	0.16 0.16	16.44 16.49	4.1.74 4.1.77

Table 4.2.14: Centerline (X-direction) NRMS results for Case 3

Model Pair 11 was created with a match-case with plume decay rate of 0 and a base-case with a plume decay rate of 0.1 (yr^{-1}) with a half-life of 6.93 years. The centerline curve plot for Model Pair 11 at 60 years, Figure 4.1.62 (ranked #6 of 13), shows a decent match between the base- and match-case curves. The centerline curve plot for Model Pair 11 at 40 years, shown in Figure 4.1.65 (ranked #4 of 13 at 40 years), shows that the curves have similar geometries and are relatively close, but that the base-case curve is at an overall higher TCE concentration. The statistical analysis for the centerline plots for Model Pair 11 agrees with the findings of the graphical analysis that the 40-year plot has a slightly higher amount of variation between the base- and match-case curves. The percent of deviation for the centerline plot for Model Pair 11 at 60 years is 5.30% and at 40 years is 6.62%.

Model Pair 12 was created with a match-case with plume decay rate of 0 and a base-case with a plume decay rate of 0.2 (yr^{-1}) with a half-life of 3.47 years. The centerline plot for Model Pair 12 at 60 years, shown in Figure 4.1.68 (ranked #7 of 13), shows that the base- and match-case curves are relatively similar to each other, but that their shapes are not the same. The centerline plot for Model Pair 12 at 40 years, shown in Figure 4.1.71 (ranked #5 of 13 at 40 years), shows that the base- and match-case curves have more similar geometries than the pair at 60 years, but that the base-case curve is overall higher in concentration than the match-case curve. The statistical analysis for the centerline plots for Model Pair 12 does not seem to agree with the graphical analysis in which the 60-year curve pair visually appears to be more similar than does the 40-year curve pair. The percent of deviation for the centerline plot for Model Pair 12 at 60 years is 14.69% and at 40 years is 12.01%. The overall amount of variation for Model Pair 12 at both 60- and 40-years is greater than that of Model Pair 11, as expected.

The Model Pair 13 match was created with a match-case with plume decay rate of 0 and a base-case with a plume decay rate of 0.3 (yr^{-1}) with a half-life of 2.31 years. The centerline plot for Model Pair 13 at 60 years, shown in Figure 4.1.74 (ranked #13 of 13), shows that the curves in this plot are not as similar as the 60-year curves in the previous two model pairs. The centerline plot for Model Pair 13 at 40 years, shown in Figure

4.1.77 (ranked #3 of 13 at 40 years), shows that the base- and match-case curves are relatively similar to each other and may be a better match than the 60-year pair of curves. The statistical analysis of the centerline plots for Model Pair 13 shows that the 60-year match and the 40-year match have almost exactly the same degree of variance between the base- and match-case curves. The percent of deviance for the centerline plot for Model Pair 13 at 60 years is 16.44% and at 40 years is 16.49%. Model Pair 13 has a higher degree of variance than either of the previous two model pairs.

Transverse plot matches (X-Y spatial plane)

Table 4.2.15, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the transverse comparison plots for the two model pairs that were examined in Case 3.

NRMS Analysis Table (Transverse: X-Y spatial plane) Case 3: Growing-connected plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
11	0.1	6.93yr	60yr 40yr	3.23 3.74	2.66	1.22 1.41	121.71 141.02	4.1.63a & b 4.1.66a & b
12	0.2	3.47yr	60yr 40yr	0.57 0.46	2.53	0.22 0.18	22.34 18.34	4.1.69a & b 4.1 72a & b
13	0.3	2.31yr	60yr 40yr	1.07 1.81	2.38	0.45 0.76	45.02 75.87	4.1.75a & b 4.1.78a & b

Table 4.2.15: Transverse (X-Y spatial plane; Z=0) NRMS results for Case 3

The transverse plume plot for Model Pair 11 at 60 years, Figures 4.1.63a & b (ranked #3 of 13), show that the base- and match-case plumes are very similar to each other with the match-case plume having a very slightly greater expanse than the base-case plume. The transverse plume plots for Model Pair 11 at 40 years, Figures 4.1.66 a &

b (ranked #1 of 13 at 40 years), show that the base- and match-case plumes are similar, with the base-case plume being slightly more expansive than the match-case plume. The statistical analysis is in agreement with the graphical analysis in that there is a slightly greater degree of variance in the 40-year plume plot than in the 60-year plume plot. The percent of deviation for the transverse plume plot for Model Pair 11 at 60 years is 121% and at 40 years is 141%.

The transverse plume plot for Model Pair 12 at 60 years, Figures 4.1.69a & b (ranked #8 of 13), shows that the base- and match-case plumes are relatively similar with the match-case plume being slightly more expansive than the base-case plume. The transverse plume plot for Model Pair 12 at 40 years, Figures 4.1.72a & b (ranked #2 of 13 at 40 years), shows that the base- and match-case plumes are nearly a match for each other in expanse and concentration with the base-case plume being only slightly more oblate than the match-case plume. The statistical analysis for Model Pair 12 is in agreement with its graphical analysis in that the 60-year plume match has a greater degree of variance than does the 40-year plume. The percent of deviation for the transverse plume plot for Model Pair 12 at 60 years is 22.34% and at 40 years is 18.34%. Model Pair 12 has an overall lesser amount of variance than Model Pair 11, which was not expected. This could be due to error in creating the visual match for Model Pair 11.

The transverse plume plot for Model Pair 13 at 60 years, Figures 4.1.75a & b (ranked #13 of 13), shows that the match-case plume is more expansive than is the base-case plume. The transverse plume plot for Model Pair 13 at 40 years, in Figures 4.1.78a & b (ranked #3 of 13 at 40 years), shows that the plumes do not match well because the base-case plume is more expansive than the match-case plume. The statistical analysis of the transverse plume plots for Model Pair 13 are in agreement with the graphical analysis in that there is a greater amount of variation between the base- and match-case plumes at 40 years than there is at 60 years. The percent of deviation for the transverse plume plots for Model Pair 13 at 60 years is 45.02% and at 40 years is 75.87%. The variation between the plumes at 60 years and at 40 years for Model Pair 13 is less than that for Model Pair 11, but greater than that for Model Pair 12.

Vertical plot matches (X-Z spatial plane)

Table 4.2.16, shown below, contains the results of the Normalized Root Mean Squared (NRMS) error analysis for the vertical comparison plots for the two model pairs that were examined in Case 3.

NRMS Analysis Table (Vertical: X-Z spatial plane) Case 3: Growing-connected plume with base-case parameter values from Liang [2009]								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**log(C_m)**	**NRMS**	**%Deviation**	**Figure Ref.**
11	0.1	6.93yr	60yr 40yr	0.54 0.75	2.73	0.20 0.28	19.85 27.70	4.1.64a & b 4.1.67a & b
12	0.2	3.47yr	60yr 40yr	1.11 1.42	2.75	0.40 0.52	40.39 51.68	4.1.70a & b 4.1.73a & b
13	0.3	2.31yr	60yr 40yr	1.40 2.09	2.63	0.53 0.79	53.38 79.33	4.1.76a & b 4.1.79a & b

Table 4.2.16: Vertical (X-Z spatial plane; Y=0) NRMS results for Case 3

The vertical plume plot for Model Pair 11 at 60 years, Figures 4.1.64a & b (ranked #12 of 13), shows that the base- and match-case plumes do not match due to the much greater vertical expanse of the match-case plume. The vertical plume plot for Model Pair 11 at 40 years, Figures 4.1.67a & b (ranked #4 of 13 at 40 years), shows that the plumes are not a match due to the greater expanse of the match-case plume. The percent of deviation for the vertical plume plots for Model Pair 11 at 60 years is 19.85% and at 40 years is 27.70%.

The vertical plume plot for Model Pair 12 at 60 years, Figures 4.1.70a & b (ranked #11 of 13), shows that there is no match between base- and match case due to the much greater vertical expanse of the match-case plume. The vertical plume plot for Model Pair 12 at 40 years, Figures 4.1.73a & b (ranked #5 of 13 at 40 years), shows that the match-case plume has a much greater vertical expanse than does the base-case plume. It is difficult to determine visually which of the plots displays a greater amount of variance due to the very poor nature of the matches. The percent of deviation for the vertical plume plot for Model Pair 12 at 60 years is 40.39% and at 40 years is 51.68%. Model Pair 12 has an overall greater degree of variation in the vertical plume plots than does Model Pair 11.

The vertical plume plot for Model Pair 13 at 60 years, Figures 4.1.76a & b (ranked #13 of 13), shows that the base- and match-case plumes do not match due to the greater vertical expanse of the match-case curve. The vertical plume plot for Model Pair 13 at 40 years, in Figures 4.1.79a & b (ranked #7 of 13 at 40 years) does not a match well due to the greater expanse of the match-case plume. It is difficult to tell visually, due to the poor nature of the matches in these plots, which has the greater degree of variation. The percent of deviation for the vertical plume plot for Model Pair 13 at 60 years is 53.38% and at 40 years is 79.33%. Model Pair 13 has an overall higher degree of variance for the vertical plume plots than do Model Pairs 11 and 12.

CHAPTER FIVE

CONCLUSIONS DRAWN FROM RESULTS

It was possible in all of the Cases to force centerline matches for the given decay rates, though at the higher decay rates it was more challenging than at the lower ones. It became more difficult to manipulate a successful match when the second dimension (X-Y spatial plane) was considered along with the centerline match. Though it was not attempted in this study, it follows that forcing a match in all three dimensions would most likely be even more challenging. The issue becomes even more complicated when time is considered. None of the 40-year (34-year) plots matched when their respective base- and match-cases were compared, with the notable exception of the centerline plot for Model Pair 13, shown in Table 4.2.14. It would seem to be nearly impossible to create a model pair that matched in not only all three spatial dimensions, but also at all points in time. At the very least, a four-dimensional match would require the design of a more complex match-making procedure.

Of all the parameters, the seven that had the most effect on the model-matching results were: C_0, M_0, V_D, R, α_L, α_T, and α_V. The Parameter Master Table (Table 4.2.1 which is located in Appendix A) is a compilation of all of the base-case and match-case parameter values for all thirteen of the model pairs. Because the parameter values are all gathered together in this table, it is possible to view and compare them all at once and to view the changes in value that were applied to the seven most influential of the parameters. The parameters C_0 and M_0 tended to control the position of the centerline curve vertically (along the axis that describes TCE concentration) and to affect the position of the concentration contours within the transverse plume plots. The effect of $V_{D,}$ and R on any of the given models was to elongate or shorten the plot of the plume in the X-direction in such a manner as to be in keeping with the parameters' inverse relationship to each other. The parameter α_L had a great amount of control over the shape of the centerline curve and was used to cause the geometries of the curves to coincide. The transverse and vertical dispersion terms, α_T and α_V, had a direct effect on the plume boundaries in the X-Y and X-Z spatial planes. It was possible in Case 3 (Growing-connected plume) for the scenarios of plume decay rates of 0.2 and 0.3 yr^{-1} to force the centerline and transverse matches by drastically increasing the value of the vertical dispersivity to beyond its usually accepted value of one hundredth or less of the value of the longitudinal dispersivity. If it were desired to use this adjustment for model calibration at an actual site, it would be critical to have data about 3-d plume extent and vertical groundwater flow at the site; also information about any structures present at the site that could contribute to vertical spreading of the plume such as fractures or perforations in low permeability layers.

Aside from these seven parameters, which were actively manipulated to force the model matches, the most important variable in distinguishing between the effects of degradation processes and those of physical dispersion and dissolution was time. The three-dimensional spatial characteristics and spread of the plumes were also important in this determination. Because of the dominance of time and plume geometry, it is crucial to collect copious plume data for multiple points in time over a given plume's lifespan in order to constrain the models to provide a better understanding of the effects of degradation versus those of physical processes within the plume.

The graphical results were useful in determining the degree of match in each of the model pairs in all three dimensions. It was simple to perceive on the centerline charts when curves matched or did not match in each of the comparisons, to see on the transverse plume plots when the X-Y-plane plume contours lined up or not, and also in vertical plume plots to view the change in the positions of the X-Z-plane contours for the vertical representation of the plumes. The statistical results, in general, were in agreement with the graphical analysis results. The graphical analysis provided the answer and was supported by the statistical analysis in answering the hypothesis of this study: it <u>is</u> possible to misinterpret natural aerobic attenuation of TCE as dispersion in models that have zero-decay rates. Though the possibility of natural decay in an aerobic plume to be masked by other model parameters exists, it is a bit more difficult to determine with absolute certainty the amount of degradation, or rate of decay, that can be masked by model parameters. Based on the increasing level of difficulty encountered in matching the base- and match-cases as the plume decay rates were increased in each of the scenarios, it could be possible that the amount of decay masked by the model parameters of the zero-decay-rate models is rather low. Keeping in mind that the actual TCE decay rates for a given site are controlled by the specific conditions at that site, based on the findings of this study, there could be the potential for natural attenuation of TCE in aerobic plumes to have plume decay rates of at least 0.1 to 0.2 (yr^{-1}) that is not accounted for in the models that assume a decay rate of zero for TCE in aerobic plumes.

APPENDICES

APPENDIX A

Parameter Master Table

Model Pair	Case	d.r. (1/yr)	$t_{1/2}$ (yr)	φ	W (m)	D (m)	V_D (m/yr)	C_o (g/L)	M_o (kg)	R	σ_v	α_L	α_T (m)	α_V (m)
Case 1: Stable plume with hypothetical parameter values														
1	base	0.1	6.93	0.3	10	3	30	0.1	1000	2	0.14142	x/100	x/1000	x/10000
	match	0		0.3	10	3	45	0.0048	171.5	2.99	0.14142	x/100	x/1000	x/10000
2	base	0.2	3.47	0.3	10	3	30	0.1	1000	2	0.14142	x/100	x/1000	x/10000
	match	0		0.3	10	3	31	0.0004	1000	2.6	0.2	x/50	x/1111	x/11110
3	base	0.3	2.31	0.3	10	3	30	0.1	1000	2	0.14142	x/100	x/1000	x/10000
	match	0		0.3	10	3	13.5	0.0004	1000	3.2	0.44721	x/10	x/1667	x/16670
4	base	0.4	1.73	0.3	10	3	30	0.1	1000	2	0.14142	x/100	x/1000	x/10000
	match	0		0.3	10	3	10	0.0004	1000	3.4	0.44721	x/10	x/1428	x/14280
5	base	0.5	1.39	0.3	10	3	30	0.1	1000	2	0.14142	x/100	x/1000	x/10000
	match	0		0.3	10	3	8.5	0.0004	1000	3.7	0.44721	x/10	x/1667	x/16670
6	base	1.0	0.69	0.3	10	3	30	0.1	1000	2	0.14142	x/100	x/1000	x/10000
	match	0		0.3	10	3	4.3	0.0004	1000	3.8	0.44721	x/10	x/2500	x/25000
Case 1b: Stable plume with base-case values from Liang [2009]														
7	base	0.1	6.93	0.33	8	3.5	8	0.006	136	2	0.31623	x/20	x/1000	x/10000
	match	0		0.33	8	3.5	10.9	0.004	200	3.7	0.44721	x/10	x/1111	x/1428
8	base	0.2	3.47	0.33	8	3.5	8	0.0006	136	2	0.31623	x/20	x/1000	x/10000
	match	0		0.33	8	3.5	7.5	0.003	200	3.7	0.44721	x/10	x/1428	x/1000
Case 2: Growing-Disconnected plume with base-case values from Liang [2009]														
9	base	0.1	6.93	0.33	10	3	20	0.1	324	2	0.14142	x/100	x/1000	x/10000
	match	0		0.33	10	3	22	0.007	35	2.2	0.14142	x/100	x/1000	x/10000
10	base	0.2	3.47	0.33	10	3	20	0.1	324	2	0.14142	x/100	x/1000	x/10000
	match	0		0.33	10	3	22	0.00032	2.7	2.2	0.14142	x/100	x/1428	x/14280
Case 3: Growing-Connected plume with base-case values from Liang [2009]														
11	base	0.1	6.93	0.33	10	3	10	0.1	1620	2	0.1	x/200	x/1000	x/10000
	match	0		0.33	10	3	11.3	0.03	5000	2.5	0.14142	x/100	x/1000	x/2500
12	base	0.2	3.47	0.33	10	3	10	0.1	1620	2	0.1	x/200	x/1000	x/10000
	match	0		0.33	10	3	10.1	0.03	5000	3.8	0.44721	x/10	x/1000	x/1000
13	base	0.3	2.31	0.33	10	3	10	0.1	1620	2	0.1	x/200	x/1000	x/10000
	match	0		0.33	10	3	8.2	0.03	5000	3.8	0.44721	x/10	x/1515	x/1250

Table 4.2.1: Parameter Master Table

APPENDIX B

NRMS Analysis Table (Centerline: X-direction)								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS***	**$\log(C_m)$**	**NRMS**	**%Deviation**	**Figure Ref.**
Case 1: Stable plume with hypothetical parameter values								
1	0.1	6.93	60yr	0.01	2.19	0.003	0.35	4.1.1
	0.1		40yr	0.42		0.19	19.40	4.1.4
2	0.2	3.47	60yr	0.47	2.10	0.22	22.29	4.1.8
	0.2		40yr	1.21		0.58	57.79	4.1.11
3	0.3	2.31	60yr	1.39	2.04	0.68	68.30	4.1.14
	0.3		40yr	1.91		0.94	93.57	4.1.17
4	0.4	1.73	60yr	1.26	2.00	0.63	62.97	4.1.20
	0.4		40yr	1.68		0.84	84.02	4.1.23
5	0.5	1.39	60yr	0.89	1.96	0.45	45.35	4.1.26
	0.5		40yr	1.71		0.87	87.17	4.1.29
6	1.0	0.7	60yr	0.90	1.86	0.48	48.30	4.1.32
	1.0		40yr	1.77		0.95	95.23	4.1.35
Case 1b: Stable plume with base-case values from Liang [2009]								
7	0.1	6.93	60yr	0.11	2.74	0.04	3.84	4.1.38
	0.1		40yr	0.28		0.10	10.38	4.1.41
8	0.2	3.47	60yr	0.27	2.61	0.10	10.18	4.1.44
	0.2		40yr	0.99		0.38	38.03	4.1.47
Case 2: Growing-disconnected plume with base-case values from Liang [2009]								
9	0.1	6.93	54yr	0.02	1.71	0.01	1.43	4.1.50
	0.1		34yr	119.36		69.78	6977.57	4.1.53
10	0.2	3.47	54yr	0.04	1.40	0.03	2.72	4.1.56
	0.2		34yr	0.86		0.61	61.40	4.1.59
Case 3: Growing-connected plume with base-case values from Liang [2009]								
11	0.1	6.93	60yr	0.20	3.79	0.05	5.30	4.1.62
	0.1		40yr	0.25		0.07	6.62	4.1.65
12	0.2	3.47	60yr	0.54	3.65	0.15	14.69	4.1.68
	0.2		40yr	0.44		0.12	12.01	4.1.71
13	0.3	2.31	60yr	0.58	3.55	0.16	16.44	4.1.74
	0.3		40yr	0.59		0.16	16.49	4.1.77
*calculated with log(C) in Equations 3.5 & 3.6								

Table 4.2.2: Centerline (X-direction) NRMS results compilation for Cases 1 through 3

NRMS Analysis Table (Transverse: X-Y spatial plane)								
Model Pair	**λ**	**$t_{1/2}$**	**Time**	**RMS**	**$\log(C_m)$**	**NRMS**	**%Deviation**	**Figure Ref.**
Case 1: Stable plume with hypothetical parameter values								
1	0.1	6.93	60yr	0.03	0.94	0.03	3.16	4.1.2a & b
	0.1		40yr	0.41		0.44	44.00	4.1.5a & b
2	0.2	3.47	60yr	1.83	0.89	2.06	205.65	4.1.9a & b
	0.2		40yr	2.10		2.37	236.99	4.1.12a & b
3	0.3	2.31	60yr	2.32	0.73	3.19	319.13	4.1.15a & b
	0.3		40yr	2.62		3.60	360.42	4.1.18a & b
4	0.4	1.73	60yr	1.76	0.51	3.47	347.16	4.1.21a & b
	0.4		40yr	3.31		6.52	652.07	4.1.24a & b
5	0.5	1.39	60yr	1.60	0.76	2.11	210.65	4.1.27a & b
	0.5		40yr	3.01		3.95	395.08	4.1.30a & b
6	1.0	0.7	60yr	2.18	0.80	2.74	273.73	3.1.33a & b
	1.0		40yr	3.75		4.70	469.69	4.1.36a & b
Case 1b: Stable plume with base-case values from Liang [2009]								
7	0.1	6.93	60yr	3.16	1.47	2.15	214.68	4.1.39a & b
	0.1		40yr	3.44		2.34	233.72	4.1.42a & b
8	0.2	3.47	60yr	1.90	1.50	1.26	126.41	4.1.45a & b
	0.2		40yr	2.50		1.67	166.62	4.1.48a & b
Case 2: Growing-disconnected plume with base-case values from Liang [2009]								
9	0.1	6.93	54yr	0.03	0.97	0.03	2.61	4.1.51a & b
	0.1		34yr	0.41		0.42	42.45	4.1.54a & b
10	0.2	3.47	54yr	2.02	0.47	4.29	429.20	4.1.57a & b
	0.2		34yr	2.20		4.68	467.68	4.1.60a & b
Case 3: Growing-connected plume with base-case values from Liang [2009]								
11	0.1	6.93	60yr	3.23	2.66	1.22	121.71	4.1.63a & b
	0.1		40yr	3.74		1.41	141.02	4.1.66a & b
12	0.2	3.47	60yr	0.57	2.53	0.22	22.34	4.1.69a & b
	0.2		40yr	0.46		0.18	18.34	4.1 72a & b
13	0.3	2.31	60yr	1.07	2.38	0.45	45.02	4.1.75a & b
	0.3		40yr	1.81		0.76	75.87	4.1.78a & b
*calculated with log(C) in Equations 3.5 & 3.6								

Table 4.2.3: Transverse (X-Y spatial plane; Z=0) NRMS results compilation for Cases 1 through 3

NRMS Analysis Table (Vertical: X-Z spatial plane)								
Model Pair	λ	$t_{1/2}$	Time	RMS*	$\log(C_m)$	NRMS	%Deviation	Figure Ref.
Case 1: Stable plume with hypothetical parameter values								
1	0.1	6.93	60yr	0.03	1.04	0.03	3.00	4.1.3a & b
	0.1		40yr	0.41		0.39	39.31	4.1.6a & b
2	0.2	3.47	60yr	0.58	0.79	0.74	74.16	4.1.10a & b
	0.2		40yr	1.50		1.90	189.99	4.1.13a & b
3	0.3	2.31	60yr	2.78	0.65	4.29	428.96	4.1.16a & b
	0.3		40yr	2.97		4.58	458.03	4.1.19a & b
4	0.4	1.73	60yr	2.30	0.56	4.13	412.66	4.1.22a & b
	0.4		40yr	4.01		7.20	719.93	4.1.25a & b
5	0.5	1.39	60yr	3.22	0.49	6.55	654.51	4.1.28a & b
	0.5		40yr	4.53		9.22	922.06	4.1.31a & b
6	1.0	0.7	60yr	4.37	0.29	14.85	1485.37	4.1.34a & b
	1.0		40yr	5.38		18.26	1825.78	4.1.37a & b
Case 1b: Stable plume with base-case values from Liang [2009]								
7	0.1	6.93	60yr	3.04	1.66	1.83	182.91	4.1.40a & b
	0.1		40yr	3.27		1.96	196.31	4.1.43a & b
8	0.2	3.47	60yr	1.85	1.61	1.15	115.13	4.1.46a & b
	0.2		40yr	2.18		1.35	135.31	4.1.49a & b
Case 2: Growing-disconnected plume with base-case values from Liang [2009]								
9	0.1	6.93	54yr	0.03	0.83	0.03	3.00	4.1.52a & b
	0.1		34yr	0.41		0.49	49.21	4.1.55a & b
10	0.2	3.47	54yr	1.28	0.36	3.56	356.19	4.1.58a & b
	0.2		34yr	2.38		6.61	661.18	4.1.61a & b
Case 3: Growing-connected plume with base-case values from Liang [2009]								
11	0.1	6.93	60yr	0.54	2.73	0.20	19.85	4.1.64a & b
	0.1		40yr	0.75		0.28	27.70	4.1.67a & b
12	0.2	3.47	60yr	1.11	2.75	0.40	40.39	4.1.70a & b
	0.2		40yr	1.42		0.52	51.68	4.1.73a & b
13	0.3	2.31	60yr	1.40	2.63	0.53	53.38	4.1.76a & b
	0.3		40yr	2.09		0.79	79.33	4.1.79a & b
*calculated with log(C) in Equations 3.5 & 3.6								

Table 4.2.4: Vertical (X-Z spatial plane; Y=0) NRMS results compilation for Cases 1 through 3

APPENDIX C

Graphical Analysis Visual Comparison Similarity Ranking				
Centerline (X-direction) plot comparisons at 60 (54) years				
Rank	**Case**	**dr**	**Figure**	**NRMS**
1	1: Stable plume	0.1	4.1.1	0.003
2	2: Growing-disconnected plume	0.1	4.1.50	0.01
3	1: Stable plume	0.2	4.1.8	0.22
4	2: Growing-disconnected plume	0.2	4.1.56	0.03
5	1b: Stable plume	0.1	4.1.38	0.04
6	3: Growing-connected plume	0.1	4.1.62	0.05
7	3: Growing-connected plume	0.2	4.1.68	0.15
8	1: Stable plume	0.5	4.1.26	0.45
9	1: Stable plume	1.0	4.1.32	0.48
10	1: Stable plume	0.4	4.1.20	0.63
11	1: Stable plume	0.3	4.1.14	0.68
12	1b: Stable plume	0.2	4.1.44	0.10
13	3: Growing-connected plume	0.3	4.1.74	0.16
Centerline (X-direction) plot comparisons at 40 (34) years				
Rank	**Case**	**dr**	**Figure**	**NRMS**
1	1b: Stable plume	0.1	4.1.41	0.1
2	1b: Stable plume	0.2	4.1.47	0.38
3	3: Growing-connected plume	0.3	4.1.77	0.16
4	3: Growing-connected plume	0.1	4.1.65	0.07
5	3: Growing-connected plume	0.2	4.1.71	0.12
6	1: Stable plume	0.1	4.1.4	0.19
7	1: Stable plume	0.2	4.1.11	0.58
8	2: Growing-disconnected plume	0.2	4.1.59	0.61
9	1: Stable plume	1.0	4.1.35	0.95
10	1: Stable plume	0.5	4.1.29	0.87
11	1: Stable plume	0.4	4.1.23	0.84
12	1: Stable plume	0.3	4.1.17	0.94
13	2: Growing-disconnected plume	0.1	4.1.53	69.78

Table 4.1.14: Ranking chart for graphical analysis of centerline (X-direction) charts

Graphical Analysis Visual Comparison Similarity Ranking				
Transverse (X-Y spatial plane) plot comparisons at 60 (54) years				
Rank	**Case**	**dr**	**Figures**	**NRMS**
1	1: Stable plume	0.1	4.1.2a & b	0.03
2	2: Growing-disconnected plume	0.1	4.1.51a & b	0.03
3	3: Growing-connected plume	0.1	4.1.63a & b	1.22
4	1b: Stable plume	0.2	4.1.45a & b	1.26
5	1b: Stable plume	0.1	4.1.39a & b	2.15
6	1: Stable plume	0.2	4.1.9a & b	2.06
7	2: Growing-disconnected plume	0.2	4.1.57a & b	4.29
8	3: Growing-connected plume	0.2	4.1.69a & b	0.22
9	1: Stable plume	1.0	4.1.33a & b	2.18
10	1: Stable plume	0.3	4.1.15a & b	3.19
11	1: Stable plume	0.4	4.1.21a & b	3.47
12	1: Stable plume	0.5	4.1.27a & b	2.11
13	3: Growing-connected plume	0.3	4.1.75a & b	0.45
Transverse (X-Y spatial plane) plot comparisons at 40 (34) years				
Rank	**Case**	**dr**	**Figures**	**NRMS**
1	3: Growing-connected plume	0.1	4.1.66a & b	1.41
2	3: Growing-connected plume	0.2	4.1.72a & b	0.18
3	3: Growing-connected plume	0.3	4.1.78a & b	0.76
4	1: Stable plume	0.1	4.1.5a & b	0.44
5	2: Growing-disconnected plume	0.1	4.1.54a & b	0.42
6	1b: Stable plume	0.1	4.1.42a & b	2.34
7	1b: Stable plume	0.2	4.1.48a & b	1.67
8	1: Stable plume	0.2	4.1.12a & b	2.37
9	1: Stable plume	0.3	4.1.18a & b	3.6
10	2: Growing-disconnected plume	0.2	4.1.60a & b	4.68
11	1: Stable plume	0.5	4.1.30a & b	3.95
12	1: Stable plume	1	4.1.36a & b	4.7
13	1: Stable plume	0.4	4.1.24a & b	6.52

Table 4.1.15: Ranking chart for graphical analysis of transverse (X-Y spatial plane) plots

Graphical Analysis Visual Comparison Similarity Ranking				
Vertical (X-Z spatial plane) plot comparisons at 60 (54) years				
Rank	**Case**	**dr**	**Figures**	**NRMS**
1	1: Stable plume	0.1	4.1.3a & b	0.03
2	2: Growing-disconnected plume	0.1	4.1.52a & b	0.03
3	1: Stable plume	0.4	4.1.22a & b	4.13
4	2: Growing-disconnected plume	0.2	4.1.58a & b	3.56
5	1: Stable plume	0.3	4.1.16a & b	4.29
6	1: Stable plume	0.2	4.1.10a & b	0.74
7	1: Stable plume	0.5	4.1.28a & b	6.55
8	1: Stable plume	1	4.1.34a & b	14.85
9	1b: Stable plume	0.2	4.1.46a & b	1.15
10	1b: Stable plume	0.1	4.1.40a & b	1.83
11	3: Growing-connected plume	0.2	4.1.70a & b	0.4
12	3: Growing-connected plume	0.1	4.1.64a & b	0.20
13	3: Growing-connected plume	0.3	4.1.76a & b	0.53
Vertical (X-Z spatial plane) plot comparisons at 40 (34) years				
Rank	**Case**	**dr**	**Figures**	**NRMS**
1	2: Growing-disconnected plume	0.1	4.1.55a & b	0.49
2	1: Stable plume	0.1	4.1.6a & b	0.39
3	2: Growing-disconnected plume	0.2	4.1.61a & b	6.61
4	3: Growing-connected plume	0.1	4.1.67a & b	0.28
5	3: Growing-connected plume	0.2	4.1.73a & b	0.52
6	1b: Stable plume	0.1	4.1.43a & b	1.96
7	3: Growing-connected plume	0.3	4.1.79a & b	0.79
8	1b: Stable plume	0.2	4.1.49a & b	1.35
9	1: Stable plume	0.2	4.1.13a & b	1.9
10	1: Stable plume	0.3	4.1.19a & b	4.58
11	1: Stable plume	0.4	4.1.25a & b	7.20
12	1: Stable plume	0.5	4.1.31a & b	9.22
13	1: Stable plume	1	4.1.37a & b	18.26

Table 4.1.16: Ranking chart for graphical analysis of vertical (X-Z spatial plane) plots

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